Dugga 1, TBMT19 and TBMT37, 2015-01-30

3 questions, with 3 points each. 7 points needed to pass. You can answer in Swedish or English, and write on both sides of the paper. Name, personal number, and Dugga-id on all papers you hand in!

1 Model components

Consider the following model

d/dt([A]) = u1 – k1*[A] – k2*[A]

d/dt([B]) = k2*[A]

[A](0) = 0.5, [B](0) = 1, k1 = 4, k2 = 3

yhat(t,p) = ky*[B]/(Km_y + [B])   ky=4, Km_y = 5

a) What are the reaction rates? b) What are the states? c) Describe the yhat-equation, what does it mean? (if you can: also describe the actual functional relationship it describes)

2 Model formulation

Consider the following reactions

(R1) E=>G   and (R2) E + G => Ø

a) Write up the differential equations. Assume that R1 has a saturation with respect to E and that R2 is governed by mass action kinetics. Don't forget to specify the initial conditions, and to give values to any parameters you may introduce.

b) Extend the model so that it describes that you can measure the rate of R2 times an unknown scaling parameter.

3) Cost function and simulation

a) What is the principle behind numerical integration of ordinary differential equations?

b) Consider the model from question 1. What is the value of B(0.1) if you take one Euler forward step to get there.

c) Consider again the model from question 1. What are the inputs and outputs of that model?

Good luck! //Gunnar

ANSWERS

1a) v1 = u, v2 = k1*[A], v3 = k2*[A]

Common mistake: to forget v1 = u (gave 0.5p deduction)

b) [A], [B]

Common mistake: to write A and B (this time, that gave no reduction in points)

c) ½ point if you say that it describes what we can measure, the other ½ point if you also say that the measurement measures [B], but with a saturation that means that the signal never goes beyond ky, independently of how big [B] becomes.

Common mistake: to say that you measure a reaction rate (it is just an expression with a saturation) without also explaining that this – if so – has to be of a reaction outside of the given model

2

a) v1 = Vmax*[E]/(Km + [E]), v2 = k2*[E]*[G]

d[E]/dt = -v1 – v2

d[G]/dt = +v1 – v2

E(0) = 1, G(0) = 0, Vmax=Km=k2 = 8

Common mistakes:

To write an ODE which starts d/dt([E] + [G]) = ….

To write v2 = k2*([E] + [G])

To not use the same expression for v2 in the two ODEs

etc

b) Add yhat = ky*v2 and ky = 4

Common mistake: to simplify and write yhat = ky*v2 = ky*k2*[E][G] = ky*[E][G] (1/2 point deduction) Then an increase in k2 does not increase yhat, which it should!

3

a) Go with the flow. I.e. start at the initial condition, calculate the derivative, take a small step in this direction, re-calculate the derivative, take another small step, and so on

Common mistakes: many different types of mistakes. However, if you answered b) correctly, and showed the calculations, you got full points anyway, because this contains the principle

b) B(0.1) = B(0) + d/dt(B)(0)*h = 1 + 3*0.5*0.1 = 1.15

c) input u, output yhat.

Common mistakes: to write the input/output of the cost function. To write that parameters are inputs. To write that the states are output. Etc.