

Using statpages.info to perform nonlinear regression <http://statpages.info/nonlin.html>

My modified page: http://ensignchemistry.com/enzymology/curve_fitting.html

Michaelis-Menten equation

Number of data points = (varies for data)

number of independent variables = 1 (x_1)

number of parameters = 2 (a, b)

Formula: $Y = a \cdot x_1 / (b + x_1)$

a = V_{max}

b = K_m

c = K_{is}

x_1 = [substrate] (independent variable 1)

x_2 = [inhibitor] (independent variable 2)

Y = velocity

- Enter data in two columns in the order x_1 , Y (paste from excel or sigmaplot)
- Enter initial guesses for parameters a and b (V_{max} and K_m)
- Click “iterate” once for each iteration cycle. Continue to click “iterate” until the values converge at a constant value. The values of V_{max} and K_m from will replace your initial guesses in 7a and 7b. $a \text{ (or } p_1) = 10.31581092113 \pm 0.084894623150$, the fit
- Seven columns of data were generated by the $b \text{ (or } p_2) = 3.175900437348 \pm 0.093749889829$, fit. Columns 1-2 are the experimental data (x_1 , Y). Column 3 contains the predicted velocity values from the curve fit. Columns 4-7 contain additional statistical data.
- Copy and paste the data generated into a basic text editing program (e.g. wordpad on PC, textedit on mac). Save the data as a .txt file. Open the .txt file in excel. Choose “delimited”, then “space delimited”. Click OK and finish. Add a row above the data to type in the headings. Save the file as an excel spreadsheet or csv file.
- The data in the first three rows are important for making your graphs (v_{expt} and v_{theor} vs. S, and corresponding inverse plots). Graph the data with your program of choice.
- Example data below:

[S]	v expt	v theor	v (expt-theor)	std error	v low	v high
0.25	0.7	0.7528	-0.0528	0.0158	0.7177	0.7879
1	2.32	2.4703	-0.1503	0.0399	2.3813	2.5593
2	4.14	3.9861	0.1539	0.0481	3.8789	4.0933
3	4.91	5.011	-0.101	0.0471	4.9059	5.1161
4	5.83	5.7503	0.0797	0.0438	5.6526	5.8479
5	6.41	6.3087	0.1013	0.0404	6.2188	6.3986
7	7.01	7.0962	-0.0862	0.0358	7.0165	7.176
10	7.72	7.8293	-0.1093	0.0352	7.751	7.9076
15	8.63	8.5133	0.1167	0.041	8.422	8.6046
20	8.92	8.9022	0.0178	0.0473	8.7967	9.0076
25	9.15	9.153	-0.003	0.0525	9.0361	9.27
30	9.28	9.3283	-0.0483	0.0565	9.2023	9.4542

Competitive inhibition:

Number of data points = (varies for data)

number of independent variables = 2 (x1, x2)

number of parameters = 3 (a, b, c)

Formula: $Y = a \cdot x_1 / (b \cdot (1 + x_2/c) + x_1)$

a = Vmax

b = Km

c = Kis

x1 = [substrate] (independent variable 1)

x2 = [inhibitor] (independent variable 2)

Y = velocity

- Enter data in three columns in the order x1, x2, Y (paste from excel or sigmaplot)
- Enter initial guesses for parameters a, b, and c
- Click “iterate” once for each iteration cycle. Continue to click “iterate” until the values converge at a constant value.
- Eight columns of data were generated by the fit. Columns 1-3 are the experimental data (x1, x2, Y). Column 4 contains the predicted velocity values from the curve fit. Columns 5-8 contain additional statistical data.
- Copy and paste the data generated into a basic text editing program (e.g. wordpad on PC, textedit on mac). Save the data as a .txt file. Open the .txt file in excel. Choose “delimited”, then “space delimited”. Click OK and finish. Deleted the data in columns 5-8. Resave the file as a csv or excel file.
- The experimental data should be plotted as data points (symbols) on a scatter plot. The predicted values should be plotted as a smoothed line and without displaying the predicted data points.

Sample data:

0.0000	0.0000	0.0000
0.2500	0.0000	2.9066
0.5000	0.0000	6.0368
0.7500	0.0000	8.8317
1.2500	0.0000	11.5147
2.5000	0.0000	18.5577
5.0000	0.0000	27.2775
7.5000	0.0000	32.4200
10.0000	0.0000	31.0785
0.5000	0.0750	2.7432
0.7500	0.0750	3.7408
1.2500	0.0750	5.8605
2.5000	0.0750	8.3544
5.0000	0.0750	15.0878
7.5000	0.0750	20.2002
10.0000	0.0750	24.1903
0.5000	0.1250	1.8863
0.7500	0.1250	2.8294
1.2500	0.1250	3.8904
2.5000	0.1250	6.7198
5.0000	0.1250	11.6712
7.5000	0.1250	16.3868
10.0000	0.1250	19.3341
1.2500	0.2500	2.3531
2.5000	0.2500	4.3140
5.0000	0.2500	7.9743
7.5000	0.2500	10.0659
10.0000	0.2500	13.9877

	Coefficient	Std. Error
Vmax	44.0879	1.4195
Km	3.2777	0.2675
Ki	0.0422	0.0027

Sequential bisubstrate:

Number of data points = (varies for data)

number of independent variables = 2 (x1, x2)

number of parameters = 4 (a, b, c, d)

Formula: $Y = a \cdot x_1 \cdot x_2 / (d + c \cdot x_1 + b \cdot x_2 + x_1 \cdot x_2)$

a = Vmax

b = Kma

c = Kmb

d = Kia

x1 = [substrate 1] (independent variable 1)

x2 = [substrate 2] (independent variable 2)

Y = velocity

Example data:

0.3000 0.0738 8.0520

0.3000 0.1642 11.9680

0.3000 0.3493 15.9980

0.3000 0.6430 18.3740

0.3000 1.0105 19.8820

0.7000 0.0738 12.0390

0.7000 0.1642 17.0890

0.7000 0.3493 22.7320

0.7000 0.6430 27.5490

0.7000 1.0105 29.4900

1.5000 0.0738 16.1990

1.5000 0.1642 23.5827

1.5000 0.3493 29.5530

1.5000 0.6430 34.5370

1.5000 1.0105 36.4190

3.0000 0.0738 18.1830

3.0000 0.1642 27.2560

3.0000 0.3493 34.0350

3.0000 0.6430 39.2700

3.0000 1.0105 41.5810

4.5000 0.0738 20.3120

4.5000 0.1642 30.5370

4.5000 0.3493 38.6740

4.5000 0.6430 44.1600

4.5000 1.0105 46.9240

Sigmatplot: $f = V_{\max} \cdot A \cdot B / (K_{ia} \cdot K_{mb} + K_{mb} \cdot A + K_{ma} \cdot B + A \cdot B)$

Results from sigmaplot:

Kmb	0.1067	0.0117
Kma	0.4634	0.0516
Kia	0.7773	0.2066
Vmax	55.0103	1.4516

Ping pong bisubstrate:

Number of data points = (varies for data)

number of independent variables = 2 (x_1 , x_2)

number of parameters = 3 (a , b , c)

Formula: $Y = a \cdot x_1 \cdot x_2 / (b \cdot x_2 + c \cdot x_1 + x_1 \cdot x_2)$

$a = V_{\max}$

$b = K_{ma}$

$c = K_{mb}$

x_1 = [substrate] (independent variable 1)

x_2 = [inhibitor] (independent variable 2)

Y = velocity

Example data:

0.2	0.025	8.6
0.25	0.025	9.2
0.333	0.025	9.9
0.5	0.025	10.6
1	0.025	11.7
2	0.025	12.2
2.5	0.025	12.3
3.33	0.025	12.42
4	0.025	12.44
5	0.025	12.5
0.2	0.05	12.2
0.25	0.05	13.5
0.333	0.05	15.1
0.5	0.05	17.1
1	0.05	19.75
2	0.05	21.3
2.5	0.05	21.75
3.33	0.05	22
4	0.05	22.2
5	0.05	22.5
0.2	0.1	15.6
0.25	0.1	17.8
0.333	0.1	20.6
0.5	0.1	25.55
1	0.1	30.3
2	0.1	34.2
2.5	0.1	35.1
3.33	0.1	36.1
4	0.1	36.6
5	0.1	37.2
0.2	0.25	18.8
0.25	0.25	22

0.333	0.25	26.4
0.5	0.25	33.2
1	0.25	44.5
2	0.25	53.75
2.5	0.25	56
3.33	0.25	58.6
4	0.25	59.9
5	0.25	61.3
0.2	0.5	20.1
0.25	0.5	23.8
0.333	0.5	29.1
0.5	0.5	37.5
1	0.5	52.8
2	0.5	66.3
2.5	0.5	69.8
3.33	0.5	73.9
4	0.5	76
5	0.5	78.3