Metabolic and regulatory networks

Computer practical course

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Day 1

Exercice 1

$$v = \frac{v_{\max} \cdot S}{(K_m + S)(1 + \frac{S}{K_i})}$$

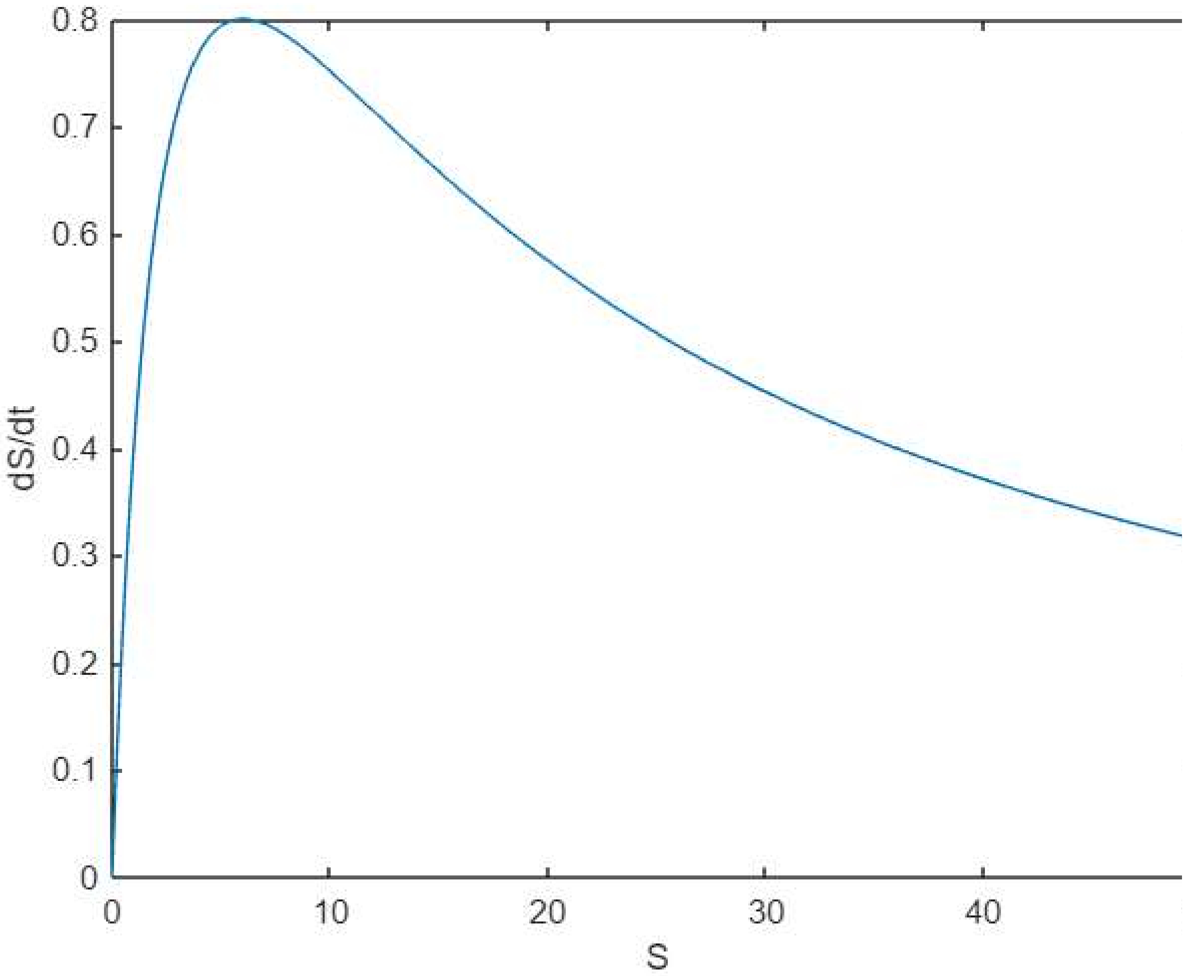
```
% Defining symbols
syms v(S) vmax S Km Ki

% Excluding negative values for S since negative concentrations are
% biologically irrelevant
assume(S >= 0)

% Defining the differential equation
v(S) = (vmax*S)/((Km+S)*(1+S/Ki))
```

v(S) =

$$\frac{S\,\mathrm{vmax}}{\left(\frac{S}{\mathrm{Ki}} + 1\right)\,(\mathrm{Km} + S)}$$

a) Plotting for $K_m = 9, v_{\max} = 5, K_i = 4$

```
fplot(subs(v, {Km,vmax,Ki},{9,5,4}), [0,50])
xlabel('S');
ylabel('dS/dt')
```



b) Find S such that $\frac{dS}{dt}$ is maximal for the given parameters

→from the plot it is apparent that there is only one extreme which is the maximum

```
solve(diff(subs(v, {Km,vmax,Ki},{9,5,4})), S)
```

ans = 6

c) Find S such that $\frac{dS}{dt}$ is maximal for any parameters

```
solve(diff(v) == 0, S)
```

Warning: Solutions are only valid under certain conditions. To include parameters and condition

ans = $\sqrt{\mathrm{Ki}\,\mathrm{Km}}$

Exercice 2

a) Perform a regression analysis for hypothtical experimental data by fitting the Michaelis-Menten-equation

```
S_values = [0.100, 0.300, 1.000, 2.000, 2.900, 4.100, 7.000, 10.000]
```

S_values = *1×8*

```
    0.1000    0.3000    1.0000    2.0000    2.9000    4.1000    7.0000   10.0000
```

```
v_values = [0.055, 0.121, 0.240, 0.425, 0.456, 0.522, 0.584,  0.805]
```

```
v_values = 1×8
    0.0550    0.1210    0.2400    0.4250    0.4560    0.5220    0.5840    0.8050
```

Km 2.9063

vmax 0.9402

Goodness of Fit:

R-square 0.9620

b) Perform a linear regression analysis in a Lineweaver-Burk-plot

```
rec_S_values = 1./S_values
```

```
rec_S_values = 1×8
   10.0000    3.3333    1.0000    0.5000    0.3448    0.2439    0.1429    0.1000
```

```
rec_v_values = 1./v_values
```

```
rec_v_values = 1×8
   18.1818    8.2645    4.1667    2.3529    2.1930    1.9157    1.7123    1.2422
```

Km 0.9871

vmax 0.5862

Goodness of Fit

R-square 0.9907

→ We observe huge differences in the resulting values

c) Excliding an outlier

Excluding the last measuring point changes the results the most, so it is the least consistent with the rest of the data

For a):

Km 1.6853

vmax 0.7312

Goodness of Fit

R-square 0.9912

For b):

Km 1.4838

vmax 0.7051

Goodness of Fit

R-square 0.9831