Baritwiga Banuna PS4 CHEME 7770
Saturday, December 21, 2019 3:05 PM

Problem 1

(1) $\frac{d[R^*]}{dt} = k_{on}[R][L] - k_{off}[R^*]$ (2) $\frac{d[X^*]}{dt} = -\frac{d[X^*]}{dt} = \frac{V_1[X]}{K_1+[X]} - \frac{V_2[X^*]}{K_2+[X^*]}$

(3) $\frac{d[Y^*]}{dt} = -\frac{d[Y]}{dt} = \frac{V_3[Y]}{K_3+[Y]} - \frac{V_4[Y^*]}{K_4+[Y^*]}$ $V_1 = \gamma_1[R^*]$ $V_3 = \gamma_3[X^*]$

(4) $R_T = [R]+[R^*]$ (5) $X_T = [X]+[X^*]$ (6) $Y_T = [Y]+[Y^*]$

a) SS solution y^* $d/dt \Rightarrow 0$

$0 = k_{on}[R][L] - k_{off}[R^*]$ $\frac{k_{on}[L]}{k_{off}}[R] = [R^*]$ $\frac{1}{K_D}(R_T - [R^*]) = [R^*]$

$\div R_T \Rightarrow \frac{1}{K_D}(1-\theta_b) = \theta_b$

$0 = \frac{V_1[X]}{K_1+[X]} - \frac{V_2[X^*]}{K_2+[X^*]}$ $\frac{V_1[X]}{K_1+[X]} = \frac{V_2[X^*]}{K_2+[X^*]}$ $V_2[X^*](K_1+[X]) = V_1[X](K_2+[X^*])$

$\frac{V_1}{V_2} = \frac{[X^*](K_1+[X])}{[X](K_2+[X^*])} = \underbrace{\frac{\gamma_1[R^*]}{V_2}}_{1/R_T} = \frac{\gamma_1\theta_b(R_T)}{V_2}$

$\frac{[X^*](K_1+X_T-[X^*])}{(X_T-[X^*])(K_2+[X^*])} \underbrace{=}_{1/X_T^2} \frac{x^*(\mathcal{K}_1+1-x^*)}{(1-x^*)(\mathcal{K}_2+x^*)}$

Eqn 3 is the same form $\Rightarrow \frac{V_3}{V_4} = \frac{y^*(\mathcal{K}_3+1-y^*)}{(1-y^*)(\mathcal{K}_4+y^*)} = \frac{\gamma_3[X^*]}{V_4} = \frac{\gamma_3 x^*}{V_4} X_T$

We want the soln to y^*, however due to the complexity of the eqns they will not be solved for explicitly. Eqn (2) can be written as a quadratic function of which the soln is of the form: $\frac{-b \pm \sqrt{b^2-4ac}}{2a}$ and solved for x^*. This value is then input into Eqn (3) which is also a quadratic and can now be solved for y^*. θ_b from Eqn (1) has an [L] dependency so x^* is a function of [L] and y^* inherits this dependency.

b) & c)

① b Plot vs. $1/\kappa_d$ + fitting $\kappa = 0.1$ & $\kappa = 10$

Curve Fitting Tool

File Fit View Tools Desktop Window Help

untitled fit 1 | untitled fit 2 | untitled fit 3 | untitled fit 4 | untitled fit 5

Fit name: untitled fit 5
X data: KD
Y data: theta
Z data: (none)
Weights: (none)

Custom Equation
y = f(x)
= (A*(x^n))/((x^n)+(C^n))

Fit Options... Auto fit Fit Stop

Results

General model:
f(x) = (A*(x^n))/((x^n)+(C^n))
Coefficients (with 95% confidence bounds):
A = 1 (1, 1)
C = 1 (1, 1)
n = 1 (1, 1)

Goodness of fit:
SSE: 4.168e-21
R-square: 1
Adjusted R-square: 1
RMSE: 2.042e-13

$n = 1$

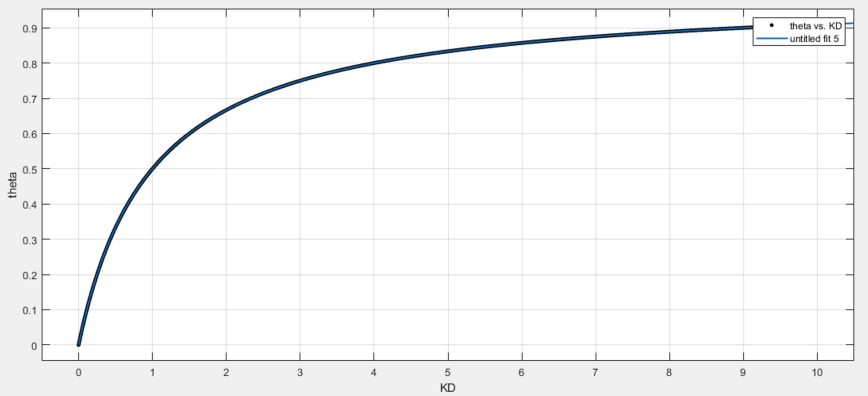


Table of Fits

Fit name	Data	Fit type	SSE	R-square	DFE	Adj R-sq	RMSE	# Coeff	Validation Data	Validation SSE	Validation RMSE
untitled fit 1	x1 vs. KD	(A*(x^n))/((x^n)+(C^n))	8.0721	0.9955	99997	0.9955	0.0090	3			
untitled fit 2	y3 vs. KD	(A*(x^n))/((x^n)+(C^n))	1.5691	0.9985	99997	0.9985	0.0040	3			
untitled fit 3	Xx1 vs. KD	(A*(x^n))/((x^n)+(C^n))	0.0033	1.0000	99997	1.0000	1.8290e-04	3			
untitled fit 4	Yy3 vs. KD	(A*(x^n))/((x^n)+(C^n))	0.0012	1.0000	99997	1.0000	1.0802e-04	3			
untitled fit 5	theta vs. KD	(A*(x^n))/((x^n)+(C^n))	4.1677e-21	1	99997	1	2.0415e-13	3			

x^* plot vs. $1/\kappa_d$ + fitting $\kappa = 0.1$

Curve Fitting Tool

File Fit View Tools Desktop Window Help

untitled fit 1 | untitled fit 2 | untitled fit 3 | untitled fit 4 | untitled fit 5

Fit name: untitled fit 1
X data: KD
Y data: x1
Z data: (none)
Weights: (none)

Custom Equation
y = f(x)
= (A*(x^n))/((x^n)+(C^n))

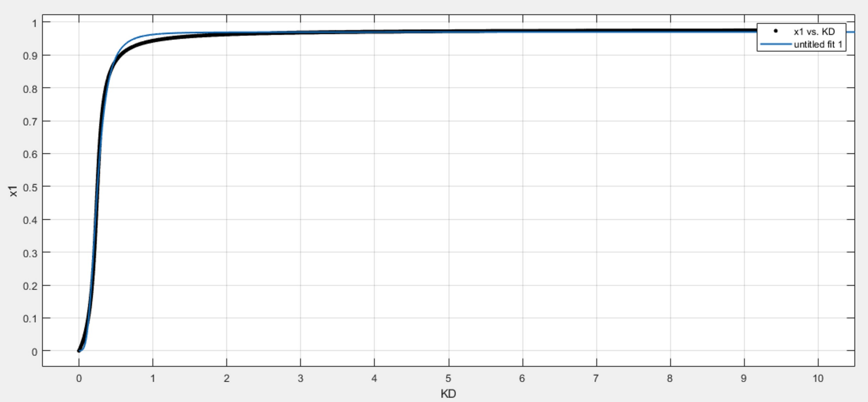
Fit Options... Auto fit Fit Stop

Results

General model:
f(x) = (A*(x^n))/((x^n)+(C^n))
Coefficients (with 95% confidence bounds):
A = 0.9698 (0.9697, 0.9698)
C = 0.2452 (0.2451, 0.2453)
n = 3.451 (3.447, 3.456)

Goodness of fit:
SSE: 8.072
R-square: 0.9955
Adjusted R-square: 0.9955
RMSE: 0.008985

$n = 3.451$



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untitled fit 5	theta vs. KD	(A*(x^n))/((x^n)+(C^n))	4.1677e-21	1	99997	1	2.0415e-13	3			

y^* plot vs. $1/\kappa a$ + fitting $\kappa = 0.1$

Curve Fitting Tool

Fit name: untitled fit 2

X data: KD

Y data: y3

Z data: (none)

Weights: (none)

Custom Equation

y = f(x)

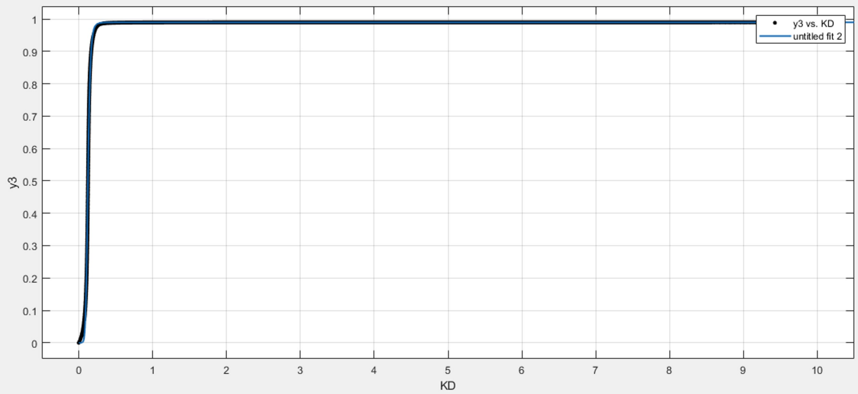
= (A*(x^n))/((x^n)+(C^n))

Results

General model:
f(x) = (A*(x^n))/((x^n)+(C^n))
Coefficients (with 95% confidence bounds):
A = 0.9895 (0.9895, 0.9895)
C = 0.1238 (0.1237, 0.1238)
n = 7.597 (7.587, 7.607)

Goodness of fit:
SSE: 1.569
R-square: 0.9985
Adjusted R-square: 0.9985
RMSE: 0.003961

$n = 7.597$



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x^* vs. $1/\kappa a$ + fitting $\kappa = 10$

Curve Fitting Tool

Fit name: untitled fit 3

X data: KD

Y data: Xx1

Z data: (none)

Weights: (none)

Custom Equation

y = f(x)

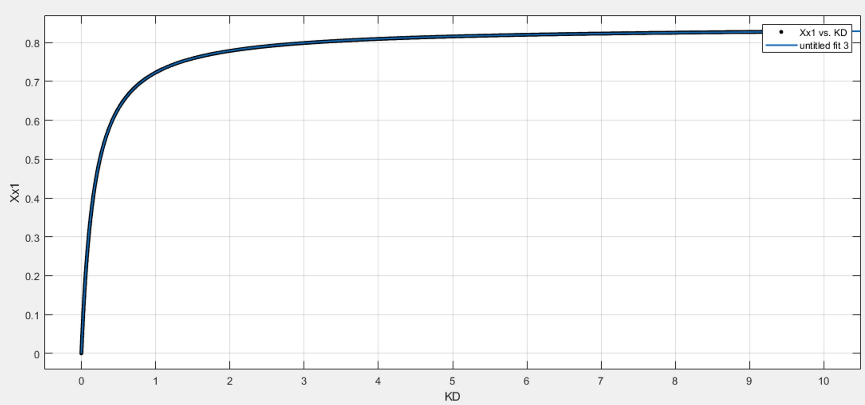
= (A*(x^n))/((x^n)+(C^n))

Results

General model:
f(x) = (A*(x^n))/((x^n)+(C^n))
Coefficients (with 95% confidence bounds):
A = 0.8412 (0.8412, 0.8412)
C = 0.1726 (0.1726, 0.1726)
n = 1.03 (1.03, 1.03)

Goodness of fit:
SSE: 0.003345
R-square: 1
Adjusted R-square: 1
RMSE: 0.0001829

$n = 1.03$



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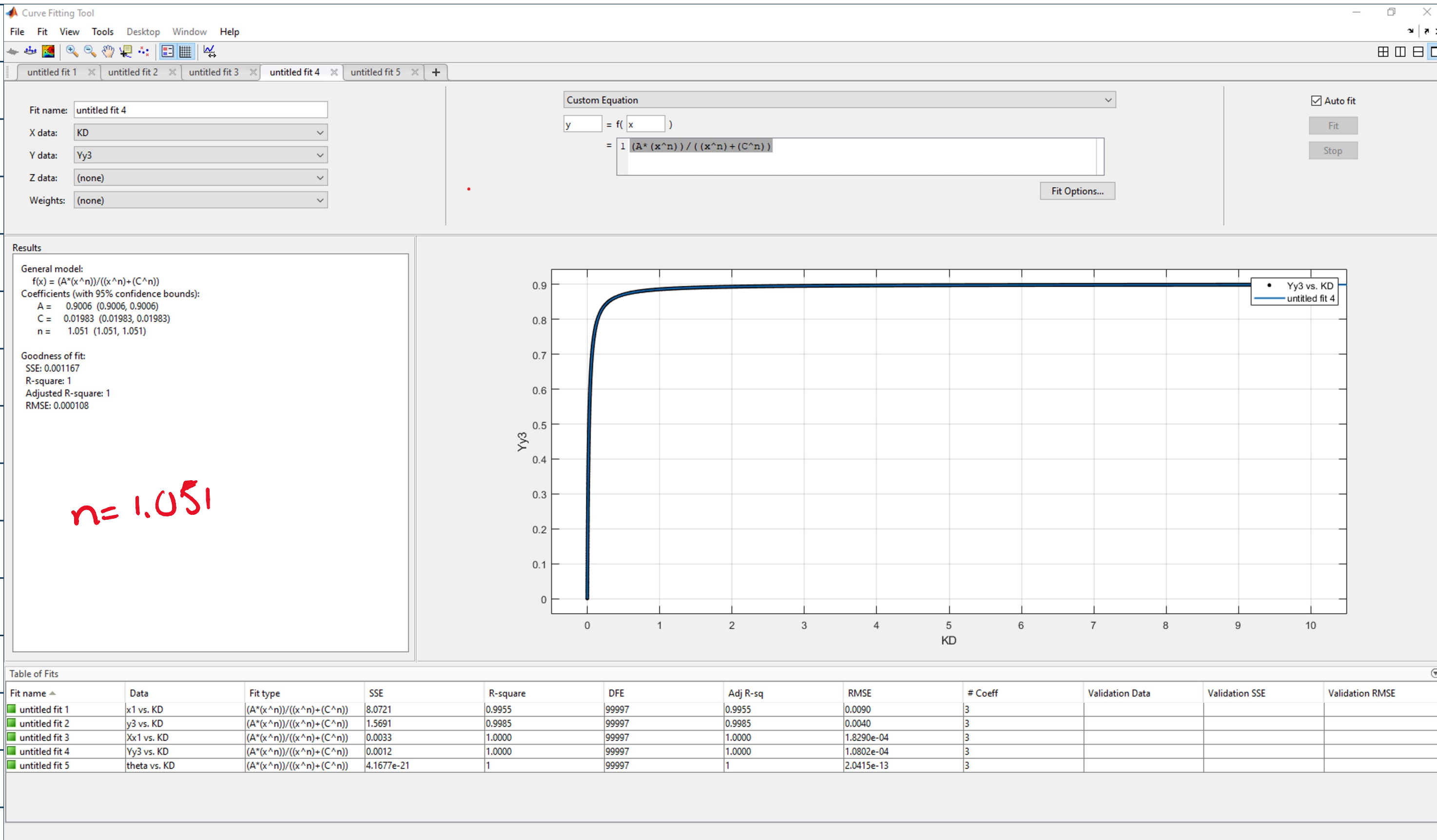
y^* vs. $1/\kappa a$ + fitting $\kappa = 10$

Curve Fitting Tool



$n = 1.051$

d) Matlab Code Output

>> PS4_Problem_1_percentchange

Output of MATLAB code for percent change. Uppercase represent values for K = 10 and lowercase K = 0.1

per_theta =

43.4783

per_x1 =

0

per_y3 =

0

Per_theta =

43.4783

Per_x1 =

Formula Used:

$$\frac{\text{final} - \text{initial}}{\text{initial}} \times 100\% = \%\ \text{change}$$

-77.1421

Per_y3 =

-78.4281

>>

e) In a system $\begin{tikzcd} Y \arrow[r, bend left, "R"] & Y^* \arrow[l, bend left, "L"] \end{tikzcd}$ output output or input amplification is heighted if

the system is a zero order ultrasensitive system ($K \ll 1$) and the system operates at saturation. This allows tuning for ultrasensitive response to small input results in a large change in output