Dugga1 , January 26, 2012

Each question gives 3p. 7p are needed to pass. For all sub-questions, there is a one-sentence answer that gives full points, but you can use longer answers if you want. 25 minutes. Good luck!

Gunnar

1) Consider the following small system, which has been described by mass action kinetics, according to normal conventions.

d/dt(x1) = -k1*x1 -k2*x1
d/dt(x2) = k2*x1

yhat(t,p) = ky*x1

x1(0) = 2, x2(0) = 3

k1 = 1, k2 = 2,
ky = 3

a) Which are the states?
b) Which are the parameters?
c) What is the interaction graph (i.e. which are the reactions) underlying this system?

2) Consider again the example above.
a) What is the simulated measurement signal at t = 0?

Assume that there are two measured values y(0) = 3, y(0.1) = 2
b) What is the residual at t = 0.1 if you use an Euler forward, with time-step h=0.1?

Assume that one of the reactions is saturated
c) Write down the new equations

3)
a) What is the input and output of a cost function, and what does it do?
b) How may an optimization algorithm help you to get parameter values?
c) What is the difference between a local and a global optimization algorithm?

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1)

a) x1, x2

b) k1,k2,ky

c)

X1 => (k1)

X1 => X2 (k2)

2)

a) yhat(0,p0) = 3*2 = 6

b) x1(0.1) = x1(0) +h*d/dt(x1)(0) = 2 + 0.1*(-1*2 - 2*2) = 2 - 0.6 = 1.4

=> residual(0.1) = y(0.1) - yhat(0.1) = 2 - 3*1.4 = -2.2

c) d/dt(x1) = - k1*(x1/(km + x1)) – k2*x1

d/dt(x2) = k2*x1

3)

a) Input to the cost function is a parameter set and output the “cost”, which is a calculation of the error between simulation data using the specified parameter set and measured data.

b) An optimization algorithm can help finding optimal parameters where the cost is minimized, i.e. where the agreement between the data and simulations is as small as possible

c) Local optimization is unable to “cross” areas of high cost (and may therefore miss the global minimum) which global optimizations are able to do; global optimization are however slower.