Mth 410/510 Inverse Problems & DA

Generalized cross-validation (GCV) method relies on statistical model validation techniques to select the regularization parameter k (TSVD) or λ (Tikhonov).

Ordinary cross-validation

$$\begin{bmatrix} b \end{bmatrix} \nearrow \begin{bmatrix} b_t \end{bmatrix}$$ training data set used to obtain x

$$\begin{bmatrix} b \end{bmatrix} \searrow \begin{bmatrix} b_v \end{bmatrix}$$ validation data set used to assess the model prediction based of x.

$\rightarrow$ denote

$$\left.\begin{aligned} b^{(i)} &= \begin{bmatrix} b_1 \\ \vdots \\ b_{i-1} \\ b_{i+1} \\ \vdots \\ b_m \end{bmatrix} \in \mathbb{R}^{m-1} \\ A^{(i)} &= \begin{bmatrix} A(1,:) \\ \vdots \\ A(i-1,:) \\ A(i+1,:) \\ A(m,:) \end{bmatrix} \in \mathbb{R}^{(m-1)\times n} \end{aligned}\right\} \text{produce regularized solution } x^{(i)}$$

for example, $x_\lambda^{(i)} = \left[A^{(i)T} A^{(i)} + \lambda^2 I_n\right]^{-1} A^{(i)T} b^{(i)}$

then evaluate $\left(A(i,:)\,x_\lambda^{(i)} - b_i\right)^2$

and repeat for all data components, b_i, $i=1:m$.

Choose regularization parameter λ that minimizes the prediction error for all data elements,

$$\min_{\lambda} \frac{1}{m} \sum_{i=1}^{m} \left(A(i,:)\,x_\lambda^{(i)} - b_i\right)^2$$

may be formulated as

$$\min_{\lambda} \frac{1}{m} \sum_{i=1}^{m} \left(\frac{A(i,:)\,x_\lambda - b_i}{1-h_{ii}}\right)^2$$

where $h \in \mathbb{R}^m$

$$h = \operatorname{diag}\left[A(A^T A + \lambda^2 I)^{-1} A^T\right]$$

Has the major drawback that it depends on the ordering of data

The <u>generalized cross validation</u> replaces each h_{ii} with the <u>average</u> of the diagonal elements,

$$\bar{h} = \frac{1}{m} \text{Trace}\left[A(A^T A + \lambda^2 I)^{-1} A^T\right]$$

to obtain the optimality criteria:

$$\min_{\lambda} \frac{1}{m} \sum_{i=1}^{m} \left(\frac{A(i;:)\, x_\lambda - b_i}{1-\bar{h}} \right)^2$$

which is equivalent with

$$\min_{\lambda} \frac{\| A x_\lambda - b \|_2^2}{m(1-\bar{h})^2}$$

Using SVD of A, we may show that

$$\text{Trace}\left[A(A^T A + \lambda^2 I)^{-1} A^T\right] = \sum_{i=1}^{n} f_i(\lambda)$$

filter coefficients for Tikhonov.

The GCV method to select the parameter λ is formulated

Choose $\lambda = \lambda_{GCV}$ as the minimizer to

$$G(\lambda) = \frac{\|Ax_\lambda - b\|_2^2}{\left(m - \sum_{i=1}^{n} f_i(\lambda)\right)^2}$$

$$f_i(\lambda) = \frac{\sigma_i^2}{\sigma_i^2 + \lambda^2}, \quad i = 1:n$$

for the TSVD method, the GCV is formulated

Choose $k = k_{GCV}$ as the minimizer to

$$G(k) = \frac{\|Ax_k - b\|_2^2}{(m-k)^2}$$

→ in practice provides good results if the noise in data is white.