Singular perturbations — enzyme kinetics

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Chemical reaction

- S ... substrate with concentration s,
- E ... enzyme with concentration e,
- C ... complex with concentration c,
- P ... product with concentration p.

Processes at work:

$$S + E \quad \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} \quad C \quad \overset{k_2}{\to} \quad E + P$$

System of equations

Chemical reaction can be modelled by the system

$$\begin{aligned}
\frac{ds}{dt} &= -k_1 se + k_{-1} c, \\
\frac{de}{dt} &= -k_1 se + (k_{-1} + k_2) c, \\
\frac{dc}{dt} &= k_1 se - (k_{-1} + k_2) c, \\
\frac{dp}{dt} &= k_2 c,
\end{aligned}$$

with initial conditions

$$\begin{aligned}
e(0) &= \bar{e} & s(0) &= \bar{s}, \\
c(0) &= 0 & p(0) &= 0.
\end{aligned}$$

Straightforward simplification

- Conservation of enzymes:

$$e + c = e(0) + c(0) = \bar{e}.$$

- Conservation of substrate:

$$s + c + p = s(0) + c(0) + p(0) = \bar{s}.$$

Can explicitly compute

$$\begin{aligned} e(t) &= \bar{e} - c(t), \\ p(t) &= \bar{s} - \bar{e} - s(t) + e(t). \end{aligned}$$

Simplified system

After elimination of e and p, we obtain

$$\begin{aligned}\frac{ds}{dt} &= -k_1\bar{e}s + k_1 sc + k_{-1}c,\\ \frac{dc}{dt} &= k_1\bar{e}s - (k_{-1} + k_2)c - k_1 sc,\end{aligned}$$

with initial conditions

$$s(0) = \bar{s}, \qquad c(0) = 0.$$

Assumption:

- $\bar{e} \ll \bar{s}$ — quantity of enzymes driving the process is much smaller than the quantity of substrate.