

## Dugga 1, TSRT17, 2013-01-23

Each question gives 3 points. 7 points are required to pass. You have approx. 45 min.

1) Consider the following model, in state-space form

$$d/dt(x_1) = -k_1*x_1 - k_2*x_1 + k_3$$

$$y(t,p) = k_y*x_1$$

$$x_1(0) = x_0$$

a) What are the states?

ANSWER:  $x_1$

COMMON MISTAKES: to answer  $d/dt(x_1)$ , or the entire equation.

b) What are the parameters?

ANSWER:  $p = (k_1, k_2, k_3, x_0, k_y)$

COMMON MISTAKES: to forget  $x_0$  or  $k_y$ .

c) What are the reactions?

ANSWER: The reactions are:

R1:  $x_1 \Rightarrow$  (corresponding to  $k_1$ )      R2:  $x_1 \Rightarrow$  (corresponding to  $k_2$ ),      R3:  $\Rightarrow x_1$  (corr to  $k_3$ )

2) Consider the following set of reactions:

(R1)  $A \Rightarrow B$

(R2)  $B \Rightarrow A$

(R3)  $A \Rightarrow$

a) What are the differential equations? Assume mass action kinetics for R1 and R3, and Michaelis-Menten kinetics for R2. Don't forget to specify the initial conditions. Specify some values for any parameters you might introduce.

ANSWER:

$$v_1 = k_1[A], v_2 = V_{\max}[B]/(K_m + [B]), v_3 = k_3[A]$$

$$d/dt([A]) = -v_1 - v_3 + v_2$$

$$d/dt([B]) = v_1 - v_2$$

$$[A](0) = [B](0) = 2; \text{ (initial conditions, arbitrary values)}$$

$$k_1 = V_{\max} = K_m = k_3 = 0.5$$

COMMON MISTAKES: To forget to give values to some of the parameters, especially the Michaelis-Menten parameters. Another common mistake is to write the equations with only mass action kinetics first, and then to change it. This is not wrong, if the second version is correct, but it is unnecessary in this situation (since you are not asked to change the kinetics).

- b) Add a measurement equation saying that you can measure something that is proportional to the sum of A and B.

ANSWER:

$$y(t,p) = k_y([A] + [B])$$

COMMON MISTAKE: to forget  $k_y$

- 3) Cost functions

- a) What is the input and output of a cost function?

ANSWER: Input: parameters. Output a cost, specifying the overall agreement between the model and the data for those parameters

- b) What are the residuals, and how do they relate to the cost function?

ANSWER: A residual is the distance between a single data point and the corresponding model simulation. A common way to get the cost function is to sum residuals together, after they have been squared, and normalized with the standard deviation of the noise.

- c) Why is the standard deviation of the measurement noise used in the expression of the cost function?

ANSWER: The standard deviation of the measurement noise is used to weigh different residuals according to how well-determined the data points are; a more well-determined data point gets a higher weight than a poorly determined data point, for the same residual.

Good luck!

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