CurveExpert Basic Documentation

Release 2.2.3

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CONTENTS

1	What is CurveExpert Basic?	1
2	Installation and Activation2.1Installation2.2Starting a Trial2.3Purchasing2.4After Purchase: licensing2.5Automated licensing	3 3 4 4 4
3	Getting started3.1Load data into CurveExpert Basic3.2Perform a Nonlinear Regression3.3Examine the Results3.4Visualize your Results	5 6 6 6
4	4.2 Toolbar 1 4.3 Results Pane 1 4.4 Graphs and Data Pane 1 4.5 Preview Pane 1 4.6 Messages Pane 1 4.7 Status bar 1	7 9 11 11 11 12 12
5	5.1 Introduction 1 5.2 Raw file import 1 5.3 CurveExpert Basic files 1	15 15 15 19
6	6.1 Introduction 2 6.2 Data statistics 2 6.3 The spreadsheet 2 6.4 Number Formatting 2	21 21 22 24 24
7	7.1 General Guidelines 2 7.2 Interpolation 2	27 27 28 29

8 CurveFinder 33 8.1 Usage 33 8.2 Cutions 34 9 Working with Results 35 9.1 Introduction 35 9.2 Color Coding 36 9.3 Badges 37 9.4 Previewing 37 9.5 Placing Results on a Graph 37 9.6 Removing Result Information 38 9.8 Querying Result Information 38 9.9 Confidence and Prediction Bands 39 9.0 Graphing 41 10.1 Introduction 41 10.2 Graph Types 41 10.4 Interacting with a graph 42 10.5 Changing Graph Properties 43 10.6 Legend 51 10.7 Scring graphs 52 10.8 Copying graphs 52 10.9 Printing graphs 53 10.10 Reproduction 61 11.2 Custom Models 61 11.2<		7.4	Nonlinear Regression 29
8.2 Cautions 34 9 Working with Results 35 9.1 Introduction 35 9.2 Color Coding 36 9.3 Badges 37 9.4 Previewing 37 9.5 Placing Results on a Graph 37 9.6 Removing Result Information 38 9.7 Copying Result Information 38 9.8 Querying Result Information 38 9.9 Confidence and Prediction Bands 39 10 Graphing 41 10.1 Introduction 41 10.2 Graph Types 41 10.3 Basics 41 10.4 Interacting with a graph 42 10.5 Changing Graph Properties 45 10.6 Legend 51 10.7 Saving graphs 53 10.9 Printing graphs 53 10.10 Keyboard Shortcuts for Graphs 53 10.10 Keyboard Shortcuts for Graphs 53 10.10 Keyboard Shortcuts	8	Curv	eFinder 33
9 Working with Results 35 9.1 Introduction 35 9.2 Color Coding 36 9.3 Badges 37 9.4 Previewing 37 9.4 Previewing 37 9.5 Placing Results on a Graph 37 9.6 Removing Results 37 9.7 Copying Result Information 38 9.8 Querying Result Details 38 9.9 Confidence and Prediction Bands 39 9.0 Graphing 41 10.1 Introduction 41 10.2 Graph Types 41 10.3 Basics 41 10.4 Interacting with a graph 42 10.5 Changing Graph Properties 43 10.6 Legend 51 10.7 Saving graphs 53 10.8 Copying graphs 53 10.9 Fraiting graphs 53 10.11 Mathext 53 </th <th></th> <th>8.1</th> <th>Usage</th>		8.1	Usage
9.1 Introduction 35 9.2 Color Coding 36 9.3 Badges 37 9.4 Previewing 37 9.4 Previewing 37 9.5 Placing Results on a Graph 37 9.6 Removing Results 37 9.7 Copying Result Information 38 9.8 Querying Result Details 38 9.9 Confidence and Prediction Bands 39 10 Graphing 41 10.2 Graph Types 41 10.3 Basics 41 10.4 Interacting with a graph 42 10.5 Changing Graph Properties 43 10.6 Legend 45 10.6 Legend 51 10.7 Saving graphs 52 10.8 Copying graphs 53 10.9 Printing graphs 53 10.10 Keyboard Shortcuts for Graphs 53 10.11 Introduction 61 11.1 Introduction 61		8.2	Cautions
9.1 Introduction 53 9.2 Color Coding 36 9.3 Badges 37 9.4 Previewing 37 9.5 Placing Results on a Graph 37 9.6 Removing Results 37 9.7 Copying Result Information 38 9.8 Querying Result Details 38 9.9 Confidence and Prediction Bands 39 10 Introduction 41 10.1 Introduction 41 10.2 Graphing 41 10.3 Basics 41 10.4 Interacting with a graph 42 10.5 Changing Graph Properties 42 10.5 Changing Graph Properties 45 10.6 Legend 51 10.7 Saving graphs 53 10.8 Copying graphs 53 10.9 Printing graphs 53 10.10 Methext 54 11.11 Introduction 61 11.1 Introduction 63	9	Work	sing with Results 35
9.2 Color Coding 56 9.3 Badges 37 9.4 Previewing 37 9.5 Placing Results on a Graph 37 9.6 Removing Results 37 9.7 Copying Result Information 38 9.8 Querying Result Details 38 9.9 Confidence and Prediction Bands 39 10 Graphing 41 10.1 Introduction 41 10.2 Graph Types 41 10.3 Basics 41 10.4 Interacting with a graph 42 10.5 Changing Graph Properties 41 10.4 Interacting with a graph 42 10.5 Changing Graph Properties 43 10.6 Legend 51 10.7 Saving graphs 52 10.8 Copying graphs 53 10.9 Printing graphs 53 10.10 Keyboard Shortcuts for Graphs 53 10.11 Introduction 61 11.2 Custom Models			
9.3 Badges 37 9.4 Previewing 37 9.5 Placing Results on a Graph 37 9.6 Removing Results on a Graph 37 9.7 Copying Result Information 38 9.8 Querying Result Details 38 9.9 Confidence and Prediction Bands 39 10 Graphing 41 10.1 Introduction 41 10.2 Graph Types 41 10.3 Basics 41 10.4 Interacting with a graph 42 10.5 Changing Graph Properties 42 10.6 Legend 51 10.6 Legend 51 10.7 Saving graphs 52 10.8 Copying graphs 53 10.9 Printing graphs 53 10.10 Keyboard Shortcuts for Graphs 53 10.11 Autoduction 61 11.1 Introduction 61 11.1 Introduction 65 13.1 Introduction 65 <th></th> <th>9.2</th> <th></th>		9.2	
9.4 Previewing 37 9.5 Placing Results on a Graph. 37 9.6 Removing Results. 37 9.7 Copying Result Information 38 9.8 Querying Result Information 38 9.9 Confidence and Prediction Bands 39 10 Graphing 41 10.1 Introduction 41 10.2 Graph Types 41 10.3 Basics. 41 10.4 Interacting with a graph 42 10.5 Changing Graph Properties 45 10.6 Legend 51 10.7 Saving graphs 53 10.8 Copying graphs 53 10.9 Printing graphs 53 10.10 Keyboard Shortcuts for Graphs 53 10.11 Mathetxt 54 11.1 Introduction 61 11.2 Custom Models 61 11.2 Custom Models 61 11.2 Custom Models 65 13.3 Exporting a drabat to text file <th></th> <th>9.3</th> <th></th>		9.3	
9.5 Placing Results on a Graph. 37 9.6 Removing Result Information 37 9.7 Copying Result Information 38 9.8 Querying Result Details 38 9.9 Confidence and Prediction Bands 39 10 Graphing 41 10.1 Introduction 41 10.2 Graph Types 41 10.3 Basics 41 10.4 Interacting with a graph 42 10.5 Changing Graph Properties 45 10.6 Legend 51 10.7 Saving graphs 52 10.8 Copying graphs 53 10.9 Printing graphs 53 10.10 Keyboard Shortcuts for Graphs 53 10.11 Autoduction 61 11.1 Introduction 61 11.1 Introduction 65 13.1 Introduction 65 13.2 Writing Data 65 13.3 Exporting a dataset to text file 65 13.4 Writin		9.4	
9.6 Removing Results 37 9.7 Copying Result Information 38 9.8 Querying Result Information 38 9.9 Confidence and Prediction Bands 39 90 Graphing 41 10.1 Introduction 41 10.2 Graph Types 41 10.3 Basics 41 10.4 Interacting with a graph 42 10.5 Changing Graph Properties 43 10.4 Interacting with a graph 42 10.5 Changing Graph Properties 43 10.6 Legend 51 10.7 Saving graphs 53 10.9 Printing graphs 53 10.9 Printing graphs 53 10.10 Keyboard Shortcuts for Graphs 53 10.11 Mathext 54 11.1 Introduction 61 11.2 Custom Models 61 11.2 Custom Models 65 13.3 Exporting a dataset to text file 55 13.4 Wri		9.5	
9.7 Copying Result Information 38 9.8 Querying Result Details 38 9.9 Confidence and Prediction Bands 39 10 Graphing 41 10.2 Graphing 41 10.3 Basics 41 10.4 Introduction 41 10.5 Changing Graph Properties 42 10.5 Changing Graph Properties 45 10.6 Legend 51 10.7 Saving graphs 52 10.8 Copying graphs 53 10.0 Printing graphs 53 10.11 Mathext 54 11.0 Printing graphs 53 10.11 Mathext 54 11.1 Introduction 61 11.2 Custom Models 61 11.1 Introduction 61 11.2 Custom Models 61 11.2 Custom Models 61 11.1 Introduction 65 13.2 Writing a dataset to text file 65			
9.8 Querying Result Details 38 9.9 Confidence and Prediction Bands 39 10 Graphing 41 10.1 Introduction 41 10.2 Graph Types 41 10.3 Basics 41 10.4 Interacting with a graph 42 10.5 Changing Graph Properties 45 10.6 Legend 51 10.7 Saving graphs 52 10.8 Copying graphs 53 10.9 Printing graphs 53 10.10 Keyboard Shortcuts for Graphs 53 10.11 Mathext 54 11.1 Introduction 61 11.2 Custom Models 61 11.1 Introduction 61 11.2 Custom Models 61 11.1 Introduction 61 11.2 Custom Models 61 11.2 Custom Models 61 12 Equation Display 63 13 Bryorting a dataset to text file 65			
9.9 Confidence and Prediction Bands 39 10 Graphing 41 10.1 Introduction 41 10.2 Graph Types 41 10.3 Basics 41 10.4 Interacting with a graph 42 10.5 Changing Graph Properties 45 10.6 Legend 51 10.7 Saving graphs 52 10.8 Copying graphs 53 10.9 Printing graphs 53 10.10 Keyboard Shortcuts for Graphs 53 10.11 Mathext 54 11 Creating Custom Models 61 11.1 Introduction 61 11.2 Custom Models 61 11.1 Introduction 61 12 Equation Display 63 13 Writing a CurveExpert (CXP) file 65 13.2 Writing a dataset to text file 65 13.3 Exporting a dataset to text file 65 13.4 Writing a dataset to text file 65 13.5		9.8	1, 6
10 Graphing 41 10.1 Introduction 41 10.2 Graph Types 41 10.3 Basics 41 10.4 Interacting with a graph 42 10.5 Changing Graph Properties 45 10.6 Legend 51 10.7 Saving graphs 52 10.8 Copying graphs 52 10.9 Printing graphs 53 10.9 Printing graphs 53 10.10 Keyboard Shortcuts for Graphs 53 10.11 Mathext 54 11 Creating Custom Models 61 11.1 Introduction 61 11.2 Custom Models 61 11.2 Custom Models 61 12 Equation Display 63 13 Writing Data 65 13.2 Writing a CurveExpert (CXP) file 65 13.3 Exporting a dataset to text file 65 13.4 Writing a graph to a picture file 65 13.5 Printing 66 14.1 Introduction 67 14.2 General Preferences 67 14.1 Introduction 67 14.2 General Preferences 70 14.3 Regression		9.9	
10.1 Introduction 41 10.2 Graph Types 41 10.3 Basics 41 10.4 Interacting with a graph 42 10.5 Changing Graph Properties 45 10.6 Legend 42 10.7 Saving graphs 52 10.8 Copying graphs 53 10.9 Printing graphs 53 10.11 Mathext 53 10.10 Keyboard Shortcuts for Graphs 53 10.11 Mathext 54 11.1 Introduction 61 11.2 Custom Models 61 12 Equation Display 63 13 Writing a CurveExpert (CXP) file 65 13.4 Writing a graph to a picture file 65 <t< th=""><th></th><th>~</th><th></th></t<>		~	
10.2 Graph Types 41 10.3 Basics 41 10.4 Interacting with a graph 42 10.5 Changing Graph Properties 45 10.6 Legend 51 10.7 Saving graphs 52 10.8 Copying graphs 53 10.9 Printing graphs 53 10.10 Keyboard Shortcuts for Graphs 53 10.11 Mathext 54 11 Creating Custom Models 61 11.1 Introduction 61 11.2 Custom Models 63 13 Writing Data 65 13.1 Introduction 65 13.2 Writing a CurveExpert (CXP) file 65 13.3 Exporting a dataset to text file 65 13.4 Writing a graph to a picture file 65 13.5 Printing 67 14.4 Graphing Preferences 70 14.5 Logging Preferences 71 14.6 Logalization Preferences 73 14.6 Lo	10		
10.3 Basics 41 10.4 Interacting with a graph 42 10.5 Changing Graph Properties 45 10.6 Legend 51 10.7 Saving graphs 52 10.8 Copying graphs 53 10.9 Printing graphs 53 10.10 Keyboard Shortcuts for Graphs 53 10.11 Mathtext 54 11 Creating Custom Models 61 11.1 Introduction 61 11.2 Custom Models 61 11.2 Custom Models 61 12 Equation Display 63 13 Writing Data 65 13.2 Writing a dataset to text file 65 13.4 Writing a graph to a picture file 65 13.5 Printing 66 14 Application Preferences 67 14.1 Introduction 67 14.2 General Preferences 67 14.3 Regression Preferences 70 14.4 Graphing Preferences 73 14.5 Logging Preferences 75 14.7 Advanced Preferences 75 14.7 Advanced Preferences 75 15.1 Executive Summary 79			
10.4 Interacting with a graph 42 10.5 Changing Graph Properties 45 10.6 Legend 51 10.7 Saving graphs 52 10.8 Copying graphs 53 10.9 Printing graphs 53 10.9 Printing graphs 53 10.10 Keyboard Shortcuts for Graphs 53 10.11 Mathext 54 11 Creating Custom Models 61 11.1 Introduction 61 11.2 Custom Models 63 13 Writing Data 65 13.4 Writing a CurveExpert (CXP) file 65 13.3 Exporting a dataset to text file 65 13.4 Writing a graph to a picture file 65 13.5 Printing 67 14.1 Introduction </th <th></th> <th></th> <th>1 71</th>			1 71
10.5 Changing Graph Properties 45 10.6 Legend 51 10.7 Saving graphs 52 10.8 Copying graphs 53 10.9 Printing graphs 53 10.9 Printing graphs 53 10.10 Keyboard Shortcuts for Graphs 53 10.11 Mathext 54 11 Creating Custom Models 61 11.1 Introduction 61 11.2 Custom Models 61 11.2 Custom Models 63 12 Equation Display 63 13 Writing Data 65 13.2 Writing a durveExpert (CXP) file 65 13.3 Exporting a dataset to text file 65 13.4 Writing a graph to a picture file 65 13.5 Printing 66 14 Application Preferences 67 14.3 Regression Preferences 70 14.4 Graphing Preferences 73 14.5 Logging Preferences 75 14.6			
10.6 Legend 51 10.7 Saving graphs 52 10.8 Copying graphs 53 10.9 Printing graphs 53 10.10 Keyboard Shortcuts for Graphs 53 10.11 Mathext 54 11 Creating Custom Models 61 11.1 Introduction 61 11.2 Custom Models 61 11.2 Custom Models 63 12 Equation Display 63 13 Writing Data 65 13.2 Writing a CurveExpert (CXP) file 65 13.3 Exporting a dataset to text file 65 13.4 Writing a graph to a picture file 65 13.5 Printing 66 14 Application Preferences 67 14.1 Introduction 67 14.2 General Preferences 70 14.4 Graphing Preferences 71 14.5 Logging Preferences 73 14.6 Localization Preferences 75 14.7 A			
10.7 Saving graphs 52 10.8 Copying graphs 53 10.9 Printing graphs 53 10.10 Reyboard Shortcuts for Graphs 53 10.11 Mathtext 54 11 Creating Custom Models 61 11.1 Introduction 61 11.2 Custom Models 61 11.2 Custom Models 63 12 Equation Display 63 13 Writing Data 65 13.1 Introduction 65 13.2 Writing a CurveExpert (CXP) file 65 13.3 Exporting a dataset to text file 65 13.4 Writing a graph to a picture file 65 13.5 Printing 66 14 Application Preferences 67 14.1 Introduction 67 14.2 General Preferences 70 14.4 Graphing Preferences 71 14.5 Localization Preferences 75 14.6 Localization Preferences 75 14.7 <th></th> <th></th> <th></th>			
10.8 Copying graphs 53 10.9 Printing graphs 53 10.10 Keyboard Shortcuts for Graphs 53 10.11 Mathext 54 11 Creating Custom Models 61 11.1 Introduction 61 11.2 Custom Models 61 11.2 Custom Models 63 12 Equation Display 63 13 Writing Data 65 13.1 Introduction 65 13.2 Writing a CurveExpert (CXP) file 65 13.3 Exporting a dataset to text file 65 13.4 Writing a graph to a picture file 65 13.5 Printing 66 14 Application Preferences 67 14.1 Introduction 67 14.2 General Preferences 67 14.3 Regression Preferences 70 14.4 Graphing Preferences 73 14.5 Logging Preferences 73 14.6 Logging Preferences 75 14.7			
10.9 Printing graphs 53 10.10 Keyboard Shortcuts for Graphs 53 10.11 Mathtext 54 11 Creating Custom Models 61 11.1. Introduction 61 11.2 Custom Models 61 11.2 Custom Models 61 11.2 Custom Models 63 13 Writing Data 65 13.1 Introduction 65 13.2 Writing a CurveExpert (CXP) file 65 13.3 Exporting a dataset to text file 65 13.4 Writing a graph to a picture file 65 13.5 Printing 66 14 Application Preferences 67 14.1 Introduction 67 14.2 General Preferences 67 14.3 Regression Preferences 70 14.4 Graphing Preferences 70 14.4 Graphing Preferences 73 14.5 Logging Preferences 73 14.6 Localization Preferences 75 14.7 Advanced Preferences 76 15.1 Executive Summary 79			
10.10 Keyboard Shortcuts for Graphs 53 10.11 Mathtext 54 11 Creating Custom Models 61 11.1 Introduction 61 11.2 Custom Models 63 13 Writing Data 65 13.1 Introduction 65 13.2 Writing a CurveExpert (CXP) file 65 13.3 Exporting a dataset to text file 65 13.4 Writing a graph to a picture file 65 13.5 Printing 66 14 Application Preferences 67 14.1 Introduction 67 14.2 General Preferences 67 14.3 Regression Preferences 70 14.4 Graphing Preferences 71 14.5 Logging Preferences 73 14.6 Localization Preferences 75 14.7 Advanced Preferences 75 14.7 Advanced Preferences 75 15.1 Executive Summary 79			
10.11 Mathtext 54 11 Creating Custom Models 61 11.1 Introduction 61 11.2 Custom Models 61 11.2 Custom Models 61 11 Equation Display 63 13 Writing Data 65 13.1 Introduction 65 13.2 Writing a CurveExpert (CXP) file 65 13.3 Exporting a dataset to text file 65 13.4 Writing a graph to a picture file 65 13.5 Printing 66 14 Application Preferences 67 14.1 Introduction 67 14.2 General Preferences 67 14.3 Regression Preferences 67 14.4 Graphing Preferences 70 14.5 Logging Preferences 73 14.6 Localization Preferences 75 14.7 Advanced Preferences 75 14.7 Advanced Preferences 76 151 Executive Summary 79			
11 Creating Custom Models 61 11.1 Introduction 61 11.2 Custom Models 61 11.2 Custom Models 61 12 Equation Display 63 13 Writing Data 65 13.1 Introduction 65 13.2 Writing a CurveExpert (CXP) file 65 13.3 Exporting a dataset to text file 65 13.4 Writing a graph to a picture file 65 13.5 Printing 66 14 Application Preferences 67 14.1 Introduction 67 14.2 General Preferences 67 14.3 Regression Preferences 70 14.4 Graphing Preferences 70 14.4 Graphing Preferences 71 14.5 Logging Preferences 73 14.6 Localization Preferences 75 14.7 Advanced Preferences 75 14.7 Advanced Preferences 76 15.1 Executive Summary 79			
11.1 Inroduction 61 11.2 Custom Models 61 12 Equation Display 63 13 Writing Data 65 13.1 Introduction 65 13.2 Writing a CurveExpert (CXP) file 65 13.3 Exporting a dataset to text file 65 13.4 Writing a graph to a picture file 65 13.5 Printing 66 14 Application Preferences 67 14.1 Introduction 67 14.2 General Preferences 67 14.3 Regression Preferences 67 14.4 Graphing Preferences 70 14.4 Graphing Preferences 73 14.6 Localization Preferences 73 14.7 Advanced Preferences 75 14.7 Advanced Preferences 76 15.1 Executive Summary 79			
11.2 Custom Models 61 12 Equation Display 63 13 Writing Data 65 13.1 Introduction 65 13.2 Writing a CurveExpert (CXP) file 65 13.3 Exporting a dataset to text file 65 13.4 Writing a graph to a picture file 65 13.5 Printing 66 14 Application Preferences 67 14.1 Introduction 67 14.2 General Preferences 67 14.3 Regression Preferences 70 14.4 Graphing Preferences 70 14.4 Graphing Preferences 73 14.6 Localization Preferences 75 14.7 Advanced Preferences 75 14.7 Advanced Preferences 76 15.1 Executive Summary 79	11		8
12 Equation Display 63 13 Writing Data 65 13.1 Introduction 65 13.2 Writing a CurveExpert (CXP) file 65 13.3 Exporting a dataset to text file 65 13.4 Writing a graph to a picture file 65 13.5 Printing 66 14 Application Preferences 67 14.1 Introduction 67 14.2 General Preferences 67 14.3 Regression Preferences 67 14.4 Graphing Preferences 70 14.4 Graphing Preferences 73 14.6 Localization Preferences 75 14.7 Advanced Preferences 76 15 Localization 79 15.1 Executive Summary 79			
13 Writing Data 65 13.1 Introduction 65 13.2 Writing a CurveExpert (CXP) file 65 13.3 Exporting a dataset to text file 65 13.4 Writing a graph to a picture file 65 13.5 Printing 66 14 Application Preferences 67 14.1 Introduction 67 14.2 General Preferences 67 14.3 Regression Preferences 67 14.4 Graphing Preferences 70 14.4 Graphing Preferences 71 14.5 Logging Preferences 73 14.6 Localization Preferences 76 14.7 Advanced Preferences 76 15 Localization 79 15.1 Executive Summary 79		11.2	Custom Models
13.1 Introduction 65 13.2 Writing a CurveExpert (CXP) file 65 13.3 Exporting a dataset to text file 65 13.4 Writing a graph to a picture file 65 13.5 Printing 65 13.5 Printing 66 14 Application Preferences 67 14.1 Introduction 67 14.2 General Preferences 67 14.3 Regression Preferences 67 14.4 Graphing Preferences 70 14.4 Graphing Preferences 73 14.5 Logging Preferences 73 14.6 Localization Preferences 75 14.7 Advanced Preferences 76 15 Localization 79 15.1 Executive Summary 79	12	Equa	tion Display 63
13.1 Introduction 65 13.2 Writing a CurveExpert (CXP) file 65 13.3 Exporting a dataset to text file 65 13.4 Writing a graph to a picture file 65 13.5 Printing 65 13.5 Printing 66 14 Application Preferences 67 14.1 Introduction 67 14.2 General Preferences 67 14.3 Regression Preferences 67 14.4 Graphing Preferences 70 14.4 Graphing Preferences 73 14.5 Logging Preferences 73 14.6 Localization Preferences 75 14.7 Advanced Preferences 76 15 Localization 79 15.1 Executive Summary 79	12	Wait	ang Data
13.2 Writing a CurveExpert (CXP) file 65 13.3 Exporting a dataset to text file 65 13.4 Writing a graph to a picture file 65 13.5 Printing 65 14 Application Preferences 67 14.1 Introduction 67 14.2 General Preferences 67 14.3 Regression Preferences 67 14.4 Graphing Preferences 70 14.4 Graphing Preferences 71 14.5 Logging Preferences 73 14.6 Localization Preferences 75 14.7 Advanced Preferences 76 15 Localization 79 15.1 Executive Summary 79	13		
13.3 Exporting a dataset to text file 65 13.4 Writing a graph to a picture file 65 13.5 Printing 66 14 Application Preferences 67 14.1 Introduction 67 14.2 General Preferences 67 14.3 Regression Preferences 67 14.4 Graphing Preferences 67 14.5 Logging Preferences 70 14.6 Localization Preferences 73 14.7 Advanced Preferences 76 15 Localization 79 15.1 Executive Summary 79			
13.4 Writing a graph to a picture file6513.5 Printing6614 Application Preferences6714.1 Introduction6714.2 General Preferences6714.3 Regression Preferences6714.4 Graphing Preferences7014.4 Graphing Preferences7114.5 Logging Preferences7314.6 Localization Preferences7514.7 Advanced Preferences7615.1 Executive Summary79			
13.5 Printing			
14 Application Preferences 67 14.1 Introduction 67 14.2 General Preferences 67 14.3 Regression Preferences 70 14.4 Graphing Preferences 70 14.5 Logging Preferences 71 14.5 Logging Preferences 73 14.6 Localization Preferences 75 14.7 Advanced Preferences 76 15 Localization 79 15.1 Executive Summary 79			
14.1 Introduction 67 14.2 General Preferences 67 14.3 Regression Preferences 70 14.4 Graphing Preferences 71 14.5 Logging Preferences 73 14.6 Localization Preferences 75 14.7 Advanced Preferences 76 15 Localization 79 15.1 Executive Summary 79			
14.2 General Preferences 67 14.3 Regression Preferences 70 14.4 Graphing Preferences 71 14.5 Logging Preferences 73 14.6 Localization Preferences 75 14.7 Advanced Preferences 75 15.1 Executive Summary 79	14		
14.3 Regression Preferences 70 14.4 Graphing Preferences 71 14.5 Logging Preferences 73 14.6 Localization Preferences 75 14.7 Advanced Preferences 76 15 Localization 79 15.1 Executive Summary 79			
14.4 Graphing Preferences 71 14.5 Logging Preferences 73 14.6 Localization Preferences 75 14.7 Advanced Preferences 76 15 Localization 79 15.1 Executive Summary 79			
14.5 Logging Preferences 73 14.6 Localization Preferences 75 14.7 Advanced Preferences 76 15 Localization 79 15.1 Executive Summary 79			
14.6 Localization Preferences 75 14.7 Advanced Preferences 76 15 Localization 79 15.1 Executive Summary 79			
14.7 Advanced Preferences 76 15 Localization 79 15.1 Executive Summary 79			
15 Localization 79 15.1 Executive Summary 79			
15.1 Executive Summary		14./	Advanced Preferences
	15	Loca	lization 79
15.2 Configuring CurveExpert Basic to match your workflow			
		15.2	Configuring CurveExpert Basic to match your workflow

	15.3 File overrides	80 80 80
16	Validation 16.1 Introduction 16.2 Running the Suite 16.3 Performing validations yourself	81 81 81 81
	Miscellaneous 17.1 Log Viewer 17.2 Running Multiple Instances 17.3 Where files are located 17.4 User License Agreement	 83 83 84 84 84 85
19	Third-Party Licensing19.1Python19.2WxWidgets and WxPython19.3Numpy19.4Scipy19.5Matplotlib19.6xlrd19.7BioPython19.8winpaths19.9Python Imaging Library (PIL)19.10Icons and Artwork19.11JPEG library	87 88 89 90 91 92 92 93 93 93
20	Appendix A: Math Functions20.1Constants20.2Transcendental Functions20.3Bessel Functions20.4Comparison Functions20.5Miscellaneous Functions20.6Array Specific Functions20.7Logical Functions	95 95 98 100 101 103 107
	Appendix B: Math Symbol Reference 21.1 Subscripts and superscripts 21.2 Fractions, binomials and stacked numbers 21.3 Using parenthesis properly 21.4 Radicals 21.5 Accents 21.6 Symbols	
22	Appendix C: Theory 22.1 Linear Regression 22.2 Nonlinear Regression	115 115 115
23	Appendix D: References	119
24	Indices and tables	121
Inc	2X	123

WHAT IS CURVEEXPERT BASIC?

CurveExpert Basic is a solution for curve fitting and data analysis for Windows. Data can be modelled using a toolbox of linear regression models and nonlinear regression models, and visualized with the built-in publication quality graphics engine.

Over 60 models are built-in, but custom regression models may also be defined by the user. Publication-quality graphing capability allows thorough examination and presentation of the curve fit. The process of finding the best fit can be automated by letting CurveExpert Basic compare your data to each model to choose the best curve. The software is designed with the purpose of generating high quality results and output while saving your time in the process.

CurveExpert Basic is a subset of the functionality contained in CurveExpert Professional and is intended for more casual/infrequent users. The major features of the software are enumerated below:

- Easy-to-use User Interface: most mathematically-intensive applications are very difficult to use. CurveExpert Basic has a very intuitive interface, which allows you to import your data, generate results, and create publication-quality plots with very minimal effort. In fact, to import a file takes only four clicks, and generating a battery of results with associated graphs takes two more.
- **Robust file import**: data files come in many shapes and sizes, and CurveExpert Basic makes importing your data files very easy. The smart file reader avoids non-data areas of your file dynamically, and attempts to find labels for each column of data in your file.
- **Publication quality graphs**: The rendering of the plots is of publication quality, with full antialiasing support and the ability to customize each graph. Graphs can be saved to a variety of graphics file formats, and they may be directly copied and pasted into another application. Graphs are interactive, with zooming, panning, and autoscaling.
- **Built-in models**: over 60 built-in nonlinear models, with high-quality automatic initial guesses, are available for use. The provided models cover all of the major families.
- **Custom models**: you can also define models yourself, using a very large library of built-in mathematical functions, and parameters in your models can take any name that you like.
- **Ranking of results**: results are automatically ranked by your choice of score, correlation coefficient, standard error, or coefficient of determination.
- Validated: validated against the Statistical Reference Datasets Project of the National Institute of Standards and Technology. These datasets can be downloaded directly at http://www.itl.nist.gov/div898/strd/general/dataarchive.html, but are also included verbatim in the CurveExpert Basic distribution for you to use yourself.
- **Quality spreadsheet**: the built-in spreadsheet allows you to manually enter data and/or modify it with a suite of data transformation tools. Data entry and cutting and pasting capabilities are as easy as Excel.
- Localization: Importing data or interoperating in European-style environments (which use a comma as a decimal) is extremely easy; regional settings are automatically obeyed, or can be selectively enabled in order to match your particular workflow.

- Logging: a log of actions is kept across sessions of the software, in case you need to recreate a particular result. A messages pane keeps you informed of the status of every computed result.
- **Documentation**: Extensive documentation in HTML and PDF format, available both directly from the software and online at https://www.curveexpert.net/support/documentation/.

TWO

INSTALLATION AND ACTIVATION

2.1 Installation

2.1.1 Windows

To install on Windows platforms, simply run the installer, either from the command line or by double clicking it in the Windows explorer. The automated installer will start and guide you through the installation process; just follow the on-screen prompts. CurveExpert Basic will install for all users (if you are the Administrator), or for you only (if you are not). This allows you to install CurveExpert Basic without any Administrator privileges.

Windows automated installs

The installer for Windows operating systems recognizes two command line switches: /S for silent installs, and /D=dirname to specify where the program should be installed. For example, in an environment where a system administrator would want to install the program silently to the directory "d:\sharedprogs", one would do:

> CurveExpertBasic-2.0.0-win64.exe /S /D=d:\sharedprogs

Windows automated uninstalls

The uninstaller for Windows operating systems can be used for silent uninstalls. If the software was installed in the directory "c:\sharedprogs", one would do:

> "c:\sharedprogs\CurveExpert Basic\uninstall" /S

Note that there are no quotes used in the last _? option, even if there are spaces in the path.

2.2 Starting a Trial

If you want to evaluate CurveExpert Basic on a trial basis, you can start a trial period by selecting *Help->Activate Trial Period*; note that an Internet connection is required for the starting of the trial period, but is not required once the trial period has been activated.

Note: If you use a proxy for Internet access, please set the appropriate proxy settings in *Edit->Preferences->Advanced* (see *Proxy settings*).

This trial period is active for approximately 30 days from activation date. During this period, all features of CurveExpert Basic are accessible. When the software is out of its trial period (either before or after), most output functions are disabled, and a watermark appears on all graphs.

After evaluation via the trial period, please consider purchasing the software at http://www.curveexpert.net/order.

2.3 Purchasing

To purchase CurveExpert Basic, visit http://www.curveexpert.net/order, and choose the product that you would like to purchase.

2.4 After Purchase: licensing

If you have purchased a CurveExpert Basic license, you will receive the license information via email. Licenses are fulfilled within 24 hours of receipt; average turnaround time between purchase and license fulfillment is 2 hours.

Proceed to *Help->Enter License*, and paste the entire email into the box. The fields below the box (Name, Company, etc.) will update, and you can then press OK to complete the process.

If you are not sure how to copy and paste the email, highlight the text of the email with your mouse (click and drag), and press Ctrl+C (Cmd+C on a Macintosh). Then, just press the *Paste* button in the *Help->Enter License* window.

Thank you for your support of CurveExpert Basic!

2.5 Automated licensing

System administrators may need a means to apply the license via the command line. To do this, save the licensing email as a text file, and then pass the text file to CurveExpert Basic on the command line as follows:

> cebasic.exe --license the_license_filename.txt --quit

Make sure that you are in the same directory as the executable when running this command, so that the executable can find its required shared libraries. This procedure works under both Mac and Linux; under Linux, simply remove the .exe from the commands above. On macOS, you will have to use the "open" command:

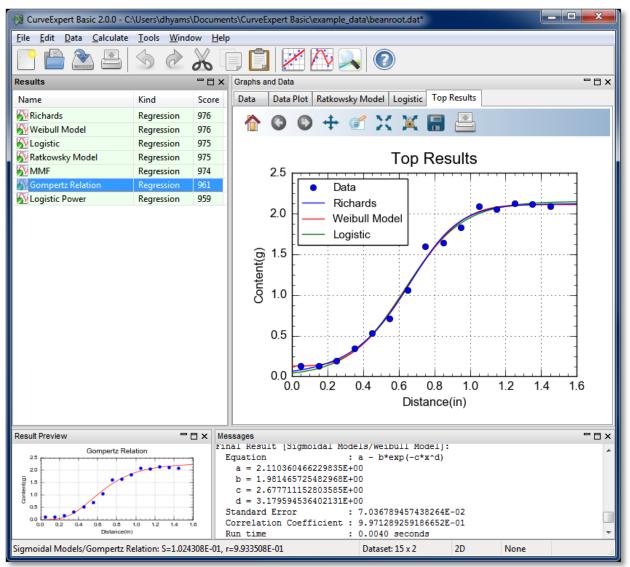
> open /Applications/CurveExpertBasic.app --args --license the_license_filename.txt --quit

The application will write a file "license.log" that prints the results of the licensing (success or failure).

THREE

GETTING STARTED

This guide leads you through the bare minimum of information you need to know in order to run CurveExpert Basic successfully. See the *User Interface* chapter for a full explanation of the interface.



3.1 Load data into CurveExpert Basic

Read a sample file supplied with CurveExpert Basic. Choose *File->Open*, double click on "example_data", set the file filter to *.dat, and double click the file "beanroot.dat". When the File Import dialog appears, simply click OK. (see *Reading Data*)

3.2 Perform a Nonlinear Regression

Choose *Calculate->Nonlinear Model Fit*. Select the Sigmoidal Models, which automatically selects all of the members of that model family for computation. Click OK. (see *Calculating Results*)

3.3 Examine the Results

As a result of the computation, the results will be shown in the left pane in CurveExpert Basic, ranked in order from the best fit to the worst fit (see *Working with Results*). Double click, or right-click and select *Details*..., on any of the results to see details (see *Querying Result Details*). Also, you can click the tabs in the graph stack (the right hand pane in the application window) to see visualizations of the results. Later, you can add graphs of your own.

3.4 Visualize your Results

In the "Graphs and Data" pane, two graphs have been automatically created for you; one that shows the data only, and one that shows the data plotted with the top few results that have been computed. You can visualize any one of the results in the "Results" pane by right clicking one (or some) of them and selecting "Send to New Plot".

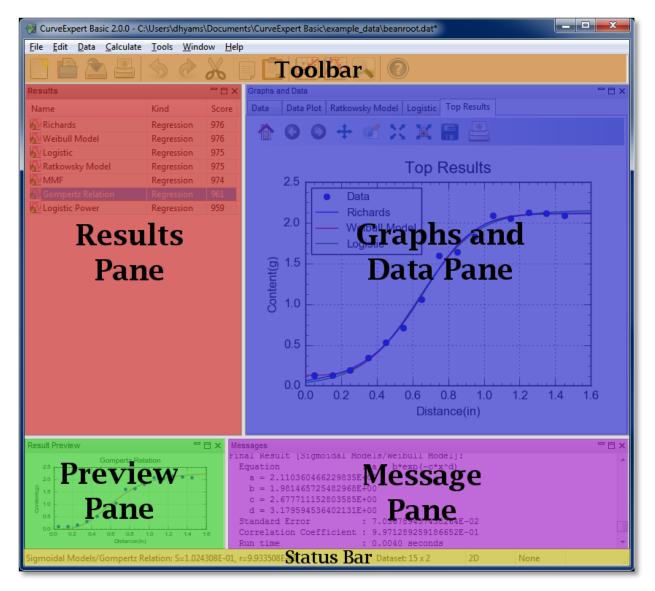
FOUR

USER INTERFACE

The CurveExpert Basic user interface is divided into panes:

- Results
- Graphs and Data
- Preview
- Messages

The panes, as well as the toolbar and status bar, are labeled in the graphic below:



All of the panes can be shown or hidden via the *Window* menu in the menu bar. Further, panes (except for the Graphs and Data pane) can be torn out from the main window; grab the pane by its title bar, and tear it out. The panes can be redocked in the main window by the reverse operation; drag the window to one of the docking indicators, and a transparent hint will appear to show where the window will be docked. Using this procedure, the panes can be rearranged inside the main window to taste.

Panes can be quickly maximized by clicking the small box at the top right of each pane; this allows the pane to fill the entire main window. Restoring the size of the pane can be performed by clicking the double-box at the top-right of the pane. This gives a quick means of viewing a particular pane (most commonly the Graphs and Data pane) in full size.

All panes can be hidden by clicking the 'X' at the top right of the pane, or by deselecting the corresponding pane name in the *Window* menu. To show a pane after being hidden, select the corresponding pane name in the *Window* menu.

4.1 Menus

If current conditions are such that a particular result cannot be computed, it will be dimmed in its *Calculate* menu. For example, with only one point in the dataset, it is not possible to compute any regressions So, all linear and nonlinear regressions in the *Calculate* menu will be dimmed and therefore unselectable. See *Menu Reference* for a quick explanation of each of the menu choices.

4.2 Toolbar

The toolbar can be shown or hidden via "Window->Toolbar".



Each button on the toolbar has a one-to-one mapping to an item in the menus. The toolbar is divided up into the following sections:

- File
- Edit
- Calculate
- Tools
- Help

The buttons are each documented below.

Icon	Meaning
·	
	File->New. Reinitializes the application with an empty dataset and no results. When New is selected, you must input the
	File->Open. Opens a new (text) data file or CurveExpert file.
	File->Save. Save the current data, results, and graphs into a CurveExpert file.
	File->Save. Save the current data, results, and graphs into a CurveExpert me.
	File->Print. Prints the contents of the spreadsheet as a data table. If you would like to print all graphs, hold SHIFT while
	Edit->Undo. Undo the last appropriate action.
C	
0.0	Edit->Redo. Redo the last appropriate undone action.
à	
	Edit->Cut. Cuts the selected item(s) to the clipboard as appropriate.
	Edit->Copy. Copies the selected item(s) to the clipboard as appropriate.
6	Edit->Copy. Copies the selected hem(s) to the enpotent as appropriate.
	Edit->Paste. Pastes data from the clipboard as appropriate.
	Calculate->Linear. Calculates a straight line regression for the data.
N .	
	Calculate->Nonlinear Model Fit. Shows the nonlinear regression picker so that you can select a model or models to comp
	Tools->CurveFinder. Runs the CurveFinder to scan models for the best fit for your data
600	$T \to C$ ($(T \to C \to T) \to C$) ($T \to C$
	Tools->Custom Models(Simple). Opens the custom model creator (simple interface)
	Help->Manual. Opens the documentation.

4.3 Results Pane

The results pane displays a list of the currently calculated results. This list is color-coded and badge-coded; see *Working with Results* for an explanation of the color codes and badges.

The items displayed in the columns of the results pane can be customized by right-clicking the column headers. The following items may be selected for display:

- Name (required; cannot be deactivated)
- Kind
- Family
- Score
- R (correlation coefficient)
- R^2 (coefficient of determination)
- Std_Err (standard error)

Remember that you can send results to a plot, remove a result, or view result details by right-clicking a particular result. See *Working with Results* for details.

4.4 Graphs and Data Pane

The "Graphs and Data" pane is a notebook where the dataset and graphs reside. Please refer to *The spreadsheet* for information on how to work with the dataset via the built-in spreadsheet. Refer to *Graphing* for documentation concerning how to work with graphs.

4.5 Preview Pane

The preview pane displays the result that is pointed to in the Result pane, or, if a result is pointed to in a graph, the preview pane also updates to the pointed-to-result. While convenient, the preview window can cause the user interface to be sluggish on older computers; to disable the preview, simply hide it by deselecting *Window->Preview*, or more straightforwardly, click the 'X' at the top right of the preview pane.

4.6 Messages Pane

The **Messages Pane** is an area where CurveExpert Basic sends all notifications for your perusal. For example, when a file is read, the a summary of the file contents appears in the Messages pane. Also, when any calculation is undertaken, a summary of the result appears in the Messages pane.

The content of the messages pane can be copied and pasted to another application by highlighting a portion, rightclicking, and selecting *Copy*, or by using Ctrl+C.

Error messages appear in the Messages pane in red, and special messages appear in blue. All messages that appear in the Message pane are automatically logged, and be accessed after-the-fact via *Tools->Log Viewer* (see *Log Viewer*).

4.7 Status bar

The status bar is divided into five sections, which show the following items:

Section	Displays
1	typically shows vital statistics for the currently pointed-to result, or displays help when appropriate.
2	size of the currrent dataset (nrows x ncolumns)
3	dimension of the dataset, which determines the mode of the application
4	current locale
5	number of helper processes present that perform calculations (see multicore). Each asterisk represents one
	helper process.

4.8 Menu Reference

4.8.1 File menu

Menu choice	Purpose
File->New	Reinitializes the application with an empty dataset and no results. When
	New is selected, you must input the desired number of columns in the new
	dataset.
File->New from Clipboard	Reinitializes the application with a dataset imported from the clipboard. The
	file import dialog allows you to fine-tune the importing process.
File->Open	Opens a new (text) data file or CurveExpert file.
File->Recent files	Opens a previously opened file.
File->Close	Closes the current file.
File->Save	Save the current data into a file.
File->Save As	Save the current data into a file, under a different name.
File->Export	exports the current dataset as a text file.
File->Print	Prints the contents of the spreadsheet as a data table. If you would like to
	print all graphs, hold SHIFT while selecting File->Print.
File->Print Preview	Shows a print preview of the spreadsheet data, optionally printing it as well.
	If you would like to print preview for all graphs, hold SHIFT while selecting
	File->Print Preview.
File->Page Setup	allows setting of preferences for margins, paper orientation, etc., for print-
	ing.
File->Exit	close CurveExpert Basic

4.8.2 Edit menu

Menu choice	Purpose
Edit->Undo	Undo the last appropriate action. For data in the spreadsheet, see Undo and
	Redo.
Edit->Redo	Redo the last appropriate undone action. For data in the spreadsheet, see
	Undo and Redo.
Edit->Cut	Cuts the selected item(s) to clipboard as appropriate. For selections of data,
	see Cutting, Copying, and Pasting.
Edit->Copy	Copies the selected item(s) to clipboard as appropriate. For selections of
	data, see Cutting, Copying, and Pasting.
Edit->Paste	Pastes items from the clipboard as appropriate. For pasting of data, see
	Cutting, Copying, and Pasting.
Edit->Clear	clears the selected data as appropriate, without placing it on the clipboard.
Edit->Select All	Selects all items as appropriate.
Edit->Preferences	Opens a dialog where the application settings/preferences can be viewed
	and/or modified. See Application Preferences.

4.8.3 Data menu

Menu choice	Purpose
Data->Sort	sort the selected data by the first column. See Operating on Data.
Data->Scale	scale the selected data by a factor. See Operating on Data.
Data->Translate	translate (add) a constant to the selected data. See Operating on Data.
Data->Transform	Apply a general transformation to the selected data. See Operating on Data.
Data->Crop	Crop the data to a selected minimum and maximum; removes points from
	the dataset. See Operating on Data.
Data->Clamp	Clamp the selected data to a minimum and maximum. See Operating on
	Data.
Data->Rotate	Rotate the columns in a dataset to the left. See Operating on Data.
Data->Add/Remove STDDEV Col-	Add or remove a standard deviation column to/from the dataset, as appro-
umn	priate.
Data->Statistics	Show the basic statistics for the dataset. See Data statistics.

4.8.4 Calculate menu

Menu choice	Purpose
Calculate->Linear Fit	Calculates a straight line regression for the data. See linreg.
Calculate->nth Order Polynomial	Calculates a polynomial fit for the data, with a user-selectable degree. See
	linreg.
Calculate->Nonlinear Fit	Shows the nonlinear regression picker so that you can select a model or
	models to compute. See nonlinreg.

4.8.5 Tools menu

Menu choice	Purpose
Tools->CurveFinder	Runs the CurveFinder to scan models for the best fit for your data. See
	CurveFinder.
Tools->Run NIST Validation	Check CurveExpert Basic against certified NIST results. See Validation.
Tools->View Logs	View the log files. See <i>Log Viewer</i> .

4.8.6 Window menu

Menu choice	Purpose
Window->Results	Toggle the Results pane on and off. See User Interface.
Window->Graphs and Data	Toggle the Graphs and Data pane on and off. See User Interface.
Window->Messages	Toggle the Messages pane on and off. See User Interface.
Window->Preview	Toggle the previewing pane on and off. See User Interface.
Window->Toolbar	Toggle the main toolbar on and off. See <i>Toolbar</i> .
Window->Dock All	Dock all floating panes back into the main window. See User Interface.
Window->Restore to Default	Restores all panes the the default layout (docked, Results pane top left, Pre-
	view bottom left, Graphs and Data top right, and Messages bottom right).
	See User Interface.

4.8.7 Help

Menu choice	Purpose		
Help->Manual	Displays the CurveExpert Basic manual (HTML version).		
Help->Web Site	Displays the Hyams Development web site.		
Help->Discussion Forum	Displays the CurveExpert user-to-user discussion forum.		
Help->Tutorial Videos	Displays the available video tutorials for CurveExpert Basic		
Help->Activate Trial Period	activates a 30 day trial period for CurveExpert Basic; see Installation and		
	Activation.		
Help->Enter License	after purchase, enter your license for the software; see Installation and Ac-		
	tivation.		
Help->Order	direct link to the website for ordering.		
Help->Check for Updates	Checks to see if your version is the latest one; requires Internet access.		
Help->Show Diagnostics	Displays diagnostic information in the Messages pane.		
About	Displays the application about box.		

READING DATA

5.1 Introduction

The first task in any data analysis program like CurveExpert Basic is to read or import your data into the software. For this, CurveExpert Basic provides a robust file import mechanism, which can be accessed simply by choosing *File->Open*. You can read in both native CurveExpert files (.cxp) and generic data files in text format.

Note: To be able to choose files with extensions other than .cxp, you must select the appropriate extension in the bottom right corner of the file choosing dialog.

Most of the time, the data to be read in is contained within a text file of some sort, with headers and comments interspersed. CurveExpert Basic tries to make the job of importing this data as easy and painless as possible. The file import intelligently examines your raw file in order to find the data, as well as finding column headers for that data, if present.

5.2 Raw file import

To read in a text file (common extensions are .dat and .txt, but can be anything that you choose), simply choose *File*->*Open*, and then the filename. Alternatively, drag and drop the file to the CurveExpert Basic spreadsheet. The file import window will display, as follows:

Importing: C:\Use	mporting: C:\Users\dhyams\Documents\CurveExpert Basic\example_data\beanroot.dat							
- File Informatio	File Information							
File name:	File name: C:\Users\dhyams\Documents\CurveExpert Basic\example_data\beanroot.dat							
File size:	0.45 KB							
Number of lin	Number of lines: 24							
File Import Options								
Number of independent variables:			1	Numeric format*:	English (3.14159)	•		
🔲 Standard d	eviation in last colum	าท	Rotate Columns Left*					
🔲 Autofill firs	t column	Start:	0.0	Increment:	1.0			
Header/footer treatment* Header skip:		8	Footer skip:	1	▲ ▼			
Comment character*			#					
* = must pres	s the "Reread file" b	utton below to see	the effect of this operatio	n.				
Reread fil	e							
Raw File Imp	ort Preview							
	Distance(in)	Content(g)						
1	0.050000000000000	0.13000000000000	0					
2	0.1500000000000000	0.13000000000000	0			=		
3	0.250000000000000	0.19000000000000	0			_		
4	0.350000000000000	0.34000000000000	0					
5	0.450000000000000	0.53000000000000	0					
6	0.550000000000000	0.71000000000000	0					
7	0.650000000000000	1.0600000000000000						
8	0.750000000000000	1.600000000000000						
9	0.850000000000000	1.640000000000000	0			-		
				(OK Cancel			

Basic information about the file is shown at the top of the window, where the complete path to the file, file size, and the number of lines detected in the file is displayed. The middle section of the window is where you set parameters necessary for reading in the file. Most of the time, default options are appropriate, and there is not much more to do except to glance at the spreadsheet preview in the bottom third of the window, and click the OK button. However, in cases where the defaults are not appropriate, there are a range of settings you can manipulate to read your file in successfully.

5.2.1 Numeric format

By default, the numeric format is set according to the settings in *Edit->Preferences->Localization* (see *Localization*). The two available settings are English (use dots for decimals) and European (use commas for decimals). Select the appropriate numeric format for your file.

5.2.2 Rotate columns left

Some raw datasets list the dependent variable first. If this is the case, checking *Rotate columns left* will shift the data in the first column to the last, moving all other columns to the left. This is the ordering that CurveExpert Basic expects (independent variables first, and the dependent variable following). For a two column dataset, this operation is equivalent to swapping the columns. To see the effects of your choice here, the *Reread file* button must be pressed.

5.2.3 Autofill

Sometimes, the independent variable is implied by the ordering of the data. If you would like to generate the first column of data as a simple range and increment, select *Autofill first column*, and then choose the starting value and increment between each data point. The result of your operation is shown instantly in the spreadsheet preview. The fill is computed as follows:

$$x = x_{start} + i\Delta x$$

where i is the point id (starting at zero for the first point), x_{start} is the starting value input, and Δx is the increment input.

5.2.4 Treatment of Header and Footer

Often, data files have text that is not part of the dataset, and this text appears either before or after the real dataset (or both). To accommodate for this, you can set the *Header Skip* and *Footer Skip*, which is the number of lines in the file that are skipped at the top and bottom, respectively, before any attempt is made at reading data. This capability can also be used to intentionally skip over certain data in your file.

The header and footer skip can be thought of as a mask that is applied to your file before any reading takes place.

CurveExpert Basic uses a sophisticated procedure to try to guess the header and footer skip correctly. In all but the most esoteric cases, the header and footer skips will be correct already, and therefore need no interaction from the user.

Note: A newline at the end of your file counts as just that; a new line. This line is skipped by CurveExpert Basic because it is a line with no data. Therefore, it is common for the footer skip to be set to 1 by the automatic header/footer algorithm.

5.2.5 Comment character

Most data files have comments interspersed throughout them, sometimes in the middle of the data. In order to skip these comments, the character that designates the comment must be specified. In the data file, then, anything that appears after a comment character is ignored. Common comment characters are '#' and '%'.

5.2.6 Refreshing the preview

If rotating columns or changing the header/footer treatment, you must press the *Reread file* button to refresh the preview.

5.2.7 File import preview and raw file preview

The file import preview shows the result of the reading of the file, augmented by the current settings discussed above. This preview shows you exactly what CurveExpert Basic will read and place in the main spreadsheet.

The raw file preview shows you a copy of the file, with no modification, so that you can see the contents. Line numbers are annotated on the left, the the header and footer skip settings are shown by dimming the areas of the file that are masked away by these settings.

5.2.8 Column Labels

CurveExpert Basic attempts to detect the labels of your columns, such that they are correctly read into the software. To detect the column labels, the file reader examines one line above the skipped header, if such a line exists. In other words, if the header skip is set to 10, line 10 is examined for the column labels. First, the line is trimmed of any white space and comment characters, and then broken into individual tokens. If the number of items on this line is the same as the detected number of columns, these tokens are treated as the column names, as long as they "look like" names. To look like a name, the labels must begin with an alphabetical character, and only contain legal punctuation "()+-*". So, your data file can look something like this:

```
Comments at the top of the file are automatically
ignored by the file reader, because
it can tell
that there is no numeric data there.
# or you can comment with a designated comment character
time(s) voltage(volts)
1.0 4.5
2.0 4.23
3.2 4.1
```

In the example above, the column labels will be automatically detected as "time(s)" and "voltage(volts)".

5.2.9 Other file metadata

To force the localization of a given text file, see File overrides for the required header information.

5.2.10 Finishing

When the file import preview looks like the desired dataset, simply hit OK; your data will be read and placed into the main spreadsheet.

5.3 CurveExpert Basic files

CurveExpert Basic files contain the data, results, graphs, and notes (notes are available in CurveExpert Pro only). To save a .cxp file, simply choose *File->Save* or *File->Save As* as appropriate. Correspondingly, to read a .cxp file, choose *File->Open*.

These files are portable across platforms (Mac, Windows, and Linux), so you can read a file in on a Mac that was generated in Windows, for example. Also, .cxp files are compatible between CurveExpert Professional and CurveExpert Basic 2.0 or later. CurveExpert Basic can read CurveExpert Pro files, and vice versa.

Also, if a particular model or function is saved as a result in a .cxp file and it is not present on the system reading the file, the model/function will automatically be created on your behalf. This newly created model/function will then be available for use in the "Imported" family, and will appear appropriately in the Nonlinear model or function pickers.

SIX

WORKING WITH DATA

6.1 Introduction

The raw data in CurveExpert Basic is handled as a simple matrix of numbers; the dataset is made up of a number of rows and a number of columns. The first column is interpreted as the independent variable, and the second column is interpreted as the dependent variable.

6.2 Data statistics

Simple statistics for the current dataset can be obtained by selecting *Data->Statistics*. The resulting window will display the number of points and columns, and the following stats for each column of your dataset:

- minimum
- maximum
- range
- average (mean)
- standard deviation

The average is computed with the standard formula:

$$\bar{x} = \frac{1}{N} \sum_{i=1}^{N} x_i$$

Standard deviation is computed with the following formula, which is called the standard deviation of the sample:

$$\sigma = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (x_i - \bar{x})^2}$$

To copy the statistics information to the clipboard, press the Copy button at the bottom of the dialog.

6.3 The spreadsheet

The spreadsheet resides in the "Graphs and Data" pane in CurveExpert Basic.

The spreadsheet allows manual entry or modification of a dataset either entry-by-entry, or by cutting and pasting from within CurveExpert Basic, or from other sources. An example of the spreadsheet is shown below;

raphs a	and Data				E
Data	Notes	Data Plot	Top Results	+	
		X 1	Y		
1	1	0.050000	0.130000		
2	2	0.150000	0.130000		
3	3 (0.250000	0.190000		
4	4 (0.350000	0.340000		
5	5 (0.450000	0.530000		
(5 (0.550000	0.710000		
7	7 (0.650000	1.060000		
8	B (0.750000	1.600000		
9	9 (0.850000	1.640000		
1	.0 (0.950000	1.830000		
1	.1 1	1.050000	2.090000		
1	2 1	1.150000	2.050000		
1	.3 1	1.250000	2.130000		
1	.4 1	1.350000	2.120000		
1	.5 1	1.450000	2.090000		
1	.6				
1	.7				
1	8				
1	.9				
2	0				
2	1				
2	2				
2	3				
۰ 📃					+

All cells that hold data are white, and cells that are not part of the dataset are colored in gray. At the end of the dataset is one light-gray row, which signifies that the cells may be typed into (in order to add data points), but are not yet part of the dataset.

Right-click the spreadsheet in order to access operations that you can perform on the data itself, in-place.

The name of a column of data can be changed by right-clicking the appropriate column header and selecting *Rename Column* (alternatively, double click the column header). These names are for user information/convenience only.

The name of a row of data can be changed by right-clicking the appropriate row header and selecting *Rename Row* (alternatively, double click the row header). These names are currently for user information only.

6.3.1 Cursor Movement

Cursor movement in the spreadsheet is normally accomplished with the TAB and RETURN keys; TAB moves the cursor to the right, and RETURN moves the cursor downward. Of course, the arrow keys and PAGEUP/PAGEDOWN may also be used to move the cursor. If it is desired to move the cursor with a carriage-return like approach (in which the RETURN key moves the cursor to the next line if at the end of a row), this can be selected in *Edit->Preferences-Seneral->Excel style cursor movement*.

To reverse the direction of cursor navigation, hold the SHIFT key.

6.3.2 Cutting, Copying, and Pasting

When copying data, the current selection in the spreadsheet is placed on the clipboard (and obeys your regional settings while doing so). If no data is selected, all data is copied. The delimiter used between columns, if applicable, is the delimiter chosen in *Edit->Preferences->General->Default Delimiter*.

A "cut" must involve all columns of the dataset. Therefore, the "Cut" item in the data menu is dimmed if your selection only involves some of the columns. This behavior is due to the fact that a cut will remove points from the dataset, and your selection should reflect that reality.

A paste from the clipboard informs CurveExpert Basic to attempt to intelligently read what is on the clipboard and turn that into an intermediate dataset for subsequent pasting. Different rows in this intermediate dataset are delimited by newlines (or carriage returns), and columns are delimited by whitespace or commas (unless using European format for incoming numbers, in which case commas are not valid as a delimiter). This intermediate dataset will then be inserted at the current cursor location in the spreadsheet, overwriting parts of your existing dataset and extending your existing dataset as necessary. A paste operation can be viewed as an insertion of a block of data at the current cursor location, following by a subsequent discarding of any data that happens to fall outside the current number of columns of your dataset.

6.3.3 Inserting Rows

To insert a row into your dataset, right click on the spreadsheet and select "Insert Row". This will cause all rows at or below the current cursor location (indicated by the black outline) to be shifted downwards, and a new row will be inserted at the current location.

To insert multiple rows at once, select a range in the spreadsheet, right click, and select "Insert Row" as before. In this case, all rows touched by the selection will be shifted downwards, and new rows are inserted at the current cursor location. The number of inserted rows will equal the number of rows in the original selection. For example, to insert three rows at row 2, select rows 2-4 (inclusive) and select "Insert Row".

6.3.4 Removing Rows

To remove rows from the dataset, select a set of rows to be removed, right click, and select "Remove Rows". This is functionally similar to cutting the rows (see above), except that the data is not copied to the clipboard.

6.3.5 Undo and Redo

All data operations are undoable and redoable to a number of levels possible by the *Edit->Preferences->Advanced->Peak Undo Memory Usage* setting. All data operations are undoable and redoable to a number of levels possible by the *Edit->Preferences->Advanced->Number of undo levels* setting. So, you can feel comfortable manipulating data knowing that any transformation, clear, or cut/paste operation can be undone.

6.4 Number Formatting

The values shown in a spreadsheet may be formatted by selecting a block via the mouse, right clicking, and selecting **Format Numbers** from the resulting menu. A dialog will appear as follows:

A **General** formatting prints a number naturally as most practitioners would write the number. **Scientific** formatting prints the number always with a mantissa and exponent part, as in "1.532e+04". **Engineering** formatting is almost the same as scientific, but the exponent is always guaranteed to be a multiple of three. **Percentage** formatting shows a decimal as a percentage, with a following percentage sign. For example, the number 0.05 would be shown as 5.0%.

The **Decimal places** field allows the user to specify the number of decimal places shown; this setting is relevant for all formatting settings listed above except for **General**.

The **Leader** and **Trailer** fields allow the user to place customized text before and/or after the number. These fields are very useful for adding units to numbers (use the trailer) or prepending a dollar sign for currencies (place \$ in the Leader field).

6.5 Operating on Data

CurveExpert Basic provides several ways that you can operate on raw data in the spreadsheet. To perform these operations, simply highlight the data that you want to work on, and select one of Sort, Scale, Translate, Transform, Crop, or Clamp from the Data menu. Alternatively, you can right click on the spreadsheet after making a selection. If no selection is made, the operation is assumed to apply to the entire dataset (all rows and all columns).

6.5.1 Sort

To sort your data against the first column of the dataset, select **Sort** from the Data menu (the entire dataset must be selected in the spreadsheet). If CurveExpert Basic has detected that the data is already sorted, this menu item will be dimmed. If the choice is nondimmed, however, it does not necessarily mean that the dataset is already sorted.

6.5.2 Scale

To multiply by or divide the selected data by a factor, select *Data->Scale*.

6.5.3 Translate

To add a constant value to the selected data, select Data->Translate.

6.5.4 Crop

To drop points from the selected part of your dataset that are above or below a certain threshold, select *Data->Crop*. After a cropping operation, there is likely to be fewer data points in your data set than before the crop. Usually, cropping is used to eliminate outliers from a dataset.

6.5.5 Clamp

To clamp points in the selected part of your dataset to a certain threshold value, select *Data->Clamp*. Clamping is usually used to correct values that are slightly over or under a valid domain for that value.

6.5.6 Rotate

To rotate columns in a dataset, select *Data->Rotate*. For a dataset with two columns, this is exactly the same as a column swap. Note that the rotation always proceeds to the left in a circular fashion; the leftmost column becomes the rightmost one after the rotation, and all other columns are displaced by one to the left.

6.5.7 Transforming Data

Data->Transform allows you to map the selected part of your dataset through a general function. If this menu item is selected, you can enter an expression, as a function of x, and all selected data will be evaluated via this function. Note that "x", in this context, just refers to the selected data.

For example:

```
x + 5
pow(x*100,0.75)
degrees(x)
```

In the transformation, you may use any functions listed in *Appendix A: Math Functions*. Note that both the Scale and Translate operations above can just as easily be done via a transformation here.

SEVEN

CALCULATING RESULTS

CurveExpert Basic supports TWO distinct classes of results:

- regressions
 - linear regressions (linear and polynomial fits)
 - nonlinear regressions (built-in and custom models)
- interpolations
 - cubic spline
 - tension spline

Calculation of these results can be accessed through the *Calculate* menu in CurveExpert Basic, or optionally via the corresponding buttons on the toolbar (see *Toolbar*).

7.1 General Guidelines

7.1.1 Scaling Datasets

For best results, always scale your data sets to the order of one. You may do this prior to reading in your data file, or after your data file has been imported using the scaling feature in CurveExpert Basic (see *Operating on Data*).

Imagine a data set with x values ranging from 1000 to 10000 and a regression model where the term $\exp(a^*x)$ is involved. Unless a very good initial guess for a is given, chances are that an exponential to a very large power (eg. $\exp(1000)$) will be taken in the course of the nonlinear regression algorithm. The calculation will overflow, and the regression will fail as a result. Even if the regression happens not to fail, the regression algorithm will have an exceedingly tough time finding the correct parameters, since a small change in the free parameters will cause a tremendous change in the size of the term. The moral of the story: always scale your data!

As another example, if you have data that describes atmospheric pressure at different elevations, you might have (in metric units) a data set that looks like:

```
x=[-100, 0, 100, 500, 1000, 4000] meters
y=[102000,101325,101000,100500,100000,99900] Pascals
```

Using the *Data->Scale* feature in the Data menu of CurveExpert Basic, you can scale this data using a scale factor of 0.001 on the x data, and 0.00001 on the y data. So, you would then have the following data set:

```
x=[-0.1, 0, 0.1, 0.500, 1, 4] kilometers
y=[1.02,1.01325,1.01,1.005,1.0,0.999] bars
```

The second example is much more likely to allow nonlinear regressions to converge, and also will allow higher order polynomial fits to be performed with more accuracy. If you have a data set that seems particularly ill-behaved, scaling can help solve this problem.

Note that CurveExpert Basic is able to perform correctly on data in any scale, as long as the calculations do not overflow or underflow. So, if a data set is giving problems, scaling it should be the first action to take.

7.1.2 Set the tolerance parameter reasonably

Don't set the tolerance parameter (in *Edit->Preferences->Regression*) too low. In regression modeling, not much advantage is to be gained by setting a very strict tolerance. Its main purpose in life is to prevent the nonlinear regression algorithm from converging on local minima, not to make the calculated parameters more accurate.

7.1.3 Data should be appropriate to the model

Make sure that the data is appropriate to the model. Especially look out for using logarithmic or exponential families of models with data that contains zeros or negatives. For example, it is not possible, in any shape or form, to obtain a negative or zero with the basic exponential model ($y=ae^{(bx)}$, assuming a is positive; the inverse problem exists for a negative a). So, it is not wise to use a model that cannot reflect the trends in the data.

7.1.4 Sometimes, it is unavoidable

Some curve fits are simply ill-behaved, i.e. prone to divergence. For some data sets, it may not be possible to converge certain nonlinear regression models.

7.2 Interpolation

7.2.1 Introduction

An interpolation, by definition, passes through every data point, and as such, the correlation coefficient will always be 1, and the standard error will always be zero. CurveExpert Basic supports cubic splines and tension splines. All splines are defined in a piecewise fashion between data points.

Note: The dataset must be sorted (based on the independent variable) in order for any spline interpolation to work. Select *Data->Sort* from the main menu in order to sort your dataset if necessary. If CurveExpert Basic detects that your dataset is not sorted, it will not allow spline interpolations to be selected.

7.2.2 Cubic Splines

To calculate a cubic spline, select *Calculate->Cubic Spline* from the main menu. The cubic spline is simply a polynomial spline of order 3; cubic splines are the most common form of spline. Cubic splines guarantee continuity in the spline, and continuity in the first and second derivatives of the spline at the data points. At the endpoints, the second derivative is set to zero, which is termed a "natural" spline at the endpoints, as the curvature goes to zero.

7.2.3 Tension Splines

To calculate a tension spline, select *Calculate->Tension Spline* from the main menu. A prompt will appear to ask for the amount of tension desired. Tension splines are based on hyperbolic functions, and simulate a cord being stretched with a defined tension (amount of force) between the data points. An extremely high tension approaches a linear spline, and low tensions will appear correspondingly "loose" around the data points, resembling a cubic spline.

7.3 Linear Regression

7.3.1 Introduction

Linear regressions, as a class of results, can be calculated directly, and do not need an iterative process like nonlinear regressions do. See *Linear Regression* in the appendices for a more in-depth explanation. A linear regression can be constructed from any model that is a linear combination of functions; the coefficients in the linear combination are the parameters to be found.

There are two types of linear regressions supported in CurveExpert: linear and polynomial. All other regressions, even if they could be calculated as a linear-type regression through a variable transformation, are computed with the nonlinear regression engine.

7.3.2 Linear Fit

In CurveExpert Basic, you can choose to calculate a straight line regression:

y = ax + b

by choosing Calculate->Linear Fit.

7.3.3 nth Order Polynomial Fit

To calculate a polynomial via linear regression, choose *Calculate->nth Order Polynomial Fit*. A prompt will appear to ask for the degree of polynomial desired. Also, in the same prompt, you can choose to force the polynomial through the origin, which forces the intercept to zero. Also, you may choose the desired weighting for each point in the dataset (see weighting for further information) After entering the degree (and origin forcing or weighting as appropriate), the polynomial will be computed and added to the result list.

7.4 Nonlinear Regression

7.4.1 Introduction

Nonlinear regressions are solved with the Marquart-Levenberg method as documented in *Nonlinear Regression* in the appendices. To calculate a nonlinear regression, select *Calculate->Nonlinear Model Fit* from the main menu.

7.4.2 Selecting a Model or Models

Upon selecting *Calculate->Nonlinear Model Fit*, the nonlinear regression picker will appear; all models appear in this picker (built-in models and custom models) that are appropriate for the number of independent variables in the dataset. A screenshot of the model picker is below:

Select Nonlinear Model(s)						
	^	Currently selected models:				
Truncated Fourier Series		Name	Equation			
Power Law Family		Geometric				
Geometric			a*x**(b*x)			
Hoerl		Hoerl	a*b^x*x^c			
Modified Geometric		Modified Geometric	a*x**(b/x)			
Modified Hoerl		Modified Hoerl	a*b^(1/x)*x^c			
Modified Power		Modified Power	a*b^x			
Power		Power	a*x^b			
Root		Root	a*b^(1/x)			
Shifted Power		Shifted Power	a*(x-b)^c			
🖳 🖃 Sigmoidal Models		Equation preview:				
Gompertz Relation	=					
Logistic		Modified Hoerl				
Logistic Power	-					
MMF						
Ratkowsky Model			- 1/ <i>m</i> - 0			
Richards	-		$y\!=\!ab^{1/x}x^c$			
۰			0			
Collapse Expand Q Search	3					
Weighting: Default 👻 🖉 Auto Initial Guesses						
OK Cancel						

On the left side of the dialog is where the desired models can be selected. Models can either be selected individually (by clicking the checkboxes next to the model), or a family at a time (by selecting the checkbox next to the desired family). All models can be selected by clicking the "root" of the tree labeled "Nonlinear Models".

A search field appears below the picker, so that you can filter the models to a certain specification. For example, typing "sig" in the search field will show all models that have "sig" in their name, or belong to a family with "sig" in its name. The search field allows you to quickly find a desired model in the hierarchy.

For convenience, the list of currently selected models will appear in the **Currently Selected Models** list in the upper right region of the picker. A preview of the equation for the currently pointed-to model is rendered in the **Equation preview** region in the bottom right area of the picker.

The *Automatic Initial Guesses* checkbox allows you to enable or disable automatic initial guessing for the calculation of the selected nonlinear models. If this box is enabled, CurveExpert Basic will provide high-quality initial guesses for built-in models, and for custom models, the custom model initialization (if any) will be called. If this box is disabled, you will be prompted for initial guesses for every model selected.

Note: if automatic initial guesses are disabled, the multicore capability, if enabled, will not be used for the currently selected batch of models.

Creating a Custom Model

The nonlinear model picker also provides for a quick way of creating a custom model (normally, custom models are created with *Tools->Custom Models*, see *Creating Custom Models*). To utilize this feature, simply click on the **Create a Custom Model** expander. This will open a small area in which you can type the name and equation for a model, and save it. Upon saving, the new custom model will be immediately available in the left pane for selecting.

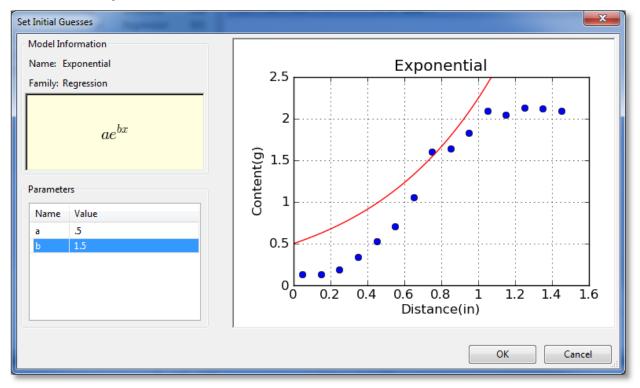
7.4.3 Setting the Weighting Scheme

To set the weighting scheme desired for the models that are to be computed, select the weighting scheme from the chooser at the bottom left of the dialog. See weighting for further details on the weighting schemes.

7.4.4 Manually setting initial guesses

Two situations cause the manual initial guess window to appear; one is if you choose to disable automatic initial guesses in the nonlinear model picker. The other is if a nonlinear regression fails, and you choose to set the initial guesses yourself in an effort to successfully calculate that model.

The manual initial guess window is shown below:



For informational purposes, the name, family, and equation for the nonlinear regression is shown in the upper left quadrant of the window. The parameters can be adjusted in the bottom left quadrant by clicking on the entries. As you adjust parameters, the graph drawn on the right will adjust accordingly. This gives real-time feedback on the parameter adjustment so that you can quickly refine the initial guesses into a reasonable state.

CHAPTER

EIGHT

CURVEFINDER

8.1 Usage

CurveFinder is a tool that you can use to search all available regressions for the best fit to your data. When CurveFinder is run, it will compute a fairly large list of results, and they will be shown in ranked order in the Results pane.

The use of the CurveFinder tool is quite straightforward; simply choose *Tools->CurveFinder* from the main menu, and then select the results that you want included in the calculation.

CurveFinder	
	CurveFinder calculates all results for your data and searches for the best fit. CurveFinder calculates all results for your data and searches for the best fit. CurveFinder calculates all results for your data and searches for the best fit. CurveFinder calculates all results for your data and searches for the best fit. CurveFinder calculates all results for your data and searches for the best fit. CurveFinder calculates all results for your data and searches for the best fit. CurveFinder calculates all results for your data and searches for the best fit. CurveFinder calculates all results for your data and searches for the best fit. CurveFinder calculates all results for your data and searches for the best fit. CurveFinder calculates all results for your data and searches for the best fit. CurveFinder calculates all results for your data and searches for the best fit. CurveFinder calculates all results for your data and searches for the best fit. CurveFinder calculates all results for your data and searches for the best fit. CurveFinder calculates all results for your data and searches for the best fit. CurveFinder calculates all results for your data and searches for the best fit. CurveFinder calculates all results for your data and searches for the best fit. CurveFinder calculates all results for your data and searches for the best fit. CurveFinder calculates all results for your data and searches for the best fit. CurveFinder calculates all results for your data and searches for the best fit. CurveFinder calculates all results for your data and searches for the best fit. CurveFinder calculates all results for your data and searches for the best fit. CurveFinder calculates all results for your data and searches for your data
Weighting: Default Vefault	Custom nonlinear regressions (6 available)
	OK Cancel

In this context "Linear Regression" refers to a polynomial of degree 1, which is the same straight line obtained from choosing *Calculate->Linear*. You can also choose the range of polynomials that should be searched, which ranges from 2 up to the lesser of 20 and the number of points in the dataset minus one. Nonlinear regressions (either built-in, custom, or both) can also be searched.

For convenience, you can use the "All On"/"All Off" button to turn all results on or off, as appropriate. After selecting the set of results that should be computed, simply press the OK button.

8.2 Cautions

Just because a particular model is ranked high in the Results pane does not mean that it is necessarily a good choice. Make sure to visually inspect the curve that represents your model. Polynomials, in particular, are very prone to oscillation, and can veer wildly away from the dataset before returning to be near the data points at each x value. Make sure that the model that you choose as best is a reasonable representation of your data.

CHAPTER

NINE

WORKING WITH RESULTS

9.1 Introduction

Once any results have been calculated, they appear in the result pane ranked in order of their score (the result pane normally is shown in the upper left part of the CurveExpert Basic application, see *User Interface*). The score reflects how closely the model adheres to the underlying data.

In the results pane, the results can also be sorted by any of the items displayed in the column header (name, kind, family, score, correlation coefficient, coefficient of determination, or standard error) simply by clicking the appropriate column header. Note that you can right-click on the column header in order to customize what is displayed in the results list; by default, the name, kind, and score is displayed.

When selecting results, you can simply click on the result (which selects it), or use multiple selection by holding down SHIFT or CTRL when clicking on results. This allows you to apply an operation to batches of results at once.

Every result in the results pane has a unique icon indicating the kind of result that it is. The table below shows meaning of each icon.

Icon	Meaning
/	Linear regression model (includes polynomials)
\sim	Nonlinear regression model (curve fit)

9.2 Color Coding

Result	Kind	Score	1
🔗 Richards	Regression	976	
🐼 Weibull Model	Regression	976	
🔂 Logistic	Regression	975	
🔊 Ratkowsky Model	Regression	975	
5 MMF	Regression	974	
🔊 Sinusoidal	Regression	968	
🔊 Truncated Fourier Series	Regression	968	
🔊 Hoerl	Regression	967	
🔊 Rational Model	Regression	964	
🔊 Gompertz Relation	Regression	961	
🔊 Gaussian Model	Regression	960	
🔊 Logistic Power	Regression	959	
💑 Vapor Pressure Model	Regression	955	
🔊 Modified Hoerl	Regression	955	L
🔊 Modified Geometric	Regression	950	
🔊 Modified Exponential	Regression	932	
🔊 Root	Regression	932	
🔊 Wavy	Regression	919	
ស Exponential Association 3	Regression	889	
🔊 Heat Capacity	Regression	874	
🔊 Shifted Power	Regression	873	
🔊 Bleasdale	Regression	873	
Section 2 Exponential Association 2	Regression	872	-

Also in the results pane, each result has a color coding of green or yellow. An example is shown below:

A green color coding indicates that the result was calculated successfully; it does **not** mean that the result is necessarily good; that is indicated by its score. The green coloring only indicates that the calculation of the result proceeded smoothly, and it is not possible to get a better result than what is given. In the common parlance of nonlinear regression, the parameters of the fit are said to be "converged".

A yellow color coding indicates that the result should only be used with caution. It indicates that the calculation succeeded, but with reservations. The most common cause for this is a nonlinear regression calculation that did not converge before the maximum number of iterations (configurable via *Edit->Preferences->Regression*) was reached. Again, the score will indicate how well the model adheres to the data.

If a result is presented in yellow, the result should be used with caution. It is possible that the parameters would have changed further if the max number of iterations is higher.

9.3 Badges

Every result is badged with either a green checkmark or a yellow exclamation point. The intention here is to inform the user when a result becomes invalid due to a change in the underlying dataset. For example, if a nonlinear regression is calculated, and then the dataset is scaled (using, say, the tools in the Data menu), that nonlinear regression becomes invalid, and an attention badge is placed on that result in the results pane to signify this.

To remedy the situation, you can update the result yourself by right clicking on the result and selecting "Update", or, if you would like to keep the old result and compute a new one, simply reselect the desired result from the *Calculate* menu, and an entirely new result will be generated.

Badge	Meaning
<u>S</u>	Data unchanged since calculation of this result
<u>Av</u>	Data changed since calculation of this result

9.4 Previewing

Pointing at a result will show its preview in the preview pane, usually at the bottom left of your application. Also, the standard error and correlation coefficient, if applicable, will display in the status bar at the bottom of the application window.

9.5 Placing Results on a Graph

There are several ways for a result to be shown on a graph; the first is automatic, in that the top scoring results (usually the top 3), are automatically placed in the "Top Results" graph whenever a new calculation is performed.

In CurveExpert Basic, you may create new graphs for each individual result. To do so, right click a result in the Results pane, and select *Send to New Plot*. This will create a new graph with the default graph theme (as selected in the application preferences), and add the selected results to that plot.

9.6 Removing Results

If you decide that a result is no longer needed, select it, right click, and pick *Remove*. This action is not undoable, but certainly the result can be calculated again by simply picking it from the *Calculate* menu.

You can remove multiple results at once by shift-clicking or control-clicking to select the results that you want to remove. If the results are shown in any graph, they are removed from the graph as well.

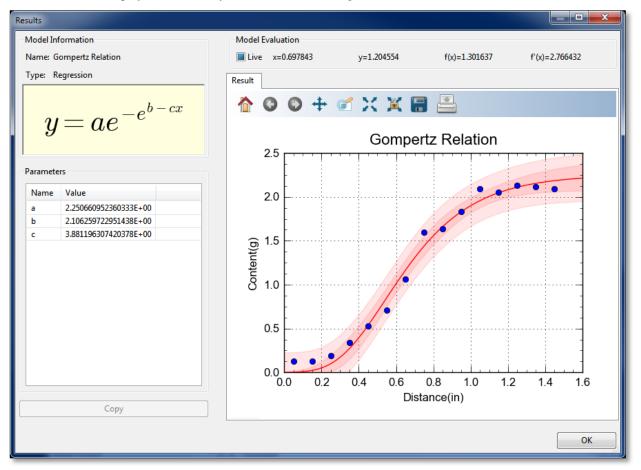
9.7 Copying Result Information

Right clicking on a result will allow you to select *Copy All Info*, which will copy a report about the selected result(s) to the clipboard.

If the selected result is a regression, the entry *Copy Parameters* will also appear. Select this to copy only the parameter name/value pairs to the clipboard, separated by the delimiter selected in the application preferences.

9.8 Querying Result Details

If you want to get more detail on a calculated result, either double-click it in the Results pane, or right-click and select *Details*. This will display a window very similar to the following:



In the result details window, you can examine a particular result much more closely. The left pane shows the name of the result, its family, and an equation for the result, if applicable. For a model, the fitted parameters are also shown on the left. To copy result details to the clipboard in text format, simply click the *Copy* button.

9.8.1 Result Graph

The result graph simply shows the data and the current result, so that you can visualize the result without the (possible) clutter of having other results on the same plot. All of the graphing capabilities (see *Graphing*) are also available here, including zooming, panning, changing the graph properties, saving the plot to file or clipboard, and printing.

As you move your pointer over the graph, the live model evaluation tool above the notebook activates and displays your current xy location, the result evaluated at x, and the result's derivative evaluated at x. A marker follows the result dependence on where the mouse pointer is placed. This behavior can be disabled by unchecking the "Live" box above the graph, or it can be made to only activate when the left mouse button is pressed (by setting the "Live" box to its intermediate state).

9.9 Confidence and Prediction Bands

For any regression (linear or nonlinear), the confidence bands and prediction bands can be shown. In order to show these bands, and/or change their appearance, right click the plot, select *Properties->Series*, and then select the appropriate series (alternatively and much more quickly, if the regression is the 3rd entry in the legend, press 3). If the series is a regression, options to control the appearance of the confidence band and prediction band will be present. See *Series Page* for more information on changing the appearance of the bands.

The confidence band is the area that has a certain likelihood (typically 95%, but you can adjust the level to your liking) of containing the true curve that fits the data.

The prediction band is the area that has a certain likelihood (typically 95%, but you can adjust the level to your liking) of containing any future data points. The prediction band is always wider than the confidence band.

CHAPTER

TEN

GRAPHING

10.1 Introduction

CurveExpert Basic contains a fully-featured graphing engine. The graphs are publication quality and are fully antialiased for the best possible appearance. The easiest way to generate a plot from a result (in the "Results" pane) is to right click the result, and select "Send to New Plot".

10.2 Graph Types

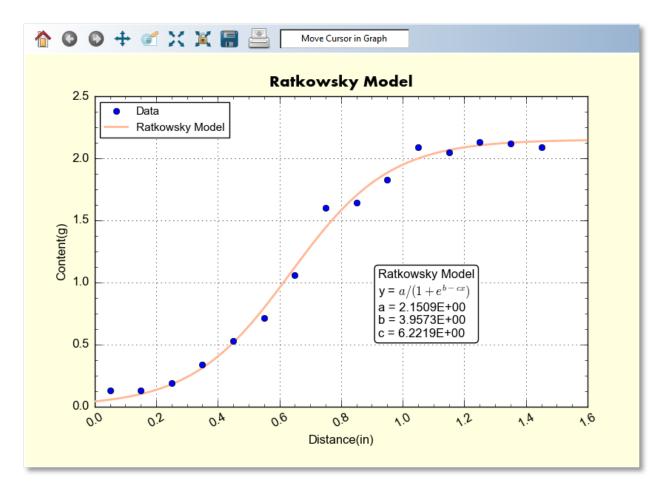
There are is one type of graph supported by CurveExpert Basic; standard XY plots. More graph types are supported in CurveExpert Pro.

10.2.1 XY Plots

XY plots, by definition, have two axes in Cartesian space. XY plots are appropriate for showing relationships between cause and effect, or equivalently, the relationship between one independent variable and one dependent variable.

10.3 Basics

The graphing area is divided into two primary portions; the toolbar, which is situated along the top of a graphing area, and the graph canvas, where the plot is drawn. The toolbar allows interactivity with the graph, such as panning, zooming, and autoscaling. Right clicking on the plot canvas shows the graphing menu, where you can customize items on the plot like the axis labels, title, and the look of the graph. Also from this menu, you can print, copy to clipboard, or save your graph in one of many picture formats. An example of a graph is shown below:



Graphs occur in quite a few places throughout CurveExpert Basic, and you can always interact with them in a very similar way. Just right-click on plots wherever you see them, in order to find out what sorts of interaction are possible.

Also, remember that anywhere that you can change the text on a graph (such as the title or axis labels), you can use mathtext for high quality rendering of mathematical expressions and symbols. For example, in the above graph, mathtext was used to render the m^2 part of the y axis label. See mathtext for details.

The hotkeys (keyboard shortcuts) for use with graphs are documented in Keyboard Shortcuts for Graphs.

10.4 Interacting with a graph

Interacting with a graph is quite straightforward; the mouse cursor always gives a hint of what can be done to various elements on a graph; a cursor that consists of four arrows indicates that the pointed-to-element is moveable, activateable, and possibly resizeable. A hand cursor means that the pointed-to-element can be activated. In this context, "activating" means to show a dialog box to modify the properties of the element in question.

Further, the frame of the graph can be moved and resized by pressing shift (or ctrl) and clicking anywhere inside of the frame. Equivalently, the 'r' key can be pressed while the mouse pointer is inside of the frame. This displays a standard set of resizing handles that you can use to move the edges of the graph frame into the desired locations.

10.4.1 Graph Toolbar

The first style of interaction with a graph is to use the toolbar. A sample of a toolbar is shown below:



All buttons have tooltip help, so if you can't remember what a button does, either watch the status bar at the bottom of the main window as you point to the buttons, or hover your mouse over a button to see its function.

Home, Back, Forward



As the graph view changes interactively, each view is saved so that you can return to a previous one at any given time. If you change the view via the zoom/pan/autoscale controls, you can return to a previous view by clicking the *Back* button, and once you have done this, you can move forward to the next view by clicking the *Forward* button. Pressing the *Home* button will return you to the initial view of your graph.

Pan



The pan button allows you to move the graph extents with your mouse. Press the pan button to begin a pan operation, press and drag in the plot to move it around, and then press the pan button again to end the pan operation. Using the right mouse button to drag during the pan manipulates each axis independently in a pseudo-zooming operation.

Zoom



The zoom button allows you to zoom in or out on a graph with your mouse. Press the zoom button to begin a zoom operation, and draw a box from top left to bottom right in order to zoom in, by clicking and dragging your left mouse button. To zoom out, drag a box with the right mouse button instead of the left.

Autoscale



The autoscale button chooses new limits and new tick intervals for your graph that fit the current dataset. See also *Autoscaling*.

Autoscale lock



CurveExpert Basic will automatically autoscale your plot as data or results are added, changed, or removed. This is done according to *Graphing Preferences*. If you click the autoscale lock, it will prevent any of these automatic autoscales from affecting this particular plot. Note that as soon as CurveExpert Basic detects that you have manually set the axis limits or tick location properties (see *Axis pages*), the autoscale lock is set on your behalf. To release the lock, obviously, just click on the autoscale lock button again.

Save



The save button allows you to save your graph in a variety of picture formats. Pressing this button shows a file chooser, so that you can select the file type and where to save the graph. See *Saving graphs* for more information, including supported image formats.

Print



The print button allows you to quickly output a hardcopy of the currently visible graph.

Locator

(0.577562,1.790783)

The locator always reports the location of your mouse, in data coordinates.

10.4.2 Dragging Elements on Graphs

Items like legends and graph titles are all draggable; meaning that they can be moved directly via interaction with the mouse. If any of these elements are not where you desire them be, simply click and drag it to the desired position.

10.4.3 Picking

If you point to a series on your graph, it will become highlighted. If you then double-click the mouse, a dialog will appear to allow you to change the properties of that series (color, marker style, etc.).

Further, if you right click on a series, you can also select *Details* in order to show the details for the underlying dataset or result associated with that particular curve. When right-clicking on a curve, there is also the opportunity to automatically add an annotation with information about that particular curve's result; choose *Autoannotate*. This generates an annotation with the name of the result, equation, and coefficients (if applicable). The content of this annotation can then be edited just like any other annotation by right clicking it and selecting *Annotation Properties*.

10.4.4 Autoscaling

Every series on a graph has its own default minimum and maximum value along each axis. Autoscaling a graph means that each (visible) series will be tested, and the extents of each axis will be set to values that encompass all of the series.

If the series is a dataset, the minimum and maximum along each axis is determined from the dataset's minimum and maximum along the corresponding axes (naturally).

Exactly when the plot automatically autoscales is determined by the current preference settings in *Graphing Preferences*. If you click the autoscale lock, it will prevent any of these automatic autoscales from affecting this particular plot. Note that as soon as CurveExpert Basic detects that you have manually set the axis limits or tick location properties, the autoscale lock is set on your behalf. To release the lock, obviously, just click on the autoscale lock button again.

10.5 Changing Graph Properties

The graph properties window is divided by functionality into pages.

10.5.1 Axis pages

Graph Properties			
X Axis Y Axis Series Overall			
Axis Type	Grid lines Major Width: 5 ✓ Minor none Width: 5 ✓ Alpha: 100 ✓ Alpha: 100 Alpha: A		
	OK Cancel Apply		

The axis page allows you to set properties such as the axis limits, labeling, and grid lines.

The Axis Type section allows you to set your axes to a normal (linear) scale, or a logarithmic scale.

The **Labeling** section can be used to either hide the axis label, or specify the label itself. Also, the font and font color of the axis label can be selected by pressing the *Font* button in this section.

The **Axis extent and major/minor spacing** section allows you to specify the minimum and maximum value of the axis (determining its limits). To have your axis run in reverse, set the maximum of the axis less than the minimum.

The major and minor spacing can each be set in one of two ways: by a fixed amount of spacing between each tick, or by the number of divisions an interval is divided into. To select the kind of spacing, click the radio buttons under the *at fixed multiples* or *by # of divisions* column as desired. If *at fixed multiples* is chosen, each tick mark (either major or minor) is set each time the multiple appears on the axis. For example, if the major ticks are set at fixed multiples of 0.2, there will be a major tick at -0.2, 0, 0.2, 0.4, etc. If *by # of divisions* is chosen, the ticks are placed such that the appropriate interval (the entire axis in the case of minor ticks, and the interval between two majors in the case of major ticks) is divided into the specified number of parts. For example, if the minor ticks are set to a # of divisions of 4, there should be four intervals between each major tick (which means that three minors will be visible).

The **Grid Lines** section allows you to specify the line style, line width, color, and transparency (alpha) of both the major and minor grid lines.

The **Appearance of tick marks and labels** section is where the size and style of tick marks, the font and color of the tick mark labels, and the numerical format of the tick mark labels can be specified. The **Major/Minor** tick size determines how large the markers are that are placed at each tick, in points. Also, the **Draw ticks inside of axis** setting determines if these tick marks are placed completely inside, outside, or across the axis. **Label minors** determines whether or not text labels are placed at each minor demarcation (most useful for log scaled plots).

The format of the tick mark labels is determined by the combination of the **Formatting** setting and the **Numerical precision** setting. **Formatting** can be set to normal for a generic style of numerical formatting, fixed point, scientific,

engineering, 10^x, or degrees. In all cases except for normal formatting and 10^x, the **Numerical precision** field determines exactly how many places are shown after the decimal in the label.

- Normal: a generic style of formatting that lets the software determine best appearance. e.g. 10245.1234
- Fixed point: exactly like normal formatting, except that the numerical precision is honored. e.g. 10245.1 (coupled with a numerical precision of 1)
- Scientific: a mantissa followed by an exponent. e.g. 1.02e4 (coupled with a precision of 2)
- Engineering: a mantissa followed by an exponent that is a power of 3. e.g. 10.25e3 (coupled with a precision of 2)
- 10^x: most useful for log scale plots, where the user desires to display the number on the axis as 10 raised to the appropriate exponent. e.g. 10²
- Degrees: most useful when the user desires to display a number *in radians* as a number *in degrees*. e.g. 60° (coupled with a precision of 0)

Any axis tick label can be preceded or followed by customized text (including mathtext) as you specify. For text to appear before each axis label, place the text in the **Leader** field; for text to appear after each axis label, place the text in the **Trailer** field. By default, no text appears before or after the axis tick label. Examples of common usage of this feature are to place a dollar sign in front of the numbers to indicate currency, or units after the label.

Finally, the set of tick labels can be rotated by a certain number of degrees, which is also configurable in this section via the **Rotation** setting.

Graph Properties	
X Axis Y Axis Series Overall	
Series: Data	▼ Visible Alpha: 100 ▼
	Markers
solid Linewidth: 10	square Size: 60
IV Fill to y=0 Alpha: 100 ▲	Edge: Visible Width: 5
	Fill: 🔽 Visible 🚺 Style: full 🔻
	Skip stride: 1
	Legend Entry
	✓ Visible
	Data
OK Can	cel <u>Apply</u>

10.5.2 Series Page

The Series page is where the settings for individual series can be changed. For quick help with any of the settings in this page, hover your mouse over any control.

The first item to choose is the **Series**; this determines which curve the settings in the dialog apply to. As the series is changed, the controls in the rest of the dialog will update appropriately. Next to the series chooser, you can set

the *Visible* flag, and the overall transparency of the series via the *Alpha* control (100 being opaque, and 0 being fully transparent).

The next section can be either **Line** or **Bar**, depending on the selection of the user. A **Line** section indicates that the series should be drawn as a line with markers at each data point (both line and markers are optional, though, based on your specific settings for these). A **Bar** section indicates that the series should be drawn as a sequence of vertical bars extending upwards from y=0. If **Bar** is selected, there is no concept of markers or confidence/prediction bands (see below), so these sections are hidden.

The **Line** section obviously sets properties for the line; the linestyle can be chosen, as well as the color and width. The *Resolution* parameter determines how many pieces make up the curve, from the current minimum extent to maximum extent of the graph. Higher resolutions look more attractive, but take longer to draw. If your curve changes sharply over a short distance, increase the resolution in order to avoid a segmented look to the curve.

The lock button adjacent to the line color selector determines whether or not the marker edge color and fill color (see below) remain the same as the line color. If left unlocked, the marker edge color and fill color may be adjusted independently from line color. If locked, the marker edge color and fill color are always governed by the line color.

The **Bar** section sets properties for the bar sequence; the color of the bar border, linestyle of the bar borders, and the line width of the bar borders can be chosen. Further, the bar can be filled with a particular color that does not necessarily match the bar borders described above. The resolution determines the number of divisions to create over the current x range of the graph. Finally, the bar width can be either prescribed specifically as a horizontal extent, or set to *Auto*, which sets the width of each bar such that each bar touches the bar before and after.

The **Marker** section obviously sets properties for markers (this section is not visible while **Bar** is selected). The marker type can be chosen from a set of 22 different markers, and the marker size can be set with the Size control. Most markers (such as circles, squares, triangles, etc.) consist of both edge and fill; the edge is the outline of the shape, and the fill is the interior of the shape. Other markers (such as X, +, etc.) consist of only an edge, and the fill property has no effect. The edge and fill properties can be set independently in order to customize the markers to the maximum degree possible. Also, the markers can be half-filled or fully-filled according to the *Style* setting. If the marker distribution is too dense, the *Skip Stride* parameter can be increased in order to decrease the marker density on any particular series. Note that for a dataset, there is one marker per data point; for a continuous result, there is one marker per resolution increment set in the **Line** section. Also note that the marker edge and fill colors may only be adjusted if the "lock" button in the line section (see above) is unlocked.

The **Legend Entry** section gives control over the series's appearance in the legend. Here, you can exclude the series from appearance in the legend, and also change the label that appears in the legend for the active series.

If the selected series at the top of the dialog is a regression, there will also be controls to manipulate the appearance of the confidence and/or prediction bands (see *Confidence and Prediction Bands*). By default, confidence and prediction bands are not drawn on normal graphs, but are in the result details window (see *Querying Result Details*). A sample of the available controls for the confidence and prediction bands is shown below:

Graph Properties	
X Axis Y Axis Series Overall	
Series: Vapor Pressure Model	▼ Visible Alpha: 100 ▲
	Markers
solid 🔻 🚺 👔 Linewidth: 10 💌	none V Size: 60
Fill to y=0 Alpha: 100 ×	Edge: 🔽 Visible 🚺 Width: 5 💌
Resolution: 100	Fill: 🔽 Visible 📕 Style: full 🔻
Confidence Band	Skip stride: 1
Visible Villed Confidence level: 95	Legend Entry
Line style: solid Alpha: 10	Visible
Prediction Band	Vapor Pressure Model
Visible Villed Confidence level: 95	
Line style: solid Alpha: 10	
OK Can	cel Apply

In both the **Confidence band** and **Prediction band** sections (these sections are not visible unless the series is a regression, and further, are not visible when **Bar** is selected), the visibility of the respective bands can be set via the *Visible* checkbox; if visibility is off, none of the other settings are significant. the *Filled* checkbox determines if the bands are drawn as a filled region or a pair of lines. The *Confidence level* allows you to set the desired probability level for the confidence bands or prediction bands; the default value for this probability is set via the *Application Preferences*. If the bands are drawn as a pair of lines, the *Linestyle* setting determines the style for those lines; the line color always matches the line color of the corresponding regression curve. If the bands are drawn as a filled region, the **Alpha** parameter determines the transparency of that region.

10.5.3 Overall Page

Graph Properties	
X Axis Y Axis Series Overall	
Canvas Aspect Ratio: 3:2 (Photo) 1.500000	Legend box
Title and Background Visible Title: Skin Friction Coefficient Font Position: 0.500 1.000 Background fill:	Placement: specified location XY Location: 0.028 Frame: Width:
Graph Frame Frame: Width: 10 Ine@ y=0 Fill: Alpha: 100 Ine@ x=0	Fill: Alpha: 100 Title: My legend title Font Visible frame Rounded corners Shadow Legend labels same color as line
✓ Use padding left ✓ Visible Image: Straight of the straight o	Label Font Scale markers: 1 Columns: 1 Points in key: 3
OK Cancel	Apply

The overall settings page is where the global settings for a plot are changed, such as the title, background, and legend box appearance. For quick help with any of the settings in this page, hover your mouse over any control.

The **Canvas Aspect Ratio** setting determines the aspect ratio of your plot. If set to Dynamic, which is the default, the plot will always fill the window that it resides in. However, there are many cases where the aspect ratio of the plot should be fixed; there are several predefined aspect ratios in the **Canvas Aspect Ratio** pulldown to select from, that fit common aspect ratios in use in various modern applications. If one of these fixed aspect ratios is set, your plot will automatically size itself in its parent window (leaving part of the parent window unpainted) appropriately in order to retain the desired aspect. If *Custom* is selected as the aspect ratio, you may type in the desired aspect (width/height) as a floating point number next to the pulldown.

The **Title and Background** section allows the title, font and color to be set. The position of the title is governed by the *Position* setting; this position is in the axes coordinate system, which is a system that is (0,0) at the bottom left corner of the axes frame, and (1,1) at the top right corner. The default position is (0.5,1.02), which places the title horizontally centered and above the top of the axes frame. Note that the title may be dragged and dropped interactively on the plot itself. The title can be turned completely off by unchecking the *Visible* box. Also, the background color (the area around the graph frame) can be set with the *Background fill* parameter.

In the **Graph Frame** section, the graph frame's line color and width, along with its fill and transparency, can also be set. The position of the graph frame's sides can be set by sliding the appropriate sliders near the bottom of this section; each side of the graph frame can also be turned on and off individually. The *Use padding* setting determines whether or not extra padding is added around the graph in order to make sure that all text (i.e., tick labels, axis labels, and titles) is visible. Turning the padding off provides finer control over the location of the axes frame (because there is not an automatic sizer involved; all sizing is explicit), but also will allow you to set the frame such that certain textual elements are not visible. Note that if you move/resize a frame interactivity in the plotting window (by pressing 'r' or shift-clicking the axes area), the padding switch is automatically turned off. A solid line, of the same thickness and color of the frame, can be drawn specifically at x=0 or y=0 by checking the appropriate box.

The Legend Box section is located in the right side of the Overall page. See Legend Properties for details.

10.6 Legend

The legend shows the mapping between a drawn entity on the plot and the dataset/function/model that it represents. Right click on a legend for the actions that be performed on the legend itself; one can change the look of the legend or reorder items in the legend (*Legend Properties*), or raise/lower legend itself in order for it to be drawn appropriately with other items on the graph.

10.6.1 Legend Properties

The legend properties can be accessed via the normal graph properties dialog (right click on the graph, choose *Properties*, and then go to the **Overall** tab), or can be accessed by right clicking on a legend itself. The legend properties dialog appears as below:

Legend properties	X	
✓ Visible Placement: specified location ▼ XY Location: 0.010 0.984 Frame: Width: 10	Legend labels New York City Philadelphia Baltimore Chicago Los Angeles]
Fill: Alpha: 100 Title: Font Visible frame Rounded corners Shadow Legend labels same color as line Label Font Scale markers: 1.00 Columns: 1 Points in key: 1	Houston]
	OK Apply Cancel	<u>ן</u>

The entire legend box can be made invisible, and its placement in the graph can be chosen from the Placement chooser. If the placement is set to "specified location", the XY location of the legend's upper left corner can be set. The XY location is in graph coordinates, which run from (0,0) at the bottom left of the graph frame to (1,1) at the top right of the frame. The XY location can certainly be set to numbers greater than 1 or less than 0, in order to move the legend into the desired position.

Still in the **Legend Box** section, the color and linewidth of the legend frame can be selected, and the fill/transparency can also be selected. A legend title may be specified (along with a font and color), that is displayed above the legend entries and inside the legend box. A set of checkboxes allow the legend frame to be visible/invisible, have a drop shadow, have rounded corners, or have the labels in the legend assume the same colors as the line that they refer to.

At the bottom of the **Legend Box** section, the font and color of the legend labels can be selected. If markers need to be made smaller or larger in the legend, a *Scale markers* setting takes care of this. To lay your legend out in a multicolumn format, increase the number of columns in the *Columns* setting. To include more than one marker in a legend key, increase the *Points in key* setting.

10.6.2 Legend label editing

Legend labels may be changed in the **Legend labels** section, by clicking an already-selected label. The label will become editable, and you can change the text to whatever is desired. Remember that mathtext can be used in a legend label as well. Also, the label can be made blank so that the series does not appear in the legend. Editing a label in this manner is exactly the same as doing so via the *Series Page* in the **Graph Properties dialog**.

10.6.3 Legend Ordering

The order of the series in of a legend can be changed by selecting the desired series's legend label in the **Legend labels** section, and pressing the appropriate arrow buttons to arrange the ordering of the series. The topmost arrow button moves the selected series to the top; while the bottommost arrow button moves the selected series to the bottom. The inner two arrow buttons move the selected series up or down by one slot as appropriate.

The ordering of items in the legend also has another important role: it determines the order in which each series is drawn in the graph. So, if you would like a particular series to be drawn on top, move it to the front in the legend ordering. Series are drawn in reverse order as the legend ordering, which means that the item appearing on top of the legend order will also appear on top of other series in the graph.

10.7 Saving graphs

To save a graph, either choose the *Save* button in the graph toolbar, or right click the graph and select *Save*. A file chooser will appear that allows you to select the location and filename of the graph to be saved, and the format of the picture file to be saved. For image (raster) files, supported filetypes are:

- portable network graphics (PNG)
- JPEG
- TIFF
- raw RGBA bitmaps (RGBA or RAW)

Supported vector graphics file formats are:

- scalable vector graphics (SVG)
- enhanced metafiles (EMF)
- encapsulated postscript (EPS)
- postscript (PS)
- portable document format (PDF)

Of these formats, the PNG format is the most common for raster-type images, and SVG is most common for vector graphics. A PNG file can be read by any graphics application, and by applications such as Microsoft Word and Powerpoint. SVG files can be read by computer illustration software, such as Adobe Illustrator or Inkscape. It should be noted that an SVG file written by CurveExpert Basic retains all object information, so you can add or remove elements from the graph after-the-fact with an illustration package, if desired.

10.8 Copying graphs

To copy a graph, right click it and select *Copy*. An image will be copied to the clipboard, which can be subsequently pasted into any application that can receive an image from the clipboard, such as Microsoft Word.

10.9 Printing graphs

To print a graph, right click it and select *Print Preview* or *Print*, depending on the desired action. Alternatively, press the Print button in the graph toolbar associated with the desired graph.

10.10 Keyboard Shortcuts for Graphs

Keyboard shortcuts can be used when a graph, or the notebook tab associated with the graph, has keyboard focus.

Keyboard Shortcut	Action	
a	autoscale. Identical to clicking the autoscale button in the graph toolbar.	
	See Graph Toolbar and Autoscaling.	
р	toggle panning mode. Identical to clicking the pan button in the graph tool-	
	bar. See Graph Toolbar.	
Z	toggle zooming mode. Identical to clicking the zoom button in the graph	
	toolbar. See Graph Toolbar.	
r	resize the graph frame interactively (pointer must be over the frame when r	
	is pressed).	
Х	Open context sensitive properties dialog. Identical to right click-	
	>Properties. See Changing Graph Properties.	
1-9	Pressing a number button (1-9) will open the graph properties dialog di-	
	rectly to the corresponding series as listed in the legend.	
Shift + 1-9	Pressing a number button (1-9) will open the Results Window (see <i>Querying</i>	
	<i>Result Details</i>) directly to the corresponding series as listed in the legend.	
Ctrl+C	if the pointer is over an image, annotation, or arrow, copy it; if over the	
	graph, copy the graph to the clipboard as an image. Identical to right click-	
	>Copy. See <i>Graph Toolbar</i> .	
Ctrl+V	paste a graph element (image, annotation, or arrow)	
,	move backward to the previous view. Identical to clicking the back button	
	in the graph toolbar. See Graph Toolbar.	
	move forward to the next view. Identical to clicking the forward button in	
	the graph toolbar. See Graph Toolbar.	
h	return to the first view. Identical to clicking the home button in the graph	
	toolbar. See Graph Toolbar.	
n	add a new annotation	
r	add a new arrow	

10.11 Mathtext

You can use a subset of TeX markup anywhere that a graph uses text (for a label, title, legend, annotation, etc.) by placing a bit of your text inside a pair of dollar signs (\$). This capability allows you to typeset quite complex mathematical expressions within any text label on any plot. Regular text and math text can be freely intermixed. For example:

Surface Area \$m^2\$

renders as:

Surface Area m²

Note: To make it easy to display monetary values such as \$100.00, if a single dollar sign is present in the entire string, it will be displayed as a dollar sign.

Greek letters and a large number of symbols are supported.

10.11.1 Subscripts and superscripts

To make subscripts and superscripts, use the '_' and '^' symbols:

\$\alpha_i > \beta_i\$

 $\alpha_i > \beta_i$

Some symbols automatically put their sub/superscripts under and over the operator. For example, to write the sum of x_i from 0 to ∞ , you could do:

\$\sum_{i=0}^\infty x_i\$

$$\sum_{i=0}^{\infty} x_i$$

10.11.2 Fractions, binomials and stacked numbers

Fractions, binomials and stacked numbers can be created with the \frac{}{}, \binom{}{} and \stackrel{}{} commands, respectively:

\$\frac{3}{4} \binom{3}{4} \stackrel{3}{4}\$

produces

 $\frac{3}{4}\begin{pmatrix}3\\4\end{pmatrix}^{3}_{4}$

Fractions can be arbitrarily nested:

```
\frac{5 - \frac{1}{x}}{4}
```

produces

 $\frac{5-\frac{1}{x}}{4}$

Note that special care needs to be taken to place parentheses and brackets around fractions. Doing things the obvious way produces brackets that are too small:

 $(\int x^{5} - \int x^{1}{x}^{4})$

The solution is to precede the bracket with \left and \right to inform the parser that those brackets encompass the entire object:

 $\left(\frac{5-\frac{1}{x}}{4}\right)$

 $\left(\frac{5 - \frac{1}{x}}{4}\right)$

$$\left(\frac{5-\frac{1}{x}}{4}\right)$$

10.11.3 Radicals

Radicals can be produced with the \sqrt[]{} command. For example:

 $\operatorname{sqrt}{2}$

Any base can (optionally) be provided inside square brackets. Note that the base must be a simple expression, and cannot contain layout commands such as fractions or sub/superscripts:

 $\sqrt{2}$

\$\sqrt[3]{x}\$

 $\sqrt[3]{x}$

10.11.4 Inline Fonts

The default font is *italics* for mathematical symbols.

To change fonts, eg, to write "sin" in a Roman font, enclose the text in a font command:

\$s(t) = \mathcal{A}\mathrm{sin}(2 \omega t)\$

 $s(t) = \mathcal{A}sin(2\omega t)$

More conveniently, many commonly used function names that are typeset in a Roman font have shortcuts. So the expression above could be written as follows:

\$s(t) = \mathcal{A}\sin(2 \omega t)\$

 $s(t) = \mathcal{A}\sin(2\omega t)$

Here "s" and "t" are variable in italics font (default), "sin" is in Roman font, and the amplitude "A" is in calligraphy font. Note in the example above the calligraphy A is extremely close to the sin. You can use a spacing command to add a little whitespace between them:

 $s(t) = \hat{A}/\hat{sin}(2 \mod t)$

 $s(t) = \mathcal{A}\sin(2\omega t)$

The choices available with all fonts are:

Command	Result
\mathrm{Roman}	Roman
\mathit{Italic}	Italic
\mathtt{Typewriter}	Typewriter
\mathcal{CALLIGRAPHY}	CALLIGRAPHY

10.11.5 Global Fonts

In CurveExpert Basic, there are three choices for the global font to use for math symbols: Computer Modern, STIX Serif, and STIX Sans Serif. To select one of these fonts, choose *Edit->Preferences->Graphing->Global mathtext font*.

The look of each font slightly different, with the Computer Modern font resembling the traditional TeX typsetting most closely, STIX Serif meant to blend with Serif-style fonts (such as Times New Roman), and STIX Sans Serif being a mathematical font without any serifs at all.

10.11.6 Accents

An accent command may precede any symbol to add an accent above it. There are long and short forms for some of them.

Command	Result
$\acute a or \'a$	á
∖bar a	ā
\breve a	ă
$\det a \text{ or } $	ä
$\det a \text{ or } a$	à
grave a or `a	à
$hat a or ^a$	â
$\ \$ a or $\$	ã
∖vec a	đ

In addition, there are two special accents that automatically adjust to the width of the symbols below:

Command	Result
\widehat{xyz}	\widehat{xyz}
\widetilde{xyz}	xyz

Care should be taken when putting accents on lower-case i's and j's. Note that in the following \imthermal{inath} is used to avoid the extra dot over the i:

r" $\ i \in \$

10.11.7 Symbols

Other symbols available in math typesetting are listed below.

Lower-case Greek

$\alpha \setminus alpha$	$\beta \setminus beta$	$\chi \setminus chi$	$\delta \setminus delta$	$F \setminus digamma$
$\epsilon \setminus epsilon$	$\eta \setminus eta$	$\gamma \setminus gamma$	ı∖iota	$\kappa \setminus kappa$
$\lambda \setminus lambda$	$\mu \setminus mu$	v ∖nu	$\omega \setminus omega$	$\phi \setminus phi$
$\pi \setminus pi$	ψ \psi	$\rho \setminus rho$	$\sigma \setminus sigma$	$\tau \setminus tau$
$\theta \setminus theta$	$v \setminus upsilon$	$\varepsilon \setminus varepsilon$	$\varkappa \setminus varkappa$	$\varphi \setminus varphi$
$\varpi \setminus varpi$	$\varrho \setminus varrho$	$\varsigma \setminus varsigma$	$\vartheta \setminus vartheta$	ξ\xi
$\zeta \setminus zeta$				

Upper-case Greek

$\Delta \setminus Delta$	$\Gamma \setminus Gamma$	$\Lambda \setminus Lambda$	$\Omega \setminus Omega$	$\Phi \setminus Phi$	П∖Рі
Ψ\Psi	$\Sigma \setminus Sigma$	Θ\Theta	Υ \Upsilon	Ξ\Xi	び \mho
$\nabla \setminus nabla$					

Hebrew

% \aleph □ \beth □ \daleth □ \gimel

Delimiters

//]]	↓\Downarrow	↑\Uparrow	∥\Vert	$\ \ backslash$
↓\downarrow	< \langle	[\lceil	[∖lfloor	∟ \llcorner	」\lrcorner
\rangle \rangle]\rceil]∖rfloor	「 \ulcorner	↑\uparrow	¬∖urcorner
\vert	{ \{	X	} \}]]	

Big symbols

$\bigcap \$	∪\bigcup	○ \bigodot	$\bigoplus \ bigoplus$	⊗ \bigotimes
\+ \biguplus	\/ \bigvee	$\wedge \$ bigwedge	∐ \coprod	∫∖int
∮∖oint	∏∖prod	$\sum \setminus sum$		

Standard function names

Pr \Pr	arccos \arccos	arcsin \arcsin	arctan \arctan
arg \arg	cos \cos	$\cosh \cosh$	cot \cot
coth ∖coth	csc \csc	deg \deg	det \det
dim \dim	exp \exp	gcd \gcd	hom \hom
inf \inf	ker \ker	lg \lg	lim \lim
liminf \liminf	lim sup \limsup	ln \ln	log \log
max \max	min \min	sec \sec	sin \sin
sinh \sinh	sup ∖sup	tan \tan	tanh \tanh

Binary operation and relation symbols

⇒ \Bumpeq	∩ \Cap	⊎ \Cup
≑\Doteq	⋈ \Join	∈ \Subset
∋\Supset	⊩ \Vdash	⊪ \Vvdash
$\approx \approx$	≊ \approxeq	* \ast
≍ \asymp	→ \backepsilon	$\sim \$ backsim
	$\overline{\wedge} \setminus barwedge$	∵ \because
≬\between	⊖\bigcirc	$\triangledown \$ bigtriangledown
$\triangle \$	◄ \blacktriangleleft	▶ \blacktriangleright
⊥ \bot	⊳\bowtie	⊡ \boxdot
⊟ \boxminus	⊞ \boxplus	⊠ \boxtimes
• \bullet	≏ \bumpeq	∩∖cap
· \cdot	∘ \circ	≜ \circeq
:- \coloneq	≅ \cong	∪∖cup
<pre></pre> <pre></pre> <pre></pre>	<pre>> \curlyeqsucc</pre>	Y \curlyvee
∧ \curlywedge	† \dag	⊣∖dashv
‡ \ddag	◊ \diamond	÷ \div
* \divideontimes	≐ \doteq	≑ \doteqdot
∔\dotplus	$\overline{\wedge} \setminus doublebarwedge$	<pre></pre>
-:∖eqcolon	$\approx \eqref{eq:sim}$	>\eqslantgtr
<pre><\eqslantless</pre>	≡ \equiv	≒\fallingdotseq

$\frown \$ frown	≥∖geq	≧ \geqq
≥∖geqslant	≫ \gg	≫ \ggg
≩ \gnapprox	≩ \gneqq	≳∖gnsim
≳\gtrapprox	>\gtrdot	≷∖gtreqless
≷∖gtreqqless	≷∖gtrless	≳∖gtrsim
∈∖in	_T ∖intercal	$\lambda \setminus $ leftthreetimes
≤\leq	≦ \leqq	≤∖leqslant
[≲\lessapprox	∢\lessdot	≶\lesseqgtr
[∮ \lesseqqgtr	≶∖lessgtr	$\lesssim \lessim$
≪ \11	« \lll	≨ \lnapprox
≨∖lneqq	≲∖lnsim	K \ltimes
\mid	⊨ \models	∓ \mp
⊯ \nVDash	⊮ \nVdash	≉ \napprox
≇ \ncong	≠ \ne	≠ \neq
≠ \neq	≢ \nequiv	≱ \ngeq
≯∖ngtr	∋∖ni	≰ \nleq
≮∖nless	∤ \nmid	∉∖notin
∦ \nparallel	⊀ \nprec	≁ \nsim
⊄∖nsubset	⊈∖nsubseteq	⊁ \nsucc
⊅ \nsupset	⊉ \nsupseteq	≮\ntriangleleft

≰ \ntrianglelefteq	⊭ \ntriangleright	≱ \ntrianglerighteq
⊭ \nvDash	⊬ \nvdash	⊙∖odot
$\ominus \setminus ominus$	$\oplus $ \oplus	⊘∖oslash
⊗∖otimes	∥\parallel	⊥ \perp
	± ∖pm	< \prec
\leq \precapprox	<pre><\preccurlyeq</pre>	≤\preceq
i ⇒ \precnapprox	$\leq \precnsim$	$\leq \precsim$
∝ \propto	\land \rightthreetimes	≓∖risingdotseq
	$\sim \$	$\simeq \$
/\slash	$\smile \$ smile	□ \sqcap
⊔ \sqcup	□ \sqsubset	□ \sqsubset
⊑ \sqsubseteq	⊐ \sqsupset	⊐\sqsupset
⊒\sqsupseteq	★ \star	⊂∖subset
⊆∖subseteq	⊆\subseteqq	⊊∖subsetneq
⊊∖subsetneqq	> \succ	≿ \succapprox
≽∖succcurlyeq	≥ \succeq	≿ \succnapprox
$\gtrsim \succnsim$	$\gtrsim \succsim$	⊃∖supset
⊇∖supseteq	⊇\supseteqq	⊋∖supsetneq
⊋∖supsetneqq	∴ \therefore	× \times
⊤ \top	⊲\triangleleft	⊴∖trianglelefteq

≜ \triangleq	ト\triangleright	⊵ \trianglerighteq
⊎ \uplus	⊧ \vDash	$\propto \$
⊲\vartriangleleft	▷ \vartriangleright	⊦ \vdash
∨ \vee	⊻ \veebar	∧ \wedge
≀\wr		

Arrow symbols

↓ \Downarrow	$\leftarrow \$ Leftarrow
$\Leftrightarrow \ Leftrightarrow$	$\in \Lleftarrow$
$\leftarrow \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \$	$\iff \setminus Longleftrightarrow$
$\implies \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \$	ጎ \Lsh
// \Nearrow	🔨 \Nwarrow
$\Rightarrow \$	$\Rightarrow \$
r ∖Rsh	📎 \Searrow
🖉 \Swarrow	↑ \Uparrow
↓ Updownarrow ↓	$\bigcirc \$ \circlearrowleft
$\bigcirc \$ \circlearrowright	$\sim \$ curvearrowleft
\frown \curvearrowright	<\dashleftarrow
> \dashrightarrow	↓ \downarrow
↓↓ \downdownarrows	<pre>↓ \downharpoonleft</pre>
↓\downharpoonright	↔ \hookleftarrow
$\hookrightarrow \setminus hookrightarrow$	\rightarrow \leadsto
$\leftarrow \leftarrow$	← \leftarrowtail
$\leftarrow \$ leftharpoondown	$\leftarrow \$ leftharpoonup
$\models \leftleftarrows$	$\leftrightarrow \$
$\leq \$ leftrightarrows	$\Rightarrow \ leftrightharpoons$
<pre></pre>	↔ \leftsquigarrow
1	

$\leftarrow \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \$	$\longleftrightarrow \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \$
$\mapsto \setminus longmapsto$	$\longrightarrow \longrightarrow$
↔ \looparrowleft	$\hookrightarrow \looparrowright$
$\mapsto \mbox{mapsto}$	$- \circ \$
∉ \nLeftarrow	⇔ \nLeftrightarrow
⇒ \nRightarrow	∕\nearrow
↔ \nleftarrow	↔ \nleftrightarrow
→ \nrightarrow	🔨 \nwarrow
$\rightarrow $ \rightarrow	\rightarrow \rightarrowtail
\rightarrow \rightharpoondown	$ ightarrow \rightharpoonup$
\rightleftharpoons \rightleftarrows	\rightleftharpoons \rightleftarrows
$\Rightarrow \$	$\Rightarrow \$
$\Rightarrow \$	$\Rightarrow \$
→\rightsquigarrow	📐 \searrow
🖌 \swarrow	\rightarrow \to
← \twoheadleftarrow	-» \twoheadrightarrow
↑ \uparrow	<pre>\$ \updownarrow</pre>
<pre>\$ \updownarrow</pre>	1 \upharpoonleft
`\upharpoonright	<pre>↑↑ \upuparrows</pre>

Miscellaneous symbols

\$\\$	Å \AA	∃∖Finv
· •		,
∂\Game	J \Im	¶ \P
R ∖Re	§ \S	∠∖angle
\\backprime	★ \bigstar	■ \blacksquare
▲ \blacktriangle	▼ \blacktriangledown	$\cdots \setminus cdots$
√ \checkmark	<pre></pre>	
♣\clubsuit	C \complement	© \copyright
\ddots	$\diamond \$	$\ell \setminus ell$
Ø∖emptyset	ð\eth	∃∖exists
♭\flat	∀\forall	$\hbar \setminus hbar$
♡\heartsuit	$\hbar \$ hslash	∭∖iiint
∬∖iint	∬∖iint	<i>i</i> \imath
∞ \infty	<i>j</i> \jmath	\ldots
∡ \measuredangle	¦\natural	¬ ∖neg
∄∖nexists	∰ \oiiint	$\partial \setminus partial$
/\prime	‡∖sharp	♦ \spadesuit
<pre>< \sphericalangle</pre>	∖ss	⊽ \triangledown
$\varnothing \setminus varnothing$	$\land \$:\vdots
℘∖wp	¥ \yen	

CHAPTER

ELEVEN

CREATING CUSTOM MODELS

11.1 Introduction

Note that you can create custom models at any time; they are saved so that you can use them when you compute nonlinear regressions or functions later, and they appear in the "Custom" part of the nonlinear regression picker when you choose *Calculate->Nonlinear Model Fit*.

11.2 Custom Models

To create a custom model, select *Tools->Custom Models*. This will show the model manager, which allows you to delete or save custom models.

Custom Models		
Models [2D] Wavy	Model File: C:\Users\dhyams\.curveexpert-basic\lib\2D\Custom\Wavy.py Show in Folder Model Equation: a*cos(2*x)+b*sin(x) Equation Preview:	
	$y\!=\!\alpha cos(2x)\!+\!\beta sin(x)$	
	Delete Save Save As	
	Close	

To get started, simply type the expression for your model into the "Model Equation" field. Do not include "y =" as a part of your equation; just the expression will suffice.

As you type, CurveExpert Basic will guess how to render your equation, even converting Greek letters into the appropriate representation. The Equation Preview (see *Equation Display*) shows how your equation will render in CurveExpert. Note that its guess is not adjustable in CurveExpert Basic; in CurveExpert Pro, the advanced code editor can be used to adjust this. Usually the equation rendering is reasonable and correct, but in those cases in which it is not, remember that the rendering does not matter as far as the calculation and mathematics are concerned.

Once your model is written the way that you like, simply hit the *Save* or *Save As* button, depending your intent. Give your model a name, and your model will then appear in the list on the left, signifying that it is now available for use within CurveExpert Basic, when you choose to compute nonlinear regressions.

11.2.1 Mathematical Operations

Obviously, the standard arithmetic operations are supported. Multiplication is performed with a *, division with /, addition with +, and subtraction with -. Raising a quantity to a power is performed with either ^ or **, with the ** notation being preferred. Grouping is performed with parentheses ().

11.2.2 Reserved Words

In any model, the independent variable is always denoted by \mathbf{x} . This variable is a reserved word and should not be used as a parameter name in your model.

All mathematical functions supported by CurveExpert Basic, such as sin, cos, tan, exp, etc., are also reserved words. See *Appendix A: Math Functions* for a complete list of the mathematical functions supported.

Any other name that CurveExpert Basic sees in your model is treated as a parameter. This powerful feature lets you name your parameters any name that you find appropriate, such that the model's syntax carries meaning. Thus, names such as beta, my_long_parameter_name, and b are all legal parameter names. Note also that names are case sensitive; the parameter a is distinct from the parameter A, for example.

CHAPTER

TWELVE

EQUATION DISPLAY

In various dialogs throughout CurveExpert Basic, the equation for a model or function is displayed. An example of an equation display is below:

$$y\!=\!\gamma\!+\!rac{1\!-\!\gamma}{1\!+\!e^{-lpha-eta x}}$$

The equation display has a couple of small, convenient features. If the mouse is right-clicked on the display, you will be given the option to copy the image onto the clipboard (so that you can use this in some other application). You can also zoom in or out on the equation, in order to make it temporarily larger or smaller than its default size.

Note: When copying the equation, it is copied using a white background.

CHAPTER

THIRTEEN

WRITING DATA

13.1 Introduction

After performing some analysis, a typical task is to write data, in some form, to disk for later retrieval. CurveExpert Basic supports several ways to extract data and graphs to a file or the clipboard.

13.2 Writing a CurveExpert (CXP) file

If you want to save all of your data, results, and graphs to disk, you can choose *File->Save* or *File->Save As* in order to write a CXP file to disk. These files can be read in later using *File->Open*, obviously. CXP files are portable across platforms (Windows, Mac, Linux) and save all possible information about your current session. CXP files are also interchangeable between CurveExpert Professional and CurveExpert Basic.

Also, if a particular model or function is saved as a result in a CXP file and it is not present on the system reading the file, the model/function will automatically be created (on the system reading the file) on your behalf. This newly created model/function will then be available for use in the "Imported" family, and will appear appropriately in the Nonlinear model picker.

13.3 Exporting a dataset to text file

To save your dataset into a text file, choose *File->Export*. The dataset will be exported using the default delimiter chosen in *Edit->Preferences->General->Default delimiter*.

13.4 Writing a graph to a picture file

To save a particular graph to a file, right click it and select *Save*. Any graph can be saved wherever it appears via this procedure. Alternatively, click the *Save* icon in the graph toolbar (if present). See *Saving graphs* for more details on supported file formats.

The same graph can be copied to the clipboard by right clicking and selecting Copy.

13.5 Printing

All graphs in the Graphs and Data pane can be printed by choosing *File->Print* or *File->Print Preview*. To print an individual graph, right click it and select *Print* or *Print Preview*.

If the margins or paper orientation is not correct, you can set these in the File->Page Setup dialog.

FOURTEEN

APPLICATION PREFERENCES

14.1 Introduction

Application preferences can be changed by choosing *Edit->Preferences* from the menu.

14.2 General Preferences

Preferences	
General Regression Graphing Logging Localization Advanced	
Show Tips at Startup	
V Automatically Send Issue Reports	
Spreadsheet Formatting: 🔘 Normal 💿 Fixed Point 🔘 Scientific 🔘 Engineering with precision: 6	
Default confidence level: 95	
Excel style cursor movement in spreadsheet	
🔲 Sort Data On File Import	
Vive Model Evaluation	
Automatically Update Results	
Default delimiter: Tab	
Data file location: C:\Users\dhyams\Documents\CurveExpert Basic Browse	
OK Cancel	

General settings apply to general items of interest in CurveExpert Basic.

14.2.1 Show Tips at Startup

When the software starts, a helpful tip can be shown. However, if you find this either unhelpful or annoying, it may be turned off (or back on) by selecting this checkbox.

14.2.2 Automatically send issue reports

CurveExpert Basic has the ability to automatically send an issue report should something go wrong with the software. The objective of doing is to find and correct problems in the most timely manner possible.

An issue report, when and if one is sent, contains no personally identifying information or any of your data, and the report itself is submitted anonymously. However, if you would like to opt-out of this behavior, uncheck this box.

14.2.3 Spreadsheet Formatting

The *spreadsheet formatting* setting allows you to set your preference for how data is displayed, by default, in the spreadsheet. The data may be displayed in a fixed point, scientific, or engineering format, with a precision (number of digits after the decimal) as specified in the *with precision* field. This default number formatting can always be overridden on a per-cell basis by selecting the cells in the spreadsheet, right clicking, and selecting *Format Numbers* as documented in *Number Formatting*.

The engineering format is the same as scientific, except that the exponent is always a multiple of three.

14.2.4 Default confidence level

In result details and in displaying confidence/prediction bands, a certain confidence level is needed. The default confidence level set in the preferences here is the starting level set throughout the application in these situations. You will be given the opportunity to change the confidence level on a result-by-result basis.

14.2.5 Excel style cursor movement in spreadsheet

By default, both the TAB and ENTER keys are treated as carraige returns in CurveExpert Basic. In other words, the cursor is moved to the left until it bumps into the right side of the dataset, in which case the cursor is moved to the beginning of the next row.

If you would rather that the cursor go right on a TAB (which is the same as the default TAB behavior), and down on an ENTER, select this box. Note that CurveExpert Basic will still keep your cursor within the bounds of the dataset.

14.2.6 Sort Data On File Import

Normally, CurveExpert Basic reads your data directly from file, accounts for the settings in the File Import window while importing, and places it in the spreadsheet. If you would also like to automatically sort the data against the first column, check this box.

14.2.7 Live Model Evaluation

In the result details window, an evaluator follows the location of your mouse to inform you of the x/y location of the mouse, the model/function evaluated at the pointed-to x coordinate, and the first derivative of the model/function. If this is not desired or is too slow, uncheck this box.

There also an intermediate state for this checkbox; if set to intermediate, the live evaluator will activate when the left mouse button is pressed only (by default).

14.2.8 Automatically Update Results

If you have already calculated results and then change the data, the results become invalid (see *Working with Results*). This state is indicated by a yellow caution badge placed on the results in the Results pane. To update these results, you can select some (or all), right click, and select *Update*. To automatically update results without having to do it yourself, check this box. As soon as a change in the data is detected, all results will be recomputed.

14.2.9 Default delimiter

In several places in the software, a delimiter is used to separate items in the same row. For example, in copying data to the clipoboard, or in generating a table, a delimiter between data items must be selected. If you have a favorite delimiter, set it here.

14.2.10 Data file location

Default directory where data files are stored. Initially, the data file location is set to \$DOCUMENTS/CurveExpert Basic, and some example data and example documents are placed there at install time.

14.3 Regression Preferences

Preferences		×
General Regression Graphing L	ogging Localization Advanced	
Ask for initial guesses when nec	essary	
Tolerance (change in residual)	1e-08	
Tolerance (change in parameters)	1e-08	
Maximum Iterations	100	
Max # of cores to utilize		
	OK Car	icel

14.3.1 Ask for initial guesses when necessary

At times, when calculating a list of nonlinear regressions at once, the calculation of the initial guess will fail for some (for various numerical reasons; a simple example is when the natural log is taken in the process of calculating the initial conditions, and there is a zero or negative in the dataset). When this happens, CurveExpert Basic will prompt you to ask if you want to attempt initial guesses manually, and give a list of the fits that failed in this manner.

If you want CurveExpert Basic to just treat initial guess failures as general model failures, uncheck this box.

14.3.2 Tolerances

The tolerances determine when CurveExpert Basic will stop calculating a given model; in any nonlinear regression, the solution is an iterative process in which the model parameters are adjusted in order to reach the best possible set. The iteration will terminate when either the overall change in the residual is below the given tolerance, or when the change in the parameters is below the given tolerance. The residual is defined as

$$\Re = \sqrt{\sum_{i}^{N} (y_i - f(\vec{x_i}; \vec{a}))}$$

14.3.3 Maximum Iterations

The iteration described in "Tolerances" above can also be terminated when the number of iterations reaches a certain threshold. That threshold is specified in this field.

14.4 Graphing Preferences

Preferences	×
General Regression Graphing Logging Localization Advanced	
Max display points: 5000	
Autoscale when model/function added: 💿 Never 💿 Always	
Autoscale when data changed: O Never O Always	
Autoscale when model/function removed: 🔘 Never 💿 Always	
I Highlight pickable objects	
🗹 Continuous redraw during pan	
Preserve aspect ratio when printing	
Automatically plot top 3 results	
Global mathtext font: Computer Modern 🔻	
Default graph theme: Elegant White	
OK Cance	:

14.4.1 Max display points

Sets the maximum number of points, per series, to display when drawing a discrete dataset on a graph. If the dataset has more points than this, it will be thinned to this number of points. The thinning is based on an appropriate stride to use in order to reduce the total number of points drawn to below the threshold given here. This option is in place to prevent extremely slow graph redraws due to attempting to draw an excessive number of points.

This option affects discrete datasets only; not continuous functions. For continuous functions, the **Resolution** parameter, in the *Series Page* of the Graph Properties dialog (see *Changing Graph Properties*), is the way to control the sampling of the function that is used for drawing.

14.4.2 Autoscale when model/function added

When a model or function is added to a graph (via a *Send to Plot* command or a drag and drop), CurveExpert Basic can automatically autoscale the graph. In this case, you can set the preference to "Never" or "Always". If the autoscale lock has been set for a graph (see *Graph Toolbar*), the graph will not be autoscaled regardless of this setting; in other words, the graph's autoscale lock takes precedence over this preference.

14.4.3 Autoscale when data changed

In order to keep the data in view at all times in all graphs, CurveExpert Basic can automatically autoscale the graphs when the underlying dataset changes. The disadvantage of doing this is that, for large datasets, the redraw can be slow. Also, if you have specified your own limits to axes in the graphs, they would be lost if the data changes. If the autoscale lock has been set for a graph (see *Graph Toolbar*), the graph will not be autoscaled regardless of this setting; in other words, the graph's autoscale lock takes precedence over this preference.

To control when autoscaling takes place, select either "Never" or "Always".

14.4.4 Autoscale when model/function removed

When a model or function is removed from a graph (either by removing the result from your document altogether, or by right clicking a result on a plot and selecting "Remove"), CurveExpert Basic can automatically autoscale the graph. In this case, you can set the preference to "Never" or "Always". If the autoscale lock has been set for a graph (see *Graph Toolbar*), the graph will not be autoscaled regardless of this setting; in other words, the graph's autoscale lock takes precedence over this preference.

14.4.5 Highlight pickable objects

As you move the mouse over a curve or data, it will highlight, signifying that you can click it to modify its properties. Also, it signifies that, on right-click, you can access the details for that series. However, the redrawing necessary for this feature can make the graph response sluggish. So, deactivate this feature if you don't need to see the highlighting or access details directly from the graph.

14.4.6 Continuous redraw during pan

During a pan, all continuous series must be regenerated on-the-fly if this feature is turned on. This can be expensive, so if it is OK not to see the curve dynamically update during a pan, turn this checkbox off. The series will then only be regenerated each time the mouse button is released during a panning operation.

As a reminder, this setting does not affect discrete datasets on the graph; only results that are continuous.

14.4.7 Automatically plot top # results

When computing batches of nonlinear regressions at once, if all of them were plotted on the "Top Results" graph, it would be quite messy. Here, you can decide how many of the results will be plotted on the graph for each batch that you compute. The default behavior is to take the best three fits for every batch that you compute. Other results that you want to visualize can always be added by right clicking them and selecting *Send to Plot*, or by dragging and dropping the result to the plot.

14.4.8 Preserve aspect ratio when printing

Normally, any graph is fit to the page when it is printed. If you would like to preserve the aspect ratio of your graph when printing, check this box. In other words, if you have a graph that is long and skinny, to keep it long and skinny when printed, check this box.

14.4.9 Global mathtext font

The font used to render equations (see mathtext) through the application can be set to Computer Modern, STIX Serif, or STIX Sans-serif. Computer Modern looks very much like TeX equations. STIX Serif looks slightly different, and is meant to blend with surrounding text that is serifed (such as Times Roman). STIX Sans-serif is obviously a non-serifed font, meant to blend with surrounding text that is nonserifed (such as Helvetica or Arial).

Preferences			
General Regression Gra	phing Logging Loc	alization Advanced	
Log detail:	info 🔻		
Maximum log file size:	2	MB	
Number of log rotations:	3		
			OK Cancel

14.5 Logging Preferences

14.5.1 Log detail

CurveExpert Basic keeps a log in \$HOME/.curveexpert-basic/logs (see *Log Viewer*); the log detail setting determines the detail of messages that are stored in the log. The default setting is "info", which logs all messages that appear in the message window, as well as internal information generated by the application. To have less information logged, move the log detail setting to *warning*, *error*, or *critical*. To log more (for example, if trying to sort out a software problem), move the log detail setting to *debug*.

Note that the logs are easily viewable by selecting *Tools->Log Viewer* in the main menu.

14.5.2 Number of log rotations

When the log reaches a maximum size (configurable below), it will be rotated. This means that if the log file in question is main.log, it will be renamed to main.log.1, and all of the other previously rotated log files will be renamed from main.log.1 to main.log.2, and so on. The number of log rotations determines how many of these files you would like to keep. A number of log rotations of three means that you plan to keep main.log, main.log.1, main.log.2, and main.log.3.

14.5.3 Maximum log file size

Choose the largest file size (in megabytes) that any log file will be allowed to reach before rotation. Note that the log files for multicore workers will be limited to one-fourth of this number. The maximum size on disk that can be taken by the collection log files is therefore

$$space(MB) = s_{max}(n_{rotations} + 1) + s_{max}(n_{rotations} + 1)n_{workers}/4$$

With the default settings of a 2MB log size and 3 rotations, the maximum amount of disk space consumed by the logs is then 16MB, assuming a quad core machine in which four worker processes are utilized.

Preferences	
General Regression Graphing Logging Localization Advanced	
Use region settings	
File I/O numeric format: Matches application 💌	
Clipboard I/O numeric format: Matches application 👻	
	OK Cancel

14.6 Localization Preferences

The localization preferences are documented in the *Localization* chapter, in the *Configuring CurveExpert Basic to* match your workflow section.

14.7 Advanced Preferences

references	×
General Regression Graphing Logging Localization Advanced	
Number of undo levels: 20	
Cache location: C:\Users\dhyams\.curveexpert-basic\.cache	
Use authenticating proxy for Internet access	
Host: http://my.proxy.net	
Port: 800	
Username:	
Password:	
OK Cance	:

14.7.1 Number of undo levels

Any undo mechanism consumes some memory to save the previous state of the application; the number of undo levels setting allows you to customize how many previous states are saved that you can undo to. The parts of CurveExpert Basic that support Undo operations are the graphs, data spreadsheet, notes, and messages.

14.7.2 Cache location

The location of a cache that CurveExpert Basic uses. It is not changeable, but it can be cleared if need be. This cache operates very similarly to a web browser's cache. Clearing it will not affect the correct operation of the program, but will force the regeneration of the information that was cached, slowing performance temporarily.

14.7.3 Proxy settings

CurveExpert Basic uses Internet access to begin your trial period (see *Installation and Activation*), check for latest versions, upload issue reports (if enabled, see *Automatically send issue reports*), and upload logs (see *Log Viewer*). If you do not use a proxy, you can leave *Use authenticating proxy for Internet access* unchecked. However, if you are behind a proxy, please fill in the host, port and port for your proxy server (https:// or http:// in the server name is optional). If your proxy server requires authentication, also fill in the username and password fields with your username/password combination for the proxy server.

FIFTEEN

LOCALIZATION

15.1 Executive Summary

CurveExpert Basic localizes itself to the same region as the operating system you are running on by default; therefore you should see the appropriate treatment of decimal points (either a comma, or a dot) throughout the application. If you do not want this behavior, but want to operate in English only, uncheck the *Use local region settings* box and restart CurveExpert Basic.

CurveExpert Basic offers the ability, when it is reading/writing data to/from the clipboard or a file, to allow the user to specify what style of decimals to use for this, presuming that it differs from the default locale.

- If you need to read files that use the dot-decimal notation most often, select "English" for *File I/O numeric format*; same comments apply for the clipboard format.
- If you need to read files that use the comma-decimal notation most often, select "European" for "File I/O numeric format"; same comments apply for the clipboard format.

15.2 Configuring CurveExpert Basic to match your workflow

15.2.1 Use local region settings

The *Use local region settings* checkbox is by default checked, and will cause the application to use your native language style for numerical formatting. This is the desired behavior in most situations. However, if you want to operate the software in English only mode (decimals will always be dots), deselect this checkbox. If you change this setting, you must restart CurveExpert Basic for the change to take effect.

15.2.2 File I/O numeric format

The *Edit->Preferences->Localization->File I/O numeric format* choice allows you to override the application-wide locale setting for file input/output, to explicitly define the numeric format for reading and writing files. This affects the file import dialog as well as *File->Export*, and the table generator in the **Result Details** window. With this setting, for example, users that utilize commas for decimals in CurveExpert Basic can choose to read and write files using dots for decimals. And vice versa.

Note: In the file import dialog (see *Raw file import*), there is still a chance to change the numeric format before reading the file. This setting simply sets the default numeric format in that dialog appropriately.

15.2.3 Clipboard I/O numeric format

The *Edit->Preferences->Localization->Clipboard I/O numeric format* choice allows you to override the applicationwide locale setting for clipboard input/output, to explicitly define the numeric format for copying and pasting. This affects the copy/paste in the spreadsheet, as well as copying numeric data out any window that might offer it. With this setting, for example, users that utilize commas for decimals in CurveExpert Basic can choose to copy and paste data to/from the clipboard using dots for decimals. And vice versa.

15.2.4 File Import: numeric format

In the file import dialog (*File->Open*), there is a switch to explicitly pick the numerical formatting (English or European style) before reading the file. This gives the user the opportunity, on a file-by-file basis, to specify the numerical format. See *Raw file import*.

15.3 File overrides

If your file contains the following within the first ten lines of the file:

#DataFileProperties: locale=EN

or:

```
#DataFileProperties: locale=EURO
```

this signals to the CurveExpert Basic file importing mechanism that the file uses English or European numerical formatting (as appropriate), and the default there (see *Raw file import*) will be set appropriately. The user may still override the default, however, but in most cases this would be a bad idea, because the file itself is stating what the correct locale is.

So, you can use this capability in your own data files if you like. All of the sample data files shipped with CurveExpert Basic contain this line, so that the samples work straightforwardly regardless of the application's current region settings. This small addition to a text datafile lets the file itself express its own numerical formatting.

15.4 CurveExpert Basic files

CurveExpert Basic files (.cxp) are not affected by region settings; therefore, they are portable across localities as well as being portable across platforms (Windows, Mac, Linux).

15.5 NIST verification files

The data files associated with the NIST datasets are explicitly US-locale, and are treated as such when they are read in as a result of *Tools->Run NIST Validation* performed within CurveExpert Basic (see *Validation*). However, if you read these files in yourself, note that you MUST select an English numerical formatting in the file import dialog, if it is not already set.

SIXTEEN

VALIDATION

16.1 Introduction

CurveExpert Basic is validated against the Statistical Reference Datasets Project of the National Institute of Standards and Technology. These datasets can be downloaded directly at http://www.itl.nist.gov/div898/strd/general/dataarchive. html, but are also included verbatim in the CurveExpert Basic distribution for you to use yourself. The datasets validated against are all of the sets in the "Linear Regression" and "Nonlinear Regression" categories.

16.2 Running the Suite

You can validate CurveExpert Basic against these datasets simply by choosing *Tools->Run NIST Validation*. All validation cases, with all "starts", will be run. The NIST test suite provides different starts (i.e., initial guesses) for each nonlinear regression validation. CurveExpert Basic covers all of these starts in the test suite, and the results are output to the message window.

Some competing packages do not include all starts in their validation sets, but CurveExpert Basic shows the results of all of them. At the time of this writing, there is one failure (dataset BoxBOD, Start #1), where, for the given start, the initial correction to parameter β_2 causes underflow in the model, and from this there is no recovery.

16.3 Performing validations yourself

If you would like to perform validations against the test data yourself, all data files are contained in the "example_data/NIST" folder in the initial data directory (see *Where files are located*). Or, you can always download the files from NIST at the link above.

Note: The NIST datasets all list the dependent variable (usually y) **before** the independent variable (usually x). So, when you read the files, select *Rotate Columns* in the file import dialog, or alternatively, rotate the columns after you read in the dataset.

All nonlinear regression validation runs are performed in the automated suite with rtol=ptol=1.0e-14, and maxiter=1000.

SEVENTEEN

MISCELLANEOUS

17.1 Log Viewer

To view the log files, select *Tools->View Logs* from the main menu. All logs are stored in the \$HOME/.curveexpertbasic/logs directory, and roll according to the preferences that you have set in *Edit->Preferences->Logging* (see *Logging Preferences*). So, you can easily view logs for previous sessions of CurveExpert Basic with this tool.

To copy a portion of the log, select the desired portion, and press the *Copy* button. Likewise, to upload a portion of the log to the CurveExpert Basic server (http://www.curveexpert.net), press the *Upload* button. Uploading of a log is typically used in conjunction with reporting or tracing a software issue. If no part of the log is selected, the entire log will be copied to clipboard or uploaded, as appropriate.

There is one log file per process that CurveExpert Basic runs. If you are using multicore capability (CurveExpert Pro only), there will be several log files (named worker.n, where n is a number from 0 to the number of helper processes minus one) in addition to the main log file. These worker log files document the actions that each worker has performed, and can be copied or uploaded in identical fashion to the main log.

See Logging Preferences for more detail on configuring the logging options.

Log Viewer
main worker.0 worker.1 worker.2 worker.3
<pre>2011-01-03 11:13:53,236 2372 INFO: During the initialization, the locale is ('English_United States', '1252') 2011-01-03 11:13:53,236 2372 INFO: During the initialization, the default locale is ('en_US', 'cp1252') 2011-01-03 11:13:53,236 2372 INFO: During the initialization, the radix is . 2011-01-03 11:13:53,236 2372 INFO: Setting locale ==> C 2011-01-03 11:13:53,236 2372 INFO: Locale = C 2011-01-03 11:13:53,236 2372 INFO: Default locale = ('en_US', 'cp1252') 2011-01-03 11:13:53,236 2372 INFO: Default locale = ('en_US', 'cp1252') 2011-01-03 11:13:53,236 2372 INFO: Locale set to (None, None) 2011-01-03 11:13:53,638 2372 INFO: Finished loading MainFrame 2011-01-03 11:13:53,638 2372 INFO: Finished loading MainFrame. 2011-01-03 11:13:53,638 2372 INFO: Finished with splash screen init. 2011-01-03 11:13:53,638 2372 INFO: Finished with splash screen init.</pre>
2011-01-03 11:13:55,492 2372 INFO: Welcome to CurveExpert Professional. 2011-01-03 11:13:55,493 2372 INFO: Thread object created: function= <function at<br="" createmulticoreworkers="">0x04C94A30> 2011-01-03 11:13:55,493 2372 INFO: Thread about to start: function=<function at<br="" createmulticoreworkers="">0x04C94A30> 2011-01-03 11:13:55,493 2372 INFO: Thread running: function=<function 0x04c94a30="" at="" createmulticoreworkers=""></function></function></function>
2011-01-03 11:13:58,484 2372 INFO: Thread object created: function= <function 0x04c948b0="" at="" getonlinesettings=""> 2011-01-03 11:13:58,484 2372 INFO: Thread about to start: function=<function 0x04c948b0="" at="" getonlinesettings=""> 2011-01-03 11:13:58,484 2372 INFO: Thread running: function=<function 0x04c948b0="" at="" getonlinesettings=""> 2011-01-03 11:13:58,661 2372 INFO: Getting latest version from latest_version_win32 2011-01-03 11:13:58,663 2372 INFO: Your version of CurveExpert Professional is the latest version.</function></function></function>
Copy Upload Close

17.2 Running Multiple Instances

Running multiple instances of CurveExpert Basic is supported; the only side effect is that, because all instances share the same log files, logging might not function properly.

17.3 Where files are located

CurveExpert Basic places files in several locations on disk; the locations are documented below.

17.3.1 Program Files

The default locations are listed below, assuming that the default is accepted during the installation process. If you have changed the location of the program files, obviously they will be placed where you specified.

Platform	Program Files Location
Windows (64 bit)	c:\Program Files (x86)\CurveExpert Basic
Windows (32 bit)	c:\Program Files\CurveExpert Basic

17.3.2 Application Settings

Platform	Application Settings Location	
Windows	in registry: HKEY_CURRENT_USER\Software\CurveExpert Basic	

17.3.3 Working/Cache Area

An area is reserved for various caches and items that are needed for normal application operation. This area is used for the cache, logs, and storage of custom user models.

Platform	Working/Cache Area Location
Windows	\$HOME\.curveexpert-basic

17.3.4 CurveExpert Basic Data Files

The data files directory can be customized using *Edit->Preferences->General*, but the default locations are below. This directory is also where the example data that ships with CurveExpert resides.

Platform	Documents Location	
Windows	\$MYDOCUMENTS\CurveExpert Basic	

EIGHTEEN

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NINETEEN

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19.8 winpaths

CurveExpert Basic utilizes a single function from winpaths in order to find the "My Documents" directory under Windows. The required MIT license follows:

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19.11 JPEG library

This software is based in part on the work of the Independent JPEG Group.

TWENTY

APPENDIX A: MATH FUNCTIONS

This section documents the math functions that are available for use in CurveExpert Basic custom models, functions, and data transformations.

All functions below, unless otherwise stated, work on either scalars (a single number) or an array (a vector). If an array is passed to any of these functions, the function is applied elementwise to each member of the array.

20.1 Constants

20.1.1 pi

The mathematical constant 3.14159....

20.1.2 exp1

The mathematical constant 2.71828.....

20.2 Transcendental Functions

20.2.1 acos(x)

Trigonometric inverse cosine. The inverse of cos so that, if y = cos(x), then x = acos(y). The domain is [-1, 1].

acos is a multivalued function: for each x there are infinitely many numbers z such that cos(z) = x. The convention is to return the angle z whose real part lies in [0, pi].

The inverse *cos* is also known as *arccos* or cos^-1.

20.2.2 acosh(x)

Inverse hyperbolic cosine.

acosh is a multivalued function: for each x there are infinitely many numbers z such that cosh(z) = x. The convention is to return the z whose imaginary part lies in [-pi, pi] and the real part in [0, inf].

20.2.3 asin(x)

Inverse sine. The inverse sine of each element in x, in radians and in the closed interval [-pi/2, pi/2].

arcsin is a multivalued function: for each x there are infinitely many numbers z such that sin(z) = x. The convention is to return the angle z whose real part lies in [-pi/2, pi/2].

The inverse sine is also known as *arcsin* or sin^{-1} .

20.2.4 asinh(x)

Inverse hyperbolic sine.

arcsinh is a multivalued function: for each x there are infinitely many numbers z such that sinh(z) = x. The convention is to return the z whose imaginary part lies in [-pi/2, pi/2].

The inverse hyperbolic sine is also known as *arcsinh* or sinh⁻¹.

20.2.5 atan(x)

Trigonometric inverse tangent. The inverse of tan, so that if y = tan(x) then x = atan(y).

atan is a multi-valued function: for each x there are infinitely many numbers z such that tan(z) = x. The convention is to return the angle z whose real part lies in [-pi/2, pi/2].

The inverse tangent is also known as *arctan* or tan^{-1} .

20.2.6 atan2(y,x)

Arc tangent of y/x choosing the quadrant correctly.

The quadrant (i.e., branch) is chosen so that $\arctan(y, x)$ is the signed angle in radians between the ray ending at the origin and passing through the point (1,0), and the ray ending at the origin and passing through the point (*x*2, *x1*). By IEEE convention, this function is defined for x = +/-0 and for either or both of y and x = +/-inf (see Notes for specific values).

Returns angle in radians, in the range [-pi, pi].

20.2.7 atanh(x)

Inverse hyperbolic tangent.

arctanh is a multivalued function: for each x there are infinitely many numbers z such that tanh(z) = x. The convention is to return the z whose imaginary part lies in [-pi/2, pi/2].

The inverse hyperbolic tangent is also known as *arctanh* or tanh^-1.

20.2.8 cos(x)

Trigonometric cosine.

20.2.9 cosh(x)

Hyperbolic cosine. Equivalent to $1/2 \times (\exp(x) + \exp(-x))$.

20.2.10 erf(x)

Error function of x defined as

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt$$

20.2.11 erfc(x)

Returns

$$\operatorname{erfc}(x) = 1 - \operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_{x}^{\infty} e^{-t^2} dt$$

20.2.12 exp(x)

Calculate the exponential.

The irrational number e is also known as Euler's number. It is approximately 2.718281, and is the base of the natural logarithm, \ln (this means that, if $x = \ln y = \log_e y$, then $e^x = y$. For real input, $\exp(x)$ is always positive.

20.2.13 ln(x)

Natural logarithm (synonym for log). The natural logarithm ln is the inverse of the exponential function, so that ln(exp(x)) = x. The natural logarithm is logarithm in base e.

20.2.14 log(x)

Natural logarithm. The natural logarithm *log* is the inverse of the exponential function, so that log(exp(x)) = x. The natural logarithm is logarithm in base *e*.

20.2.15 log10(x)

Return the base 10 logarithm. NaNs is returned if x is negative.

20.2.16 sin(x)

Trigonometric sine.

20.2.17 sinh(x)

Hyperbolic sine, element-wise. Equivalent to $1/2 \times (\exp(x) - \exp(-x))$.

20.2.18 sqrt(x)

Return the positive square-root. Returns NaN if x is negative.

20.2.19 tan(x)

Compute tangent. Equivalent to sin(x)/cos(x).

20.2.20 tanh(x)

Compute hyperbolic tangent. Equivalent to $\sinh(x)/\cosh(x)$.

20.3 Bessel Functions

20.3.1 bessel_j0(x)

The Bessel function of order 0 at x.

20.3.2 bessel_j1(x)

The Bessel function of order 1 at x.

20.3.3 bessel_jn(n,x)

Bessel function of integer or real order n.

20.3.4 bessel_y0(x)

The Bessel function of the second kind of order 0 at x.

20.3.5 bessel_y1(x)

The Bessel function of the second kind of order 1 at x.

20.3.6 bessel_yn(n,x)

Bessel function of the second kind of integer or real order n at x.

20.3.7 bessel_i0(x)

Modified Bessel function of the first kind, order 0.

20.3.8 bessel_i1(x)

Modified Bessel function of order 1 at x.

20.3.9 bessel_k0(x)

Modified Bessel function of the second kind (sometimes called the third kind) of order 0 at x.

20.3.10 bessel_k1(x)

Modified Bessel function of the second kind (sometimes called the third kind) of order 1 at x.

20.3.11 bessel_kn(n,x)

Modified Bessel function of the second kind (sometimes called the third kind) for integer or real order n at x.

20.3.12 bessel_i0e(x)

Exponentially scaled modified Bessel function of order 0 at x. $bessel_i0e(x) = exp(-|x|) * bessel_i0(x)$.

20.3.13 bessel_i1e(x)

Exponentially scaled modified Bessel function of order 0 at x. $bessel_i1e(x) = exp(-|x|) * bessel_i1(x)$.

20.3.14 bessel_k0e(x)

Exponentially scaled modified Bessel function of the second kind (sometimes called the third kind) of order 0 at x. $bessel_k0e(x) = exp(x) * bessel_k0(x)$.

20.3.15 bessel_k1e(x)

Exponentially scaled modified Bessel function of the second kind (sometimes called the third kind) of order 1 at x. $bessel_k1(x) = exp(x) * bessel_k1(x)$.

20.3.16 bessel_jvp(n,x,i)

Return the ith derivative of bessel_jn(n,x).

20.3.17 bessel_yvp(n,x,i)

Return the nth derivative of bessel_yn(n,x).

20.3.18 bessel_kvp(n,x,i)

Return the nth derivative of bessel_kn(n,x).

20.3.19 bessel_ivp(n,x,i)

Return the nth derivative of bessel_in(n,x).

20.4 Comparison Functions

20.4.1 maximum(a,b)

Element-wise maximum of array elements; compares two arrays and returns a new array containing the elementwise maxima. If one of the elements is a NaN, that element is returned.

20.4.2 minimum(a,b)

Element-wise minimum of array elements; compares two arrays and returns a new array containing the elementwise minima. If one of the elements is a NaN, that element is returned.

20.4.3 max(array)

Return the maximum of an array (returns a scalar). Optionally, the keyword 'axis' can be given to specify, for a 2D dataset, if the max should be taken down the columns (axis=0) or across the rows(axis=1).

20.4.4 min(array)

Return the minimum of an array (returns a scalar). Optionally, the keyword 'axis' can be given to specify, for a 2D dataset, if the min should be taken down the columns (axis=0) or across the rows(axis=1).

20.5 Miscellaneous Functions

20.5.1 abs(x)

Calculate the absolute value.

20.5.2 ceil(x)

Returns the ceiling of the input. The ceil of the scalar x is the smallest integer i, such that $i \ge x$.

20.5.3 copysign(x1,x2)

Change the sign of x1 to that of x2.

20.5.4 degrees(x)

Convert angles from radians to degrees.

20.5.5 factorial(n)

Take the factorial of an integer n.

20.5.6 floor(x)

Return the floor of the input. The floor of the scalar x is the largest integer i, such that $i \le x$.

Some spreadsheet programs calculate the "floor-towards-zero", in other words floor (-2.5) == -2. Here, however, we use the a definition of *floor* such that *floor*(-2.5) == -3.

20.5.7 fmod(x1,x2)

Return the remainder of division. Returns the remainder of the division of x1 by x2.

The result of the modulo operation for negative dividend and divisors is bound by conventions. In *fmod*, the sign of the remainder is the sign of the dividend. In *remainder*, the sign of the divisor does not affect the sign of the result.

20.5.8 hypot(x1,x2)

Given the "legs" of a right triangle, return its hypotenuse. Equivalent to sqrt(x1**2 + x2**2).

20.5.9 isinf(x)

Test for positive or negative infinity.

20.5.10 isnan(x)

Test for Not a Number (NaN).

20.5.11 legendre(n,x)

Legendre function of order n evaluated at x. Orthogonal over [1,1] with weighting function 1.

20.5.12 lstsq_solve(A,B)

Solve a least squares problem, where A is a rectangular matrix. Returns a tuple of four quantities: x (the least squares solution), residuals (array ncol long), rank (integer indicating the effective rank of A), and s (the singular values of a). Common usage is as follows:

```
(soln,resid,rank,s) = solve_lstsq(A,B)
```

Can throw an exception if the computation is too ill-conditioned.

20.5.13 sh_legendre(n,x)

Shifted Legendre function of order n evaluated at x. Orthogonal over [0,1] with weighting function 1.

20.5.14 radians(x)

Convert angles from degrees to radians.

20.5.15 round(a,number_of_decimals)

Round an array to a given number of decimals. number_of_decimals is an integer denoting the number of decimal places to retain.

20.5.16 special_beta(p,q)

Returns

$$\beta(p,q) = \Gamma(p)\Gamma(q)/\Gamma(p+q)$$

20.5.17 special_lambda(nu,x)

Returns

$$\Lambda_{\nu}(x) = \frac{J_{\nu}(x)}{\left(\frac{1}{2}x\right)^{\nu}}$$

The Bessel function used here is the same as special_jn(n,x).

20.5.18 special_gamma(x)

Gamma function. The gamma function is often referred to as the generalized factorial since x*gamma(x) = gamma(x+1) and gamma(n+1) = n! for natural number n.

Note that the domain is limited to [1.0e-6,10].

20.5.19 trunc(x)

Return the truncated value of the input. The truncated value of the scalar x is the nearest integer i which is closer to zero than x is. In short, the fractional part of the signed number x is discarded.

20.6 Array Specific Functions

20.6.1 append(array)

Append values to the end of an array.

20.6.2 array(object)

Create an array from an array_like object, like a Python list or another array.

20.6.3 asarray(object)

Convert the input to an array. a is an array_like object, like a Python list.

20.6.4 arange(start, stop, step)

Return evenly spaced values within a given interval.

Values are generated within the half-open interval [start, stop) (in other words, the interval including *start* but excluding *stop*).

20.6.5 average(a)

Compute the arithmetic average (identical to the mean) of an array (returns a scalar). Optionally, the keyword 'axis' can be given to specify, for a 2D dataset, if the average should be taken down the columns (axis=0) or across the rows(axis=1).

$$\bar{x} = \frac{\sum_{i=1}^{n} x_i}{n}$$

20.6.6 column_stack((a,b,c,d,...))

Stack 1D arrays as columns into a 2D array.

20.6.7 copy(object)

Return an array copy of the given object.

20.6.8 concatenate((a1,a2,a3,...))

Join a sequence of arrays together.

20.6.9 dot(a,b)

Dot product of two arrays a and b (returns a scalar)

20.6.10 empty(shape)

Return a new array of given shape, without initializing entries. If the new array should be one dimensional, just an integer will suffice for the shape. If the new array should be multidimensional, then $my_array = empty((n,3))$ is an appropriate example.

20.6.11 eye(n)

Return a 2-D array with ones on the diagonal and zeros elsewhere.

20.6.12 fliplr(a)

Flip (reverse) an array in the left/right direction (columnwise).

20.6.13 flipud(a)

Flip (reverse) an array in the up/down direction (rowwise).

20.6.14 hstack((a,b,c,d,....))

Stack arrays in sequence horizontally (columnwise)

20.6.15 identity(n)

Return the identity array. The identity array is a square array with ones on the main diagonal.

20.6.16 linspace(start,stop,n)

Return evenly spaced numbers over a specified interval.

Returns *n* evenly spaced samples, calculated over the interval [*start*, *stop*].

20.6.17 mean(a)

Compute the arithmetic mean (identical to the average) of an array (returns a scalar). Optionally, the keyword 'axis' can be given to specify, for a 2D dataset, if the mean should be taken down the columns (axis=0) or across the rows(axis=1).

$$\bar{x} = \frac{\sum_{i=1}^{n} x_i}{n}$$

20.6.18 median(a)

Compute the median of an array along the specified column. Returns the median of the array elements. Optionally, the keyword 'axis' can be given to specify, for a 2D dataset, if the median should be taken down the columns (axis=0) or across the rows(axis=1).

Given a vector V of length N, the median of V is the middle value of a sorted copy of V, $V_sorted - i.e.$, $V_sorted[(N-1)/2]$, when N is odd. When N is even, it is the average of the two middle values of V_sorted .

20.6.19 nonzero(a)

Returns as an integer array, the indices of the elements are are nonzero. This can be used for indexing into another array.

20.6.20 ones(shape)

Return a new array of given shape, filled with ones. For example, $my_array = ones(n)$ If the new array should be one dimensional, just an integer will suffice for the shape. If the new array should be multidimensional, then $my_array = ones((n,3))$ is an appropriate example.

20.6.21 ones_like(a)

Returns an array of ones with the same dimension as the given array.

20.6.22 roll(a)

Roll array elements rowwise; rows that roll beyond the last position are reintroduced at the first.

20.6.23 rand(nrow,ncol)

Returns an array of the given dimension (nrow x ncol) and fill it with random samples from a uniform distribution over [0,1).

20.6.24 sort(a)

Return an ascending sorted copy of the array.

20.6.25 standarddev(a)

Return the standard deviation of an array. Optionally, the keyword 'axis' can be given to specify, for a 2D dataset, if the standard deviation should be taken down the columns (axis=0) or across the rows(axis=1). Also optionally, the keyword 'ddof' can be given to determine the divisor used in the calculations. By default, ddof is 1.

$$\sigma = \sqrt{\frac{1}{n - DOF} \sum_{i=1}^{n} (x_i - \bar{x})^2}$$

20.6.26 unique(a)

Find the unique elements of an array; returns the sorted unique elements of an array. Works on only 1D arrays; the array will be flattened if it is not already 1D.

20.6.27 variance(a)

Return the variance of the array. Optionally, the keyword 'axis' can be given to specify, for a 2D dataset, if the variance should be taken down the columns (axis=0) or across the rows(axis=1).

20.6.28 vstack((a,b,c,d,...))

Stack arrays in sequence vertically (rowwise).

20.6.29 zeros(shape)

Return a new array of given shape, filled with zeros. For example, $my_array = zeros(n)$. If the new array should be one dimensional, just an integer will suffice for the shape. If the new array should be multidimensional, then $my_array = zeros((n,3))$ is an appropriate example.

20.6.30 zeros_like(other_array)

Return an array of zeros with the same dimension as a given array. For example, $my_array = zeros_like(x)$

20.7 Logical Functions

20.7.1 array_and(b1,b2)

Applies the logical and operator, elementwise, to two boolean arrays b1 and b2. Returns another boolean array.

20.7.2 array_or(b1,b2)

Applies the logical or operator, elementwise, to two boolean arrays b1 and b2. Returns another boolean array.

20.7.3 array_xor(b1,b2)

Applies the logical xor operator, elementwise, to two boolean arrays b1 and b2. Returns another boolean array.

20.7.4 array_not(b1)

Applies the logical not operator, elementwise, to a boolean array b1. Returns another boolean array.

20.7.5 array_gt(x1,x2)

Returns a boolean array that tests x1 > x2 elementwise.

20.7.6 array_lt(x1,x2)

Returns a boolean array that tests $x_1 < x_2$ elementwise.

20.7.7 array_le(x1,x2)

Returns a boolean array that tests $x_1 \le x_2$ elementwise.

20.7.8 array_ge(x1,x2)

Returns a boolean array that tests $x_1 \ge x_2$ elementwise.

20.7.9 array_eq(x1,x2)

Returns a boolean array that tests x1 == x2 elementwise.

20.7.10 array_neq(x1,x2)

Returns a boolean array that tests $x_1 = x_2$ elementwise.

20.7.11 array_almost_eq(x1,x2, rtol, atol)

Tests two arrays x1 and x2, elementwise, to see if they are nearly equal within the tolerances specified in rtol and atol. Returns a boolean array. rtol is a relative tolerance, and atol is an absolute tolerance. To determine closeness, the relative difference rtol*abs(b) and the absolute difference atol are added together to compare against the absolute difference between the elements of a and b.

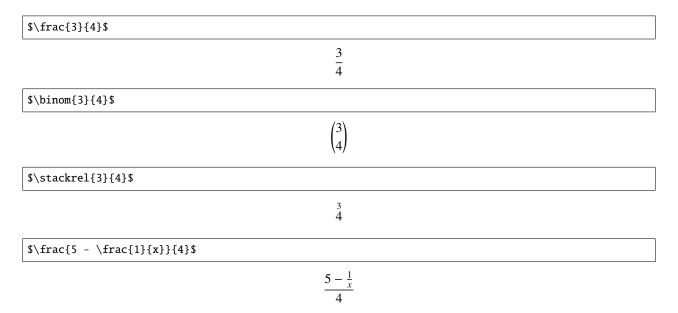
TWENTYONE

APPENDIX B: MATH SYMBOL REFERENCE

21.1 Subscripts and superscripts

Command	Result
\$alpha_i > beta_i\$	$\alpha_i > \beta_i$
\$alpha^2 > beta_i^a\$	$\alpha^2 > \beta_i^a$

21.2 Fractions, binomials and stacked numbers



21.3 Using parenthesis properly

 $(\int x^{5} - \int x^{1}{x}^{4})$

$$(\frac{5-\frac{1}{x}}{4})$$

Notice how the parenthesis do not properly wrap the object inside. To address this, use the \left and \right qualifiers in front of your parenthesis.

 $\left(\frac{5 - \frac{1}{x}}{4}\right)$

$$\left(\frac{5-\frac{1}{x}}{4}\right)$$

21.4 Radicals

 $\operatorname{Sqrt}{2}$

 $\sqrt{2}$

\$\sqrt[3]{x}\$

 $\sqrt[3]{x}$

21.5 Accents

Command	Result
$\ acute \ a \ or \'a$	á
∖bar a	ā
\breve a	ă
$\det a \text{ or } a$	ä
$\det a \text{ or } a$	à
grave a or `a	à
$hat a or ^a$	â
\tilde a or \~a	ã
\vec a	đ
\widehat{xyz}	\widehat{xyz}
\widetilde{xyz}	xyz

21.6 Symbols

Lower-case Greek

$\alpha \setminus alpha$	$\beta \setminus beta$	$\chi \setminus chi$	$\delta \setminus delta$	$F \setminus digamma$
$\epsilon \setminus epsilon$	$\eta \setminus eta$	$\gamma \setminus gamma$	ı∖iota	$\kappa \setminus kappa$
$\lambda \setminus lambda$	$\mu \setminus mu$	v ∖nu	$\omega \setminus omega$	$\phi \setminus phi$
$\pi \setminus pi$	ψ \psi	$\rho \setminus rho$	$\sigma \setminus sigma$	$\tau \setminus tau$
$\theta \setminus theta$	$v \setminus upsilon$	$\varepsilon \setminus varepsilon$	$\varkappa \setminus varkappa$	$\varphi \setminus varphi$
$\varpi \setminus varpi$	$\varrho \setminus varrho$	$\varsigma \setminus varsigma$	$\vartheta \setminus vartheta$	ξ\xi
ζ\zeta				

Upper-case Greek

$\Delta \setminus Delta$	$\Gamma \setminus Gamma$	$\Lambda \setminus Lambda$	$\Omega \setminus Omega$	$\Phi \setminus Phi$	П∖Рі
Ψ\Psi	$\Sigma \setminus Sigma$	$\Theta \setminus Theta$	Υ \Upsilon	Ξ\Xi	び∖mho
$\nabla \setminus nabla$					

Hebrew

ℵ \aleph □ \beth □ \daleth □ \gimel

Delimiters

//	[[↓\Downarrow	↑\Uparrow	∥\Vert	$\ \ backslash$
↓\downarrow	< \langle	[\lceil	[∖lfloor	∟ \llcorner	_ \lrcorner
\rangle \rangle]\rceil]\rfloor	「 \ulcorner	↑\uparrow	¬∖urcorner
\vert	{ \{	X	} \}]]	

Big symbols

$\bigcap \$	∪∖bigcup	○ \bigodot	$\bigoplus \ bigoplus$	\otimes \bigotimes
\+ \biguplus	\/ \bigvee	$\land \$	∐ \coprod	∫∖int
∮∖oint	∏ \prod	$\sum \setminus sum$		

Standard function names

Pr \Pr	arccos \arccos	arcsin \arcsin	arctan \arctan
arg \arg	cos \cos	cosh ∖cosh	cot \cot
coth ∖coth	csc \csc	deg \deg	det \det
dim \dim	exp \exp	gcd \gcd	hom \hom
inf \inf	ker \ ker	lg ∖lg	lim \lim
liminf \liminf	lim sup \limsup	ln \ln	log \log
max \max	min \min	sec \sec	sin \sin
sinh \sinh	sup ∖sup	tan \tan	tanh \tanh

Binary operation and relation symbols

⇒ \Bumpeq	∩ \Cap	⊎ \Cup
≑\Doteq	⋈ \Join	∈ \Subset
∋\Supset	⊩ \Vdash	⊪ \Vvdash
$\approx \approx$	≊ \approxeq	* \ast
≍ \asymp	→ \backepsilon	$\sim \$ backsim
	$\overline{\wedge} \setminus barwedge$	∵ \because
≬\between	⊖\bigcirc	$\triangledown \$ bigtriangledown
$\triangle \$	◄ \blacktriangleleft	▶ \blacktriangleright
⊥ \bot	⊳\bowtie	⊡ \boxdot
⊟ \boxminus	⊞ \boxplus	⊠ \boxtimes
• \bullet	≏ \bumpeq	∩∖cap
· \cdot	∘ \circ	≜ \circeq
:- \coloneq	≅ \cong	∪∖cup
<pre></pre> <pre></pre> <pre></pre>	<pre>> \curlyeqsucc</pre>	Y \curlyvee
∧ \curlywedge	† \dag	⊣∖dashv
‡ \ddag	◊ \diamond	÷ \div
* \divideontimes	≐ \doteq	≑ \doteqdot
∔\dotplus	$\overline{\wedge} \setminus doublebarwedge$	<pre></pre>
-:∖eqcolon	$\approx \eqref{eq:sim}$	>\eqslantgtr
<pre><\eqslantless</pre>	≡ \equiv	≒\fallingdotseq

$\frown \$ frown	≥∖geq	≧ \geqq
≥∖geqslant	≫ \gg	≫ \ggg
≩ \gnapprox	≩ \gneqq	≳∖gnsim
≳\gtrapprox	>\gtrdot	≷∖gtreqless
≷∖gtreqqless	≷∖gtrless	≳∖gtrsim
∈∖in	_T ∖intercal	$\lambda \setminus $ leftthreetimes
≤\leq	≦ \leqq	≤∖leqslant
[≲\lessapprox	∢\lessdot	≶\lesseqgtr
[∮ \lesseqqgtr	≶∖lessgtr	$\lesssim \lessim$
≪ \11	« \lll	≨ \lnapprox
≨∖lneqq	≲∖lnsim	K \ltimes
\mid	⊨ \models	∓ \mp
⊯ \nVDash	⊮ \nVdash	≉ \napprox
≇ \ncong	≠ \ne	≠ \neq
≠ \neq	≢ \nequiv	≱ \ngeq
≯∖ngtr	∋∖ni	≰ \nleq
≮∖nless	∤ \nmid	∉∖notin
∦ \nparallel	⊀ \nprec	≁ \nsim
⊄∖nsubset	⊈∖nsubseteq	⊁ \nsucc
⊅ \nsupset	⊉ \nsupseteq	≮\ntriangleleft

≰ \ntrianglelefteq	⊭ \ntriangleright	≱ \ntrianglerighteq
⊭ \nvDash	⊬ \nvdash	⊙∖odot
$\ominus \setminus ominus$	$\oplus $ \oplus	⊘∖oslash
⊗∖otimes	∥\parallel	⊥ \perp
	± ∖pm	< \prec
\leq \precapprox	<pre><\preccurlyeq</pre>	≤\preceq
i	$\leq \precnsim$	$\leq \precsim$
∝ \propto	\land \rightthreetimes	≓∖risingdotseq
	$\sim \$	$\simeq \$
/\slash	$\smile \$ smile	□ \sqcap
⊔ \sqcup	∟ \sqsubset	□ \sqsubset
⊑ \sqsubseteq	⊐ \sqsupset	⊐\sqsupset
⊒\sqsupseteq	★ \star	⊂∖subset
⊆∖subseteq	⊆\subseteqq	⊊∖subsetneq
⊊∖subsetneqq	> \succ	≿ \succapprox
≽∖succcurlyeq	≥ \succeq	≿ \succnapprox
$\gtrsim \succnsim$	$\gtrsim \succsim$	⊃∖supset
⊇∖supseteq	⊇\supseteqq	⊋∖supsetneq
⊋∖supsetneqq	∴ \therefore	× \times
⊤ \top	⊲\triangleleft	⊴∖trianglelefteq

≜ \triangleq	ト\triangleright	⊵ \trianglerighteq
⊎ \uplus	⊧ \vDash	$\propto \$
⊲\vartriangleleft	▷ \vartriangleright	⊦ \vdash
∨ \vee	⊻ \veebar	∧ \wedge
≀\wr		

Arrow symbols

↓ \Downarrow	$\leftarrow \Leftarrow$
$\Leftrightarrow \ Leftrightarrow$	$\in \$ Lleftarrow
$\leftarrow \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \$	$\iff \setminus Longleftrightarrow$
$\implies \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \$	ጎ \Lsh
🖉 \Nearrow	🔨 \Nwarrow
$\Rightarrow \$	$\Rightarrow \$
r ∖Rsh	📎 \Searrow
🖉 \Swarrow	↑ \Uparrow
↓ Updownarrow ↓	$\bigcirc \$ \circlearrowleft
$\bigcirc \$ \circlearrowright	$\sim \$ curvearrowleft
\frown \curvearrowright	<\dashleftarrow
> \dashrightarrow	↓ \downarrow
↓↓ \downdownarrows	<pre>↓ \downharpoonleft</pre>
↓\downharpoonright	↔ \hookleftarrow
$\hookrightarrow \setminus hookrightarrow$	\rightarrow \leadsto
$\leftarrow \leftarrow$	← \leftarrowtail
$\leftarrow \$ leftharpoondown	$\leftarrow \$ leftharpoonup
$\models \leftleftarrows$	$\leftrightarrow \$
$\leq \$ leftrightarrows	$\Rightarrow \ leftrightharpoons$
<pre></pre>	↔ \leftsquigarrow
1	

$\leftarrow \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \$	$\longleftrightarrow \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \$	
$\mapsto \setminus longmapsto$	$\longrightarrow \longrightarrow$	
↔ \looparrowleft	$\leftrightarrow \looparrowright$	
$\mapsto \mbox{mapsto}$	$\multimap \mbox{multimap}$	
∉ \nLeftarrow	⇔ \nLeftrightarrow	
⇒ \nRightarrow	↗\nearrow	
↔ \nleftarrow	↔ \nleftrightarrow	
→ \nrightarrow	🔨 \nwarrow	
$\rightarrow $ \rightarrow	\rightarrow \rightarrowtail	
\rightarrow \rightharpoondown	$ ightarrow \$	
\rightleftharpoons \rightleftarrows	\rightleftharpoons \rightleftarrows	
$\Rightarrow \$	$\Rightarrow \$	
$\Rightarrow \$	$\Rightarrow \$	
→\rightsquigarrow	💪 \searrow	
🖌 \swarrow	$\rightarrow \$ to	
← \twoheadleftarrow	->> \twoheadrightarrow	
↑ \uparrow	<pre>\$ \updownarrow</pre>	
<pre>\$ \updownarrow</pre>	1 \upharpoonleft	
`\upharpoonright	<pre>↑↑ \upuparrows</pre>	

Miscellaneous symbols

- + · · ·	· ·	
\$\\$	À \AA	∃∖Finv
∂ \Game	$\Im \setminus Im$	¶ \P
ℜ ∖Re	§ \S	∠∖angle
\\backprime	★ \bigstar	■ \blacksquare
▲ \blacktriangle	▼ \blacktriangledown	$\cdots \setminus cdots$
√ \checkmark	<pre></pre>	(§)\circledS
<pre>♣ \clubsuit</pre>	<pre></pre>	© \copyright
·.\ddots	$\diamond \$	$\ell \setminus ell$
Ø∖emptyset	ð\eth	∃∖exists
♭\flat	∀\forall	$\hbar \setminus hbar$
♡\heartsuit	$\hbar \$	∭∖iiint
∬∖iint	∬∖iint	<i>i</i> \imath
∞ \infty	j∖jmath	\ldots
∡ \measuredangle	¦\natural	¬ ∖neg
∄∖nexists	∰ \oiiint	$\partial \setminus partial$
/\prime	#∖sharp	♦ \spadesuit
< \sphericalangle	\ss	⊽ \triangledown
$\emptyset \setminus varnothing$	$\land \$:\vdots
℘∖wp	¥ \yen	

TWENTYTWO

APPENDIX C: THEORY

22.1 Linear Regression

Models which consist of a linear combination of a particular set of functions X_k are called linear models, and linear regression can be used to minimize the difference between the model and data. The general form of this kind of model is

$$y(x) = \sum a_k X_k(x)$$

where $X_k(x)$ are fixed functions of x that are called the basis functions, and a_k are the free parameters. Note that "linear" refers only to dependence of the model on the parameters a_k ; the functions $X_k(x)$ may be nonlinear. Minimization of the above linear model is performed with respect to the merit function

$$S(a) = \sum_{i=1}^{n} \left[y_i - \sum_{k=1}^{np} a_k X_k(x_i) \right]^2$$

The minimum of the above equation occurs where the derivative of S with respect to the parameters disappears. Substituting the linear model into this function, taking the first derivative, and setting this equal to zero gives the normal equations that can be solved directly for the parameters a_k .

22.2 Nonlinear Regression

22.2.1 Introduction

This program uses the Levenberg-Marquardt method to solve nonlinear regressions. This method combines the steepest-descent method and a Taylor series based method to obtain a fast, reliable technique for nonlinear optimization. This statement will be repeated later, but can bear stating at the beginning of this discussion: neither of the above optimization methods are ideal all of the time; the steepest descent method works best far away from the minimum, and the Taylor series method works best close to the minimum. The Levenberg-Marquardt (LM) algorithm allows for a smooth transition between these two methods as the iteration proceeds.

22.2.2 Development

In general, the data modeling equation (with any number of independent variables) can be written as follows:

$$y = y(\vec{x}; \vec{a})$$

The above expression simply states that the dependent variable y can be expressed as a function of the independent variables \vec{x} and vector of parameters \vec{a} of arbitrary length. Note that using the ML method, any nonlinear equation with an arbitrary number of parameters can be used as the data modeling equation. Then, the merit function we are trying to minimize is

$$\chi^2(\vec{a}) = \sum_{i=1}^n \left(\frac{y_i - y(\vec{x}_i; \vec{a})}{\sigma_i}\right)^2$$

where N is the number of data points, $\vec{x_i}$ denotes the x data points, y_i denotes the y data points, σ_i is the standard deviation (uncertainty) at point i, and $y(x_i; a)$ is an arbitrary nonlinear model evaluated at the ith data point. This merit function simply measures the agreement between the data points and the parametric model; a smaller value for the merit function denotes better agreement. Commonly, this merit function is called the chi-square.

Now, we will take a step back to provide a framework of optimization methods. From the area of pure optimization, which will not be explained here, two basic ways of finding a function minimum are a Taylor series based method and the steepest-descent method. The Taylor series method states that sufficiently close to the minimum, the function can be approximated as a quadratic. Without detailed explanation of that method, a step from the current parameters a to the best parameters amin can be written as

$$\vec{a}_{min} = \vec{a}_{cur} + H^{-1} \left[-\Delta \chi^2(\vec{a}_{cur}) \right]$$

where H is the Hessian matrix (a matrix of second derivatives). If the approximation of the function as a quadratic is a poor one, then we might instead use the steepest-descent method, where a step to the best parameters from the current parameters is

$$\vec{a}_{min} = \vec{a}_{cur} - c\Delta\chi^2(\vec{a}_{cur})$$

This equation simply states that the next guess for the parameters is a step down the gradient of the merit function. The constant c is forced to be small enough that a small step is taken and the gradient is accurate in the region that the step is taken.

Since we know the chi-square function, we can directly differentiate to obtain the gradient vector and the Hessian matrix. Taking the partial derivatives of the merit function with respect to a gives

$$\frac{\partial \chi^2}{\partial a_k} = -2\sum_{i=1}^n \frac{y_i - y(\vec{x}_i; \vec{a})}{\sigma_i^2} \frac{\partial y(\vec{x}_i; \vec{a})}{\partial a_k}$$

To obtain the Hessian matrix, take the gradient of the gradient above (so that we have a matrix of partial second derivatives):

$$\frac{\partial^2 \chi^2}{\partial a_k \partial a_l} = -2 \sum_{i=1}^n \left[\frac{1}{\sigma_i^2} \frac{\partial y(\vec{x}_i; \vec{a})}{\partial a_k} \frac{\partial y(\vec{x}_i; \vec{a})}{\partial a_l} - \frac{y_i - y(\vec{x}_i; \vec{a})}{\sigma_i^2} \frac{\partial^2 y(\vec{x}_i; \vec{a})}{\partial a_l \partial a_k} \right]$$

Now, for convenience, define the gradient vector and the curvature matrix as

$$G_{k} = -\frac{1}{2} \frac{\partial \chi^{2}}{\partial a_{k}} = \sum_{i=1}^{n} \left[\frac{y_{i} - y(\vec{x}_{i}; \vec{a})}{\sigma_{i}^{2}} \frac{\partial y(\vec{x}_{i}; \vec{a})}{\partial a_{k}} \right]$$
$$C_{kl} = \frac{\partial^{2} \chi^{2}}{\partial a_{k} \partial a_{l}} = \sum_{i=1}^{n} \left[\frac{1}{\sigma_{i}^{2}} \frac{\partial y(\vec{x}_{i}; \vec{a})}{\partial a_{k}} \frac{\partial y(\vec{x}_{i}; \vec{a})}{\partial a_{l}} \right]$$

[Note that the second derivative term in C will be ignored because of two reasons: it tends to be small because it is multiplied by $(y - y_i)$, and it tends to destabilize the algorithm for badly fitting models or data sets contaminated with outliers. This action in no way affects the minimum found by the algorithm; it only affects the route in getting there.] So, the Taylor series method (inverse Hessian method) can be written as the following set of linear equations:

$$\sum_{k=1}^{np} C_{kl} \delta a_l = G_k[1]$$

where NP is the number of parameters in the model that is being optimized. This linear matrix will be our workhorse for this method after some modification; it can be solved for the increments da that, when added to the current approximation for the parameters, gives the next approximation. Likewise, we can substitute our "convenient" definitions into the steepest descent formula to obtain

$$\delta a_l = cG_l[2]$$

Neither of the aforementioned optimization methods are ideal all of the time; the steepest descent method works best far away from the minimum, and the Taylor series method works best close to the minimum. The Levenberg-Marquardt (LM) algorithm allows for a smooth transition between these two methods as the iteration proceeds.

The first issue in deriving the LM method is to attach some sort of scale to the constant c in the steepest-gradient method (equation 2). Typically, there is no obvious way to determine this number, even within an order of magnitude. However, in this case, we have access to the Hessian matrix; examining its members, we see that the scale on this constant must be $1/C_{ll}$. But, that still may be too large, so let's divide that scale by a nondimensional factor (l) and plan on setting this much larger than one so that the step will be reduced (for safety and stability).

The second issue to formulate the LM method is noting that the steepest-descent and Taylor series methods may be combined if we define a new matrix Mij by the following:

$$M_{ii} = C_{ii}(1 + \lambda), i = j$$
$$M_{ii} = C_{ii}, i \neq j$$

This matrix combines equations [1] and [2] into a convenient and compact form. So finally, we have a means of calculating the step da in the parameters by the following system of linear equations:

$$\sum_{k=1}^{np} M_{kl} \delta a_l = G_k[3]$$

Note that when l is large, the matrix M is forced to be diagonally dominant; consequently, the above equation is equivalent to the steepest descent method (equation 2). Conversely, when the parameter l goes to zero, the above equation is equivalent to the Taylor series method (equation 1). So, we vary l to switch between the two methods, continually calculating a parameter correction da that we apply to our most recent guess for the parameter vector.

22.2.3 Procedure

The steps that are taken in the LM algorithm are as follows:

- 1. Compute $\chi^2(a)$
- 2. Pick a conservative value for λ (0.001 in CurveExpert)
- 3. Solve the linear equations (equation 3) for δa
- 4. Evaluate $\chi^2(a + \delta a)$
- 5. If $\chi^2(a + \delta a) \ge \chi^2(a)$, increase λ by a factor (10 in CurveExpert) and go back to step [3].
- 6. If $\chi^2(a + \delta a) < \chi^2(a)$, decrease λ by a factor (10 in CurveExpert), correct the parameter vector by $a = a + \delta a$, and go back to step [3].

Iteration is stopped when $|\chi^2(a + \delta a) - \chi^2(a)| < \epsilon$. This tolerance ϵ is the value specified by the user.

TWENTYTHREE

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TWENTYFOUR

INDICES AND TABLES

• genindex

• search

INDEX

A

activate, 4 administrator, 3 annotation, 44 aspect, 72 autoannotate, 44 autofill, 17 automated install, 3 automatically plot, 72 automatically update results, 69 autoscale, 43, 45, 71 autoscale lock, 43 average, 21 axis properties, 45

В

background, 49 badges, 36 bessel functions, 98 bug, 68 built-in math functions, 95

С

cache, 76 calculate, 29 calculation, 25, 27, 36 clamp, 25 clipboard, 77 color coding, 35 column labels, 18 comma as decimal, 77 comment, 17 confidence bands, 39, 47 confidence bounds, 45 confidence level, 68 constants, 95 copy, 23, 45 copy parameters, 37 copy underlying data, 45 copying graphs, 52 copying result info, 37 crop, 25

cursor, 22, 68 curve data, 45 curve fit, 29, 115 CurveExpert Basic files, 18, 80 CurveExpert files, 65 curvefinder, 31 custom, 30, 60, 61 cut, 23 CXP file, 65 CXP files, 18, 80

D

data, 21, 24, 25 data column labels, 18 data file, 69 data file location, 69 data files, 15, 63, 77 data operations, 24 deleting results, 37 delimiter, 69 details, 38 drag and drop, 37 dragging, 44

Е

element, 44 EMF, 52 EPS, 52 equation, 62 equation display, 62 equations, 108 EULA, 84 Excel, 68 export, 65

F

features, 1 file locations, 84 files, 69 font, 73 footer, 17 formatting, 24

```
functions, 60
functions, array, 103
functions, bessel, 98
functions, comparison, 100
functions, constants, 95
functions, logical, 107
functions, misc, 101
functions, transcendental, 95
```

G

```
getting started, 4
graph properties, 45
graph themes, 53
graph toolbar, 42
graphing, 39
graphs and data pane, 7, 11
guide, 4
```

Н

header, 17 hiding panes, 8 highlight, 72 hotkeys, 53

I

```
image, 44
import, 15
initial guesses, 30, 31, 70
inserting rows, 23
install, 3
internet, 77
interpolation, 28
introduction, 1
issues, 68
```

J

JPEG, 52

L

legend, 44, 51 legend order, 52 legend properties, 51 Levenberg-Marquardt, 115 license, 3, 4, 84 licensing (third party), 86 line data, 45 line properties, 47 linear regression, 29, 115 localization, 74, 77 locator, 44 log viewer, 83 logging, 73, 74 logs, 83

Μ

```
marker properties, 47
math functions, 95
math symbols, 108
mathtext, 53, 62, 73, 108
mathtext reference, 53
maximize, 8
memory, 76
menu reference, 12
menus, 8
messages pane, 7, 11
models, 29, 30, 60
multicore, 11
multiple instances, 83
```

Ν

NIST, 80 nonlinear regression, 29, 115 numeric format, 77

0

online, 77 operating on data, 24 overall graph properties, 49

Ρ

pan, 43, 72 panes, 7 paste, 23 PDF, 52 pi,95 pick, 44, 72 plot toolbar, 42 PNG, 52 polynomial, 29 prediction bands, 39, 47 prediction bounds, 45 preview pane, 7, 11 print,44 printing, 53, 65, 72 printing graphs, 53 proxy, 77 PS. 52 purchase, 4

Q

querying results, 38

R

RAW, 52 reading data files, 15 redo, 23 redraw, 72 references, 117

region settings, 77 removing columns, 23 removing results, 37 removing rows, 23 reports, 68 reserved words, 62 residual.70 restore, 8 result badges, 36 result color coding, 35 result details, 38 result icons, 35 result pane, 7 result preview, 37 results, 34 results pane, 10 results update, 36 **RGBA**, 52 rotate, 25

S

save graph, 44 saving data, 63 saving graphs, 52, 65 scale, 24 shortcuts, 53 silent install, 3 simple, 61 sort, 24, 68 splines, 28 spreadsheet, 21, 68 standard deviation, 21 standard math operations, 62 statistics, 21 status bar, 11 subscript, 108 superscript, 108 surface properties, 47 SVG, 52 system administrator, 3

Т

table, 45 tension splines, 28 themes, 53 theory, 115 TIFF, 52 tips, 67 title, 49 tolerance, 28, 70 toolbar, 9, 42 toolbar reference, 9 transform, 25 translate, 24 trial,3

U

undo, 23, 76 updating results, 36 user interface, 6

V

validation, 80 verification, 80

W

weighting, 29, 31 window menu, 8 windows, 3 writing data, 63

Х

xy plot, 41

Ζ

zoom, 43