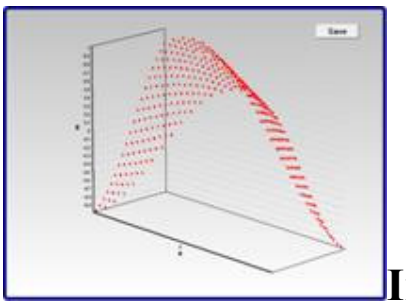
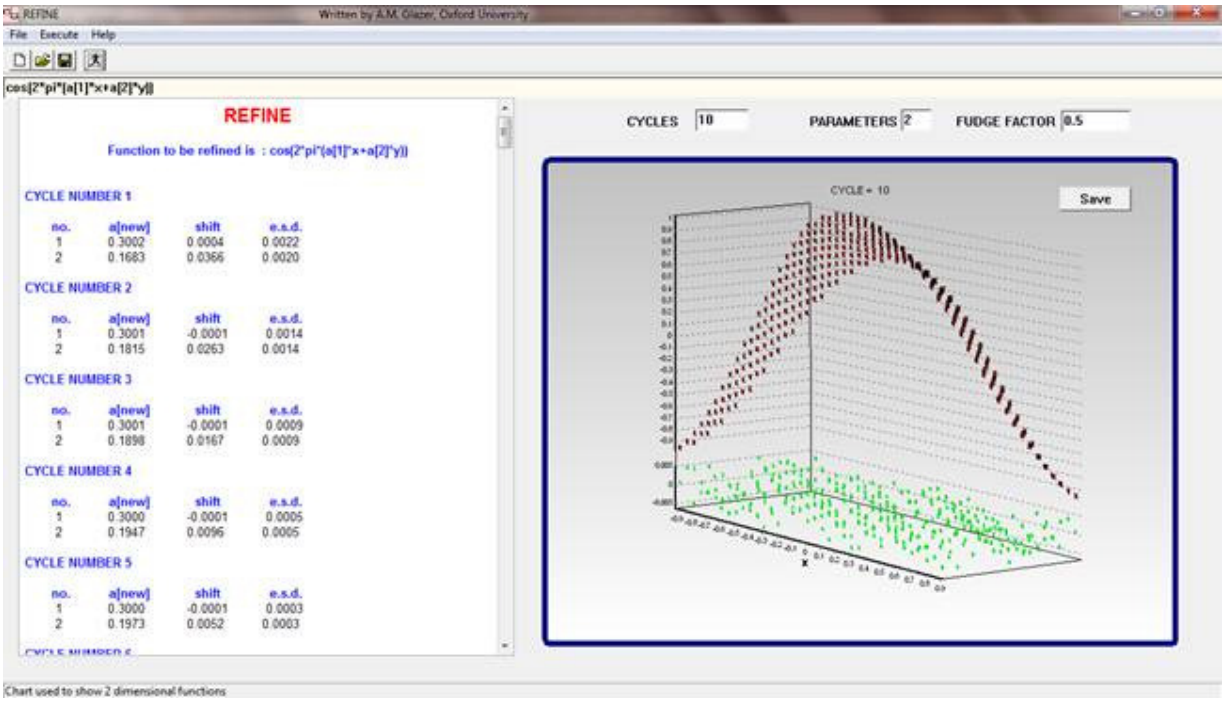
REFINE



Introduction (Version 1.0)

REFINE is a program that carries out a non-linear least-squares fit to data with a user-defined function.

Below is shown a typical screen view.



In the top box the function to be refined is entered. The datafile has as its first line the function, but this can be edited directly after reading in. REFINE refines the parameters a[1], a[2], a[]3, ….. a[10]. Left-hand panel shows the results of the refinement and the chart shows the progress of the least-squares fitting procedure.

REFINE

How to use REFINE

Operation of the program is very simple.

1. It is first necessary to input the data from a file in (*x,y*) format. The data will then be shown plotted on the graph. The first line of the file should be the function to be refined.

2. The mathematical function is entered into the function box, but can be edited). Right click on

the Function Box will open up a list of selectable function. Left click will then enter the selected function. The unknown parameters are a[1], a[2], a[3] etc, and *x* ,y,z are the variables. As you add more unknown parameters you should see the parameter count increase accordingly in the PARAMETERS box.

3. In the CYCLES box enter the number of cycles of refinement required.

4. The FUDGE FACTOR determines how big the shifts should be applied on each cycle.

5. Either use menu item Execute/Run or click on the Run button to carry out refinement.

More:

File

Execute

Help

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File

More:

New (Ctrl+N)

Open (Ctrl+O)

Print(Ctrl+P)

Save (Ctrl+S)

Export Graph(Ctrl+E)

Exit(Ctrl+X)

New (Ctrl+N)

Start a new calculation

Open (Ctrl+O)

To read in the datafile. The datafile should have as its first line the function.

If the function is (f(x) i.e. 1-dimensional then the datafile has two columns of data, the first column being the observed values, the second column being x.

If the function is (f(x,y) i.e. 2-dimensional then the datafile has three columns of data, the first column being the observed values, the second and third columns being x and y.

If the function is (f(x,y,z) i.e. 3-dimensional then the datafile has four columns of data, the first column being the observed values, the second, third and fourth columns being x , y and z.

Check that the function specified in the datafile (and in the function box at the top) is of the correct form.

For 1-dimensional case it is f(a[1],a[2],….,x)

For 2-dimensional case it is f(a[1],a[2],….,x,y)

For 3-dimensional case it is f(a[1],a[2],….,x,y,z)

 **Print(Ctrl+P)**

To output the results to a printer.

 **Save (Ctrl+S)**

To save the output in html format.

Export Graph(Ctrl+E)

Creates a JPEG of the graph.

Exit(Ctrl+X)

Closes the program.

REFINE > How to use REFINE

Execute

More:

 Run(Ctrl+R)

man.bmp **Run(Ctrl+R)**

Carries out the refinement process. The program automatically knows if the function to be refined is f(x), f (x,y) or f(x,y,z). The following dialog box is opened:

This is a pull-down box that enables you to change the trial starting parameters a[1], a[2],….

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Help

More:

Help Refine (Ctri+H)

Examples

About

Help Refine (Ctri+H)

This help file

Examples

Some example data files to try.

About

Help file explaining use of space group routine.

REFINE

Charts

More:

1 and 3 dimensional case

2 dimensional case

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1 and 3 dimensional case

The chart can be zoomed using the left mouse button. To return to unzoomed view rapidly move left mouse button up towards the left. Right mouse button allows plot to be translated across the screen. The Save button sends the chart to the Report.

REFINE > Charts

2 dimensional case

The chart can be zoomed using the left mouse button. To return to unzoomed view rapidly move left mouse button up towards the left. Right mouse button rotates the plot. The Save button sends the chart to the Report.

REFINE

Function List

Clicking with the right mouse button on the Function Box brings up a list of functions. Click with left mouse button to select. The following are the functions available.

Adding:	x + y	adds x and y
Subtracting:	x - y	subtracts y from x
Multiplying:	x * y	multiplies x and y
	fac(n)	factorial of n, n!
Dividing:	x / y	divides x through y
	n div m n \ m	integer division
	rez(x)	reciprocal value of x
	n mod m n % m	integer modulo
	modulo(x;y)	rest of division x/y
Powers:	x ^ y	x to the power of y
	sqr(x)	square of x
	exp(x)	exponential of x
Roots:	sqrt(x)	Square root of x
	cbrt(x)	cubic root of x
	root(n;x)	n-th root of x
Logarithms:	ln(x)	log. with base e of x
	lg(x)	log. with base 10 of x
	lb(x)	log. with base 2 of x
	log(b;x)	common log. with base b of x
Trigonometric Functions:	sin(x)	sine of x
	cos(x)	cosine of x
	tan(x)	tangent of x
	cot(x)	cotangent of x
	sec(x)	secant of x
	cosec(x)	cosecant of x
Arc Functions:	arcsin(x)	arc sine of x

	arccos(x)	arc cosine of x
	arctan(x)	arc tangent of x
	atan2(y;x)	arc tangent of y/x
	arccot(x)	arc cotangent of x
Hyperbolic Functions:	sinh(x)	hyperbolic sine of x
	cosh(x)	hyperbolic cosine of x
	tanh(x)	hyperbolic tangent of x
	coth(x)	hyperbolic cotangent of x
Area Functions:	arsinh(x)	inverse hyperbolic sine of x
	arcosh(x)	inverse hyperbolic cosine of x
	artanh(x)	inverse hyperbolic tangent of x
	arcoth(x)	inverse hyperbolic cotangent of x
Statistical Function:	gauss(x)	normal distribution of x
	erf(x)	error function of x
	inverf(x)	inverse of error function of x
	n over k bino(n;k)	binomial coefficient n over k
	poisson(mu;n)	Poisson distribution of n with average mu
	poicum(mu;n)	cumulated Poisson distribution up to n with average mu
Random Numbers:	rnd(x)	random number in [0,x[
	rand(a;b)	random number in [a,b[
	poirand(mu)	Poisson distributed random numbers with average mu
Bessel Functions:	J0(x)	0th order of x
	J1(x)	1st order of x
	J2(x)	2nd order of x
	J3(x)	3rd order of x
	J4(x)	4th order of x
	J5(x)	5th order of x
	J(n;x)	n-th order of x
Integral Functions:	Si(x)	sine integral of x
	Ci(x)	cosine integral of x
	Ei(x)	exponential integral of x
	li(x)	logarithm integral of x
Gammafunction:	gamma(x)	gamma function of x
Stepfunctions:	theta(x)	=1 if x >0, else =0
	sgn(x)	Sign function of x
	int(x)	integer part of x
	round(x)	x rounded to next integer value
	ceil(x)	x rounded to higher integer value
	floor(x)	x rounded to lower integer value
Periodical Functions:	triangle(x)	triangle waveform (period 2π)
	sawtooth(x)	sawtooth waveform (period 2π)
	square(x)	square waveform (period 2π)
Absolute Values:	abs(x)	absolute |x|
	cabs(x;y)	absolute |x+iy|
Miscellaneous:	frac(x)	non-integer part of x
	max(x;y)	maximum value of x and y
	min(x;y)	minimum value of x and y
	odd(n)	=1 if n is odd, =0 if n is even
	gcd(n;m)	greatest common divisor of n and m
	lcm(n;m)	least common multiple of n and m
	ramp(x;a;b)	=0 if x<a, =1 if x>b, else continuation between a and b
Bitwise and Logical Functions:	a and b a & b	bitwise logic AND
	a or b a | b	bitwise logic OR
	(a) xor (b)	bitwise logic XOR
	bnot(a)	bitwise NOT
	not(a) !a	logical NOT
	a shl b a >> b	shifts a b bit positions to the left
	a shr b a >> b	shifts a b bit positions to the right
Relational Operators:	x = y	=1 if x is equal to y, else =0
	x < > y x != y	=1 if x is not equal to y, else =0
	x < = y	=1 if x is less or equal to y, else =0

	x < y	=1 if x is less than y, else =0
	x > = y	=1 if x is greater or equal to y, else =0
	x > y	=1 if x is greater than y, else =0
IF- Function:	if(c;x;y)	if condition c=1 then x, else if c=0 then y
Properties of complex numbers:	abs(z)	absolute |z|
	arg(z)	argument (phase) of z
	re(z)	real part of z
	im(z)	imaginary part of z
	CC(z) ~z	complex conjugate of z
Mathematical Constants:	pi	circumference/diameter of circle
	e	base of natural logarithms
	C	Euler's constant
	i	imaginary unit, sqrt(-1)
	TRUE	logical value 1.0
	FALSE	logical value 0.0
	INFINITY	symbolical value for ∞
	NEGINFINITY	symbolical value for -∞
	NaN	Not a Number (aborts evaluation)
Number Formats:	N	integer numbers
	X	floating point numbers
	Z	complex numbers
	$n	hexadecimal numbers

REFINE

Constants

Vacuum speed of light [m/s]	C0 = 2.99792458e8
Planck's constant [J s]	H = 6.626176e-34
Electrical charge of electron [C]	EE = 1.6021892e-19
Boltzmann's constant [J/K]	K = 1.380662e-23
Gravitational constant [m^3 / kg / s^2]	GAMMA = 6.672e-11
Earth acceleration due to gravity [m / s^2]	G = 9.80665e0
General gas constant [J / mol / K]	R = 8.31441e0
Molar norm volume of an ideal gas [m^3 / mol]	VM = 22.41383e-3
Avogadro's constant [mol^(-1)]	NA = 6.022045e23
Loschmidt's constant [m^(-3)]	NL = 2.686754e25
Stefan-Boltzmann's constant [W / m^2 / K^4]	SIGMA = 5.67032e-8
Vacuum permittivity [F / m]	EPSILON0 = 8.85418782e-12
Magnetic permeability of vacuum [H / m]	MY0 = pi*4e-7
Faraday's constant [C / mol]	F = 9.648456e4
Quantum of angular momentum [J s]	HQUER = 1.0545887e-34
Atomic mass unit [kg]	U = 1.6605655e-37
Rydberg's constant for hydrogen [m^(-1)]	RH = 1.096776e7
Rydberg's constant for large nuclei [m^(-1)]	RINF = 1.0973731e7
Ionisation energy of hydrogen [eV]	EH = 1.36058e1
Absolute zero [°C]	T0 = -273.15e0
Square of sine of Weinberg's angle	SIN2THETAW = 0.2259e0
Sommerfeld's fine structure constant	ALPHA = 7.29735e-3
Mass of electron [MeV]	ME = 0.511004e0
Classical radius of electron [m]	RE = 2.81794e-15
Compton wavelength for electrons [m]	LAMBDACE = 2.42611e-12
Mass of neutron [MeV]	MN = 9.39553e2

Mass of proton [MeV]	MP = 9.38259e2
Mass of Z-boson [MeV]	MZ = 91.161e3
Mass of W-boson [MeV]	MW = 80.6e3
Bohr magneton [A m^2]	MYB = 9.27408e-24
Nuclear magneton [A m^2]	MYK = 5.0508e-27
Bohr radius [m]	A0 = 5.29177e-11