Scientific Computing in Python / 2027 Lecture 3

Linear observations and a two-compartment exchange model

Zan Ahmad

Proposed 2027; calendar dates pending

Recovering the initial masses

$$\begin{pmatrix} 1 & 0.2 \\ 0.1 & 1 \end{pmatrix} \begin{pmatrix} m_A(0) \\ m_B(0) \end{pmatrix} = \begin{pmatrix} 8.4 \\ 2.8 \end{pmatrix}.$$

The solution is $(m_A(0), m_B(0)) = (8, 2)$ mg.

The detector determinant

$$\det A = 1 - 0.02 = 0.98.$$

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m0 = np.linalg.solve(A, signal)
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Check Am_0 against the observed signal. Noise sensitivity is a separate question.

Conservative exchange

$$\dot{m}_A = -k(m_A - m_B), \qquad \dot{m}_B = k(m_A - m_B).$$

$$\frac{\mathrm{d}}{\mathrm{d}t}(m_A + m_B) = 0.$$

Conserved and decaying coordinates

Define $M = m_A + m_B$ and $d = m_A - m_B$.

$$\dot{M} = 0, \qquad \dot{d} = -2kd.$$

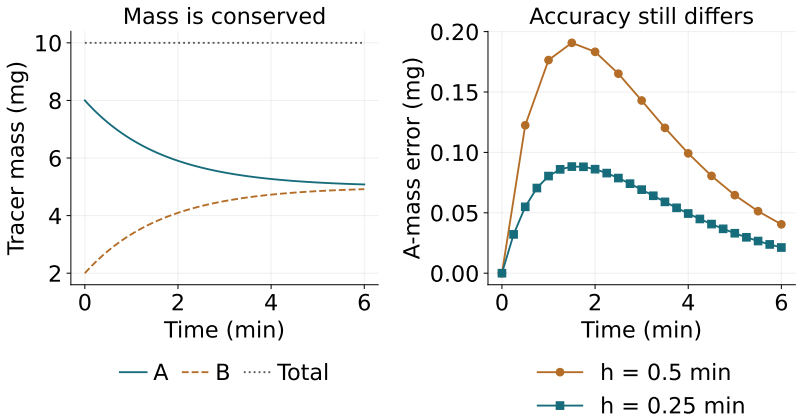
The change of coordinates separates the two modes.

Exact solution

$$M(t) = 10, \qquad d(t) = 6e^{-2kt}.$$

$$m_A(t) = 5 + 3e^{-2kt}, \qquad m_B(t) = 5 - 3e^{-2kt}.$$

Exchange and error



Matrix eigenmodes

$$\dot{m} = k \begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix} m.$$

Eigenvectors $(1, 1)^\mathsf{T}$ and $(1, -1)^\mathsf{T}$ have eigenvalues 0 and $-2k$.

Euler stability and positivity

$$\begin{pmatrix} m_A^{n+1} \\ m_B^{n+1} \end{pmatrix} = \begin{pmatrix} 1-kh & kh \\ kh & 1-kh \end{pmatrix} \begin{pmatrix} m_A^{n} \\ m_B^{n} \end{pmatrix}.$$

Nonnegative coefficients require $0 \le kh \le 1$.

The difference-mode multiplier

$$d_{n+1} = (1 - 2kh)d_n.$$

Decay requires $0 < kh < 1$. Monotone decay requires $0 < kh \leq 1/2$. A conserved total can coexist with an inaccurate or oscillating state.

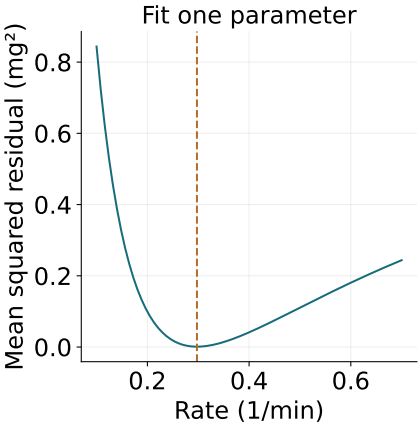
Step refinement

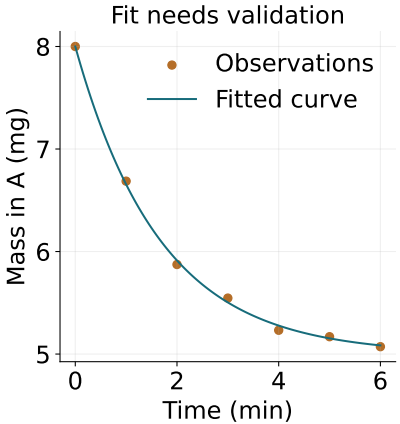
$$\epsilon_M = \max_n |m_A^n + m_B^n - 10|,$$

$$E(h) = \max_n \|m^n - m(t_n)\|_2.$$

For Euler, $E(h) = O(h)$ under ordinary smoothness assumptions.

Parameter evidence





A local truncation calculation

$$e^{-2kh} = 1 - 2kh + 2k^2h^2 + O(h^3).$$

Euler retains only the first two terms. The one-step difference is $O(h^2)$ and the accumulated fixed-time error is $O(h)$.

Estimating the exchange coefficient

$$J(k) = \sum_i [5 + 3e^{-2kt_i} - y_i]^2, \qquad k > 0.$$

$$\partial_k m_A(t; k) = -6te^{-2kt}.$$

Informative observation times

The initial measurement carries no sensitivity to k when the initial state is fixed. Late measurements approach 5 mg for every positive k. The magnitude te^{-2kt} is largest at $t = 1/(2k)$.