Scientific Computing in Python / 2027 Lecture 3

Linear observations and a two-compartment exchange model

Lecture notes

Two equal-volume compartments exchange a conserved substance. Detectors report linear mixtures of the two stored masses. We first recover the initial state from those observations, then derive the exact dynamics, construct Euler's method, and estimate an exchange coefficient from synthetic measurements.

1 Recovering the initial masses

Slides for this section

Let m_A, m_B be stored masses in milligrams. The calibrated detector map mixes them into two signals. Its determinant is nonzero, so the initial masses are identifiable under the assumed calibration. This inverse calculation precedes the dynamical model.

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

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

The detector determinant

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

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

2 Conservative exchange

Slides for this section

For equal-volume, well-mixed compartments, take the net transfer rate from A to B to be $k(m_A - m_B)$. The same transfer appears with opposite signs in the two mass balances. Here k has units of inverse time. This law would require modification if the transfer depended on unequal-volume concentrations.

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

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

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.

3 Exact solution

Slides for this section

The conserved total is $M = 10$ mg and the initial difference is $d(0) = 6$ mg. Solving the scalar decay equation gives both masses. The equilibrium is equal storage, while the difference decays on the time scale $1/(2k)$.

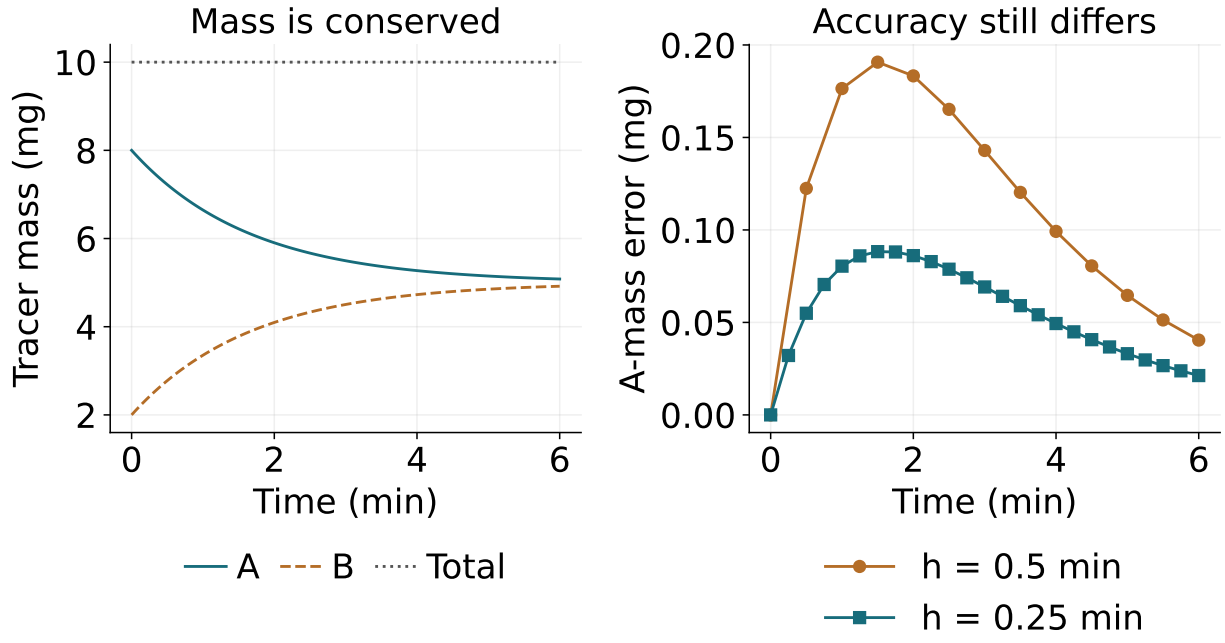
$$M(t) = 10, \qquad d(t) = 6e^{-2kt}.$$

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

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 $-2k$.



The two masses sum to 10 mg. Forward Euler preserves this total for both displayed step sizes, yet the individual-state error is smaller with the finer step.

4 Euler stability and positivity

Slides for this section

Forward Euler preserves the total exactly because the two updates still contain equal and opposite transfers. This conservation says nothing by itself about the accuracy of the difference mode. Positivity of each mass follows when the update is a convex combination of the old masses, giving a step condition that must be examined separately from monotone relaxation.

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

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 $0 < kh \le 1/2$. A conserved total can coexist with an inaccurate or oscillating state.

The companion uses the stricter condition $2kh \le 1$ so the concentration difference decays without sign changes. This monotonicity requirement is stronger than positivity and absolute stability alone.

5 Step refinement

Slides for this section

Compare both numerical state trajectories with the exact solution on a common output grid. A mass residual checks cancellation of transfers. A state error checks approximation of the nonzero eigenmode. The two diagnostics should be reported separately.

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

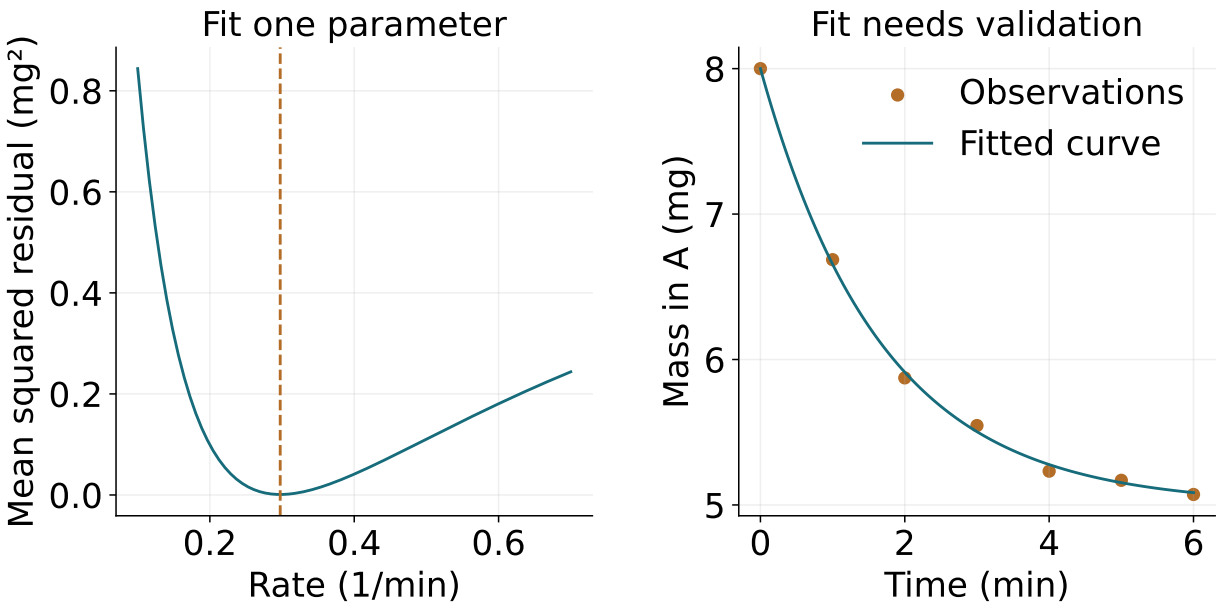
$$E(h) = \max_n \|m^n - m(t_n)\|_2.$$

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

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 $O(h)$.



The fit uses exact model values and seven synthetic perturbed observations of A, keeping parameter residuals separate from numerical integration error. Search bounds are 0.01–1 min^{-1}; the displayed objective window is narrower.

6 Estimating the exchange coefficient

Slides for this section

Suppose only compartment A is observed. With the initial state fixed, fit k by minimizing residuals between the exact model and the measurements. Using the exact formula here keeps parameter-fitting error separate from integration error. Positivity and a declared search interval restrict admissible coefficients.

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

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

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 $t = 1/(2k)$.

Exercises

P27-3-1. Interpret a sensor solve

A new observation map gives readings u=mA+0.5mB and v=mB. Measured readings are (7,4) mg-equivalent. Total: 10 points.
a Recover both masses and substitute them into both channels.

b State the matrix and vector shapes and residual units.

c If both channels instead measure mA+mB, what can and cannot be determined?

P27-3-2. Transfer and a hand step

Two equal-volume reservoirs start at 9 and 3 mg with k=0.2 min^{-1}. Use an Euler step h=0.5 min. Total: 10 points.
a Calculate the initial transfer rate and both derivatives with units.

b Calculate the next Euler state and check total mass.

c Find the difference multiplier and state whether the teaching monotonicity condition holds.

P27-3-3. An invariant is not an accuracy estimate

Two simulations both preserve a 12 mg total. At one time their A-state errors against a known exact solution are 0.4 and 0.1 mg. Total: 10 points.
a What does conservation establish, and what does it fail to establish?

b A coarse step gives the first error and a smaller step gives the second. What bounded conclusion is supported?

c Explain why a library output grid is not necessarily its internal integration grid.

P27-3-4. What does a fitted rate mean?

The model's initial masses are known and unequal. A colleague fits k from observations of A. Total: 10 points.

a Why do repeated observations at time zero fail to determine k?

b Define a mean squared residual objective and give its units when observations are mg.

c Name one numerical verification check and one independent scientific validation observation.

References

Original Python Lecture 3. PDF pages 8–13.
https://zanahmad.com/files/scientific-python/Lecture_3__Intro_to_Python.pdf

Original Python Lecture 4. PDF pages 9–13.
https://zanahmad.com/files/scientific-python/Lecture_4__Intro_to_Python.pdf

SciPy solve_ivp documentation. Initial-value problem, t_eval and error tolerance parameters.
https://docs.scipy.org/doc/scipy/reference/generated/scipy.integrate.solve_ivp.html

SciPy minimize_scalar documentation. Bounded scalar minimization and success result.
https://docs.scipy.org/doc/scipy/reference/generated/scipy.optimize.minimize_scalar.html

Python source materials: Phillip Kerger (2023). Course adaptation and additional exposition: Zan Ahmad.