

My Dugga-id is:

## Dugga 2, TBMT19/37, 2015-02-06

3 questions, with 3 points each. 7 points needed to pass. You can answer in Swedish and write on both sides of the paper. Don't forget to write name and personal number on all papers you hand in. If you want to know your results from the public results list: also write and remember your Dugga-id.

### 1 Model formulation

Consider the following model:

$$d/dt([glc]) = u_1 + k_{1b}*[Pyr] - k_{1f}*[glc]$$

$$d/dt([Pyr]) = k_{1f}*[glc] - k_{1b}*[Pyr] - k_{out}*[Pyr]$$

$$[glc](0) = 0.5, [Pyr](0) = 1. \quad k_{1f} = 2, \quad k_{1b} = 2.5, \quad k_{out} = 3.$$

$$\hat{y}(t,p) = k_y*[glc] + k_{y2} \quad k_y = 4, \quad k_{y2} = 5$$

- Which are the reactions? (or alternatively: What is the interaction graph?)
- What are the new equations if the  $k_{out}$ -reaction is changed into a Michaelis-Menten expression? Give values to any new parameters that may be introduced.
- How could you describe the  $\hat{y}$ -equation in words; what does it mean?

ANSWER: a)  $\Rightarrow glc \Leftrightarrow Pyr \Rightarrow$

b)  $d/dt([Pyr]) = k_{1f}*[glc] - k_{1b}*[Pyr] - k_{out}*[Pyr]/(K_m + [Pyr])$  and  $K_m = 8.79$

c) you can measure something that depends linearly on the concentration of glucose, i.e. there is an offset  $k_{y2}$ , and a scaling constant  $k_y$

### 2. Statistical tests

- Name at least one benefit of testing a model with respect to independent validation data.
- What is the null-hypothesis of a whiteness test? What do you conclude if it is not rejected?
- What do you conclude if you reject a likelihood ratio test?

ANSWER:

- You can more easily identify overfitting
- That the residuals are uncorrelated. If you reject the test, the residuals are correlated, and the model should be rejected/improved
- That the model that has a lower cost is significantly better, even when accounting for the difference in complexity

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### 3. Closing the loop

a) You have a well-determined prediction in a model M1, the concentration of A at  $t=20$  lies in the range 3.5-4.5. The same prediction  $A(20)$  for another model M2 is  $A(20) = 20$ , but we do not yet know the uncertainty. Is this a reason to measure A at time  $t=20$ ? Do we know that the experiment will give us something? Motivate your answer.

b) Does the situation in A improve if we also know the uncertainty of the model M2? Can we then guarantee to conclude something more from the experiment? If you answer yes, give a scenario when this is the case.

c) For model M1, you have another prediction, of the reaction rate  $v_2$ , at time point  $t=20$ . This prediction, however, is very uncertain, more than that of many other predictions. How could that uncertainty be a reason to measure this rate at this time point?

ANSWER: a) Yes, you can use the experiment to test if M1 is good, since there is a scenario when M1 will be rejected: if the data lies outside of the 3.5-4.5 region

b) Yes, if the uncertainty of the prediction for M2 lies further away from the 3.5-4.5 region than the measurement uncertainty, you can guarantee that the proposed experiment will be able to discriminate between the models

c) Measuring  $v_2(20)$  would be good if the objective is to optimally identify the uncertain parameters in the model