Scientific Computing in Python Lecture 3

NumPy arrays and linear inverse problems

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The observation matrix

$$y = Ac, \qquad A = \begin{pmatrix} 1 & 0.25 \\ 0.20 & 1.20 \end{pmatrix}, \quad c = \begin{pmatrix} c_A \\ c_B \end{pmatrix}.$$

$$y_1 = c_A + 0.25 c_B, \qquad y_2 = 0.20 c_A + 1.20 c_B.$$

Matrix entries and units

A_{ij} is the response of detector i to one concentration unit of constituent j.

$$[A_{ij}] = \frac{\text{signal}}{\text{concentration}}, \qquad [Ac] = \text{signal}.$$

The row and column meanings are part of the model.

Rows of observations

$$C \in \mathbb{R}^{n \times 2}, \quad A \in \mathbb{R}^{2 \times 2}, \quad Y = CA^{\mathsf{T}} \in \mathbb{R}^{n \times 2}.$$

$$Y_{ri} = \sum_{j=1}^{2} C_{rj} A_{ij}.$$

Array multiplication

```
Y = C @ A.T
```

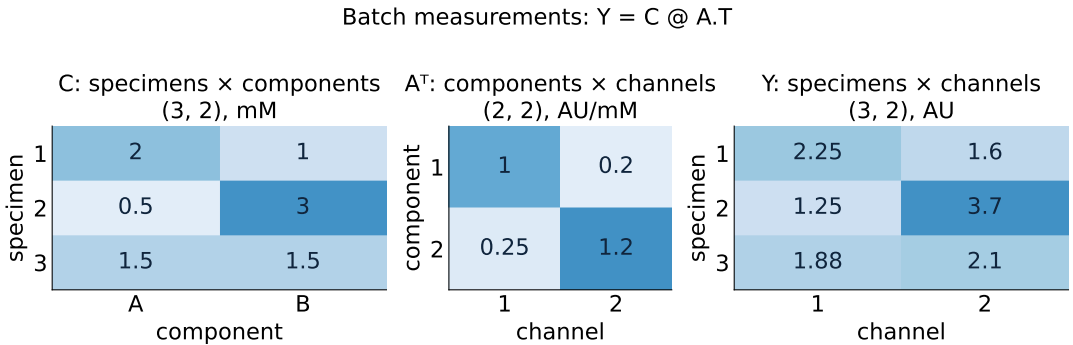
`@` contracts the shared index. Entrywise `C*A` is a different operation and need not even have compatible shapes.

Solving the calibration equations

$$\det A = 1(1.20) - 0.25(0.20) = 1.15 \neq 0.$$

```
c_hat = np.linalg.solve(A, y)
residual = A @ c_hat - y
```

The calibration map



Elimination by hand

Subtract 0.20 times the first detector equation from the second:

$$1.15 c_B = y_2 - 0.20 y_1.$$

Then $c_A = y_1 - 0.25 c_B$. The numerical solve carries out equivalent linear algebra.

Residual and reconstruction error

$$r = A\widehat{c} - y, \qquad e = \widehat{c} - c_{\text{true}}.$$

If $y = Ac_{\text{true}} + \delta y$ and $r = 0$, then

$$Ae = \delta y.$$

A residual scaled to the problem

A dimensionless residual measure is

$$\eta = \frac{\|A\widehat{c} - y\|_2}{\|A\|_2\|\widehat{c}\|_2 + \|y\|_2}.$$

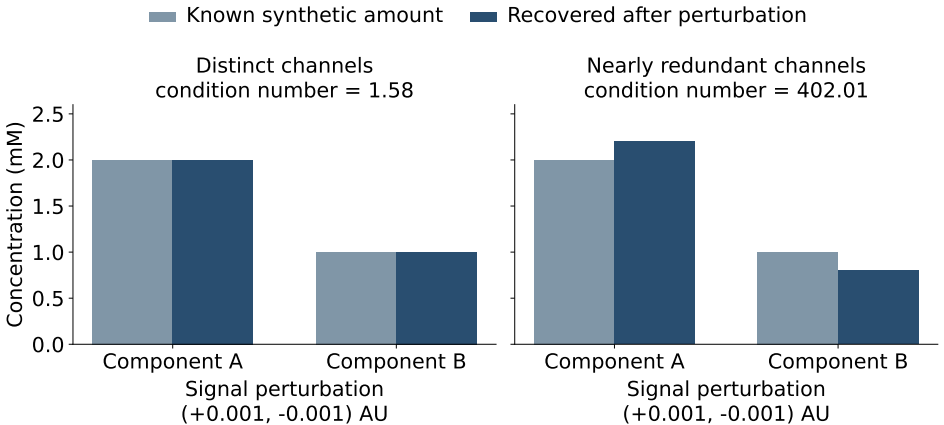
A small η supports the algebraic solve. It does not establish accurate calibration or accurate observations. If both numerator and denominator are zero, report the exact zero residual separately.

Conditioning and redundant detectors

$$\delta c = A^{-1}\delta y, \qquad \frac{\|\delta c\|_2}{\|c\|_2} \leq \kappa_2(A)\frac{\|\delta y\|_2}{\|y\|_2}.$$

The bound assumes A is fixed and nonsingular. This relative bound assumes $c \neq 0$ and $y \neq 0$.

Sensitivity to detector noise



Singular values

If $A = U\Sigma V^{\mathsf{T}}$, then

$$\kappa_2(A) = \frac{\sigma_{\max}}{\sigma_{\min}}.$$

A small $\sigma_{\min}$ identifies a concentration direction that produces little signal.

Batch solves and physical constraints

```
C_hat = np.linalg.solve(A, Y.T).T
```

This solves the same calibrated map for every row of observations.

A constrained alternative

With noisy signals one may instead define

$$\min_{c \geq 0} \|Ac - y\|_2^2.$$

The constraint changes the mathematical problem. Its residual is generally nonzero.