Dugga A 2019

TBMT37 / TBMT19

Please, write your Dugga-ID on all pages and your answers in Swedish or English. You need 12/15 points to pass.
Good luck! /Elin & Gunnar

1 Model formulation

Consider the following model

$$\begin{aligned} [\dot{A}] &= -k1[A] + k3[C] & [A](0) &= 1 & \hat{y} &= ky([A] + [C]) \\ [\dot{B}] &= -k2[B] + k1[A] & [B](0) &= 0 \\ [\dot{C}] &= -k3[C] + k2[B] & [C](0) &= 0 \end{aligned}$$

(a) List all model states! (1 point)

(b) List all model parameters! (1 point)

(c) What can be measured? Explain in words. (1 point)

2 Model simulation and cost function

Consider the following model

$$\begin{aligned} [\dot{A}] &= -k1[A] + k2 & k1 &= 1 \\ [A](0) &= 3 & k2 &= 2 \end{aligned}$$

(a) Calculate $[A](0.5)$ with one step of Euler forward. (1 point)

(b) What are the reactions? (1 point)

(c) What do you need to compute the value of a cost function? (1 point)

3 Model formulation

Consider the following reactions

$$A + B \rightarrow C \tag{1}$$

$$C \rightarrow \varnothing \tag{2}$$

(a) Write down the differential equations that corresponds to these reactions. Assume mass action kinetics for reaction 1 and assume that reaction 2 is saturated with respect to the concentration of C. Introduce parameters and initial conditions with values of your choice. (2 points)

(b) Add a measurement equation. You can measure something that is proportional to the rate of reaction 1. (1 point)

4 Statistical tests

(a) Formulate the null hypothesis underlying a $\chi 2$-test (1 point)

(b) What do you conclude when you reject a likelihood ratio test? (1 point)

(c) What do you conclude when you cannot reject a whiteness test? (1 point)

5 Predictions and experimental design

(a) What is a core prediction? (1 point)

(b) How would you convince an experimental collaborator that core predictions that separate between two hypotheses is useful in the design of a new experiment? (2 points)

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1

(a) $[A], [B], [C]$

(b) $k1, k2, k3, ky, [A](0), [B](0), [C](0)$

(c) The measurement equation, $\hat{y} = ky([A] + [C])$ shows that we can measure something that is proportional to the sum of the concentrations of A and C.

2

(a) $[A](0.5) = [A](0) + [\dot{A}](0)\Delta t = 3 + (-1 * 3 + 2) * 0.5 = 2.5$

(b) $\varnothing \rightarrow A$ and $A \rightarrow \varnothing$

(c) We need data to compute the mean and the standard error of the mean, we need model simulations, i.e. a model structure and a set of parameters to be able to do the simulations.

3

(a)

$$
\begin{aligned}
[\dot{A}] &= -k1[A][B] & [A](0) &= 1 \\
[\dot{B}] &= -k1[A][B] & [B](0) &= 2 \\
[\dot{C}] &= \frac{-Vmax[C]}{(Km + [C])} + k1[A][B] & [C](0) &= 0 \\
k1 &= 3, Km = 2, Vmax = 0.1
\end{aligned}
$$

(b) $\hat{y} = ky * k1[A][B]$

4

(a) The model behaves like the biological system that gave rise to the data
or
The residuals between model and data are small compared to the uncertainty of data .

(b) You conclude that one of the models (the model with the lower cost) is better than the other model at explaining the data.

(c) You do not conclude anything when you do not reject the null hypothesis.

5

(a) A core prediction is a uniquely defined prediction of a model property that can be tested experimentally.

(b) The measurement will always provide new knowledge. Regardless of the outcome of the experiment, we would be able to draw at least one of these conclusions: to reject model A, to reject model B, or to reject both models.