general

Least squares fitting

matrix eq. derivation

Nikki Rider

F2020

general least squares fitting

$$y(x) = \sum_{j=0}^{m-1} a_j f_j(x)$$

example from (d)

$$y(x) = a + bx$$

$$f_0 = 1 \quad , \quad f_1 = x$$

$$a_0 = a \quad , \quad a_1 = b$$

current example

$$y(x) = a + bx + c\sin(x)$$

$$f_0 = 1 \quad , \quad f_1 = x \quad , \quad f_2 = \sin x$$

$$a_0 = a \quad , \quad a_1 = b \quad , \quad a_2 = c$$

$$\frac{\partial}{\partial a_k}\chi^2 = \frac{\partial}{\partial a_k}\sum_{i=0}^{n-1}\left(\frac{y_i - \sum_{j=0}^{m-1} a_j f_j(x_i)}{\sigma_i}\right)^2$$

(24) $$= -2\sum_{i=0}^{n-1}\left(\frac{y_i - \sum_{j=0}^{m-1} a_j f_j(x_i)}{\sigma_i^2}\right) f_k(x_i) \equiv 0$$

for minimum χ^2

define

$$A_{ij} \equiv \frac{f_j(x_i)}{\sigma_i}$$

$$b_i \equiv \frac{y_i}{\sigma_i}$$

$$0 = \sum_{i=0}^{n-1} \left(\frac{y_i - \sum_{j=0}^{m-1} a_j f_j(x_i)}{\sigma_i^2} \right) f_k(x_i)$$

$$= \sum_i \frac{y_i}{\sigma_i} \frac{f_k(x_i)}{\sigma_i} - \sum_i \sum_j a_j \frac{f_j(x_i)}{\sigma_i} \frac{f_k(x_i)}{\sigma_i}$$

$$= \sum_i b_i A_{ik} - \sum_i \sum_j a_j A_{ij} A_{ik}$$

$$= \sum_i A^T_{ki} b_i - \sum_i \sum_j A^T_{ki} A_{ij} a_j$$

notation: i use 2 underlines for a matrix, and 1 for vectors

$$0 = \underline{\underline{A}}^T \underline{b} - \underline{\underline{A}}^T \underline{\underline{A}}\, \underline{a}$$

$$(\underline{\underline{A}}^T \underline{\underline{A}})^{-1} \underline{\underline{A}}^T \underline{\underline{A}}\, \underline{a} = (\underline{\underline{A}}^T \underline{\underline{A}})^{-1} \underline{\underline{A}}^T \underline{b}$$

$$\boxed{\underline{a} = (\underline{\underline{A}}^T \underline{\underline{A}})^{-1} \underline{\underline{A}}^T \underline{b}}$$

```
np.linalg.inv(A)
np.transpose(A)
np.dot(A, B)
np.diagonal(A)
```