

Generalized singular value decomposition (GSVD)

in the general form of the Tikhonov regularization, the solution $x_{\lambda, L}$ is obtained by minimizing

$$J_{\lambda, L}(x) = \|Ax - b\|_2^2 + \lambda^2 \|L(x - x_0)\|_2^2$$

where $A \in \mathbb{R}^{m \times n}$, $b \in \mathbb{R}^m$, $L \in \mathbb{R}^{p \times n}$
 $x_0 \in \mathbb{R}^n$ is a prior estimate / guess.

We assume $m \geq n \geq p$ and

$$W(A) \cap W(L) = \{0\}$$

Then there is a unique solution $x_{\lambda, L}$ obtained by solving the system

$$(A^T A + \lambda^2 L^T L) x = A^T b + \lambda^2 L^T L x_0$$

For simplicity, we may assume $x_0 = 0$.

The solution $x_{2,L}$ may be expressed as a filtered solution and analyzed using GSVD.

Definition Let $A \in \mathbb{R}^{m \times n}$, $L \in \mathbb{R}^{p \times n}$ such that $m \geq n \geq p$. Assume that $\text{rank}(L) = p$ and $\mathcal{N}(A) \cap \mathcal{N}(L) = \{0\}$.

The generalized singular value decomposition (GSVD) of (A, L) is a decomposition in the form

$$A = U \begin{pmatrix} S & 0 \\ 0 & I_{n-p} \end{pmatrix} X^{-1}$$

$$L = V \begin{pmatrix} M & 0 \end{pmatrix} X^{-1}$$

where $U \in \mathbb{R}^{m \times n}$ and $V \in \mathbb{R}^{p \times p}$ are orthogonal matrices

$$U^T U = I_n, \quad V^T V = I_p$$

$X \in \mathbb{R}^{n \times n}$ is a nonsingular matrix
 $S \in \mathbb{R}^{p \times p}$ and $M \in \mathbb{R}^{p \times p}$ are diagonal matrices

$$S = \text{diag}(\sigma_1, \dots, \sigma_p)$$

$$M = \text{diag}(\mu_1, \dots, \mu_p)$$

where $0 \leq \sigma_1 \leq \dots \leq \sigma_p \leq 1$

$$1 \geq \mu_1 \geq \dots \geq \mu_p > 0$$

satisfy $\sigma_i^2 + \mu_i^2 = 1, \quad i = 1:p$

The generalized singular values δ_i of the pair (A, L) are defined as

$$\delta_i = \frac{\sigma_i}{\mu_i}, \quad i = 1:p$$

Remark: Notice that δ_i are ordered such that

$$0 \leq \delta_1 \leq \dots \leq \delta_p$$

Denoting $U = [u_1 \dots u_n]$

$$V = [v_1 \dots v_p]$$

$$X = [x_1 \dots x_n]$$

we have the following properties :

1) $Ax_i = \sigma_i u_i$, $Lx_i = \mu_i v_i$, $i=1:p$

$$Ax_i = u_i$$
 , $Lx_i = 0$, $i = p+1:n$

in compact form,

$$X^T A^T A X = \begin{pmatrix} S^2 & 0 \\ 0 & \underline{I}_{n-p} \end{pmatrix}$$

$$X^T L^T L X = \begin{pmatrix} M^2 & 0 \\ 0 & 0 \end{pmatrix}$$

2) $A^T A x_i = \delta_i^2 L^T L x_i$, $i=1:p$

such that (δ_i^2, x_i) are generalized eigenpairs to $(A^T A, L^T L)$.

in particular, $(\delta_p, \frac{1}{\mu_p} x_p)$ satisfy

$$\delta_p = \max_{\|Lx\|=1} \|Ax\| = \frac{1}{\mu_p} \|Ax_p\|$$

When L is the identity matrix, $L = I_n$

then U and V in the GSVD are identical with U and V in $\text{svd}(A)$, whereas the generalized singular values of (A, I_n) are the singular values of A in reverse order.

For a general L matrix there is no connection between the generalized singular values/vectors and the ordinary singular values/vectors.

Property Assuming $x_0 = 0$, the solution $x_{\lambda, L}$ to the general form of the Tikhonov regularization is expressed as

$$x_{\lambda, L} = \sum_{i=1}^p f_i(\lambda, L) \frac{u_i^T \cdot b}{\sigma_i} x_i + \sum_{i=p+1}^n (u_i^T \cdot b) x_i$$

where $f_i(\lambda, L)$ are the general-form Tikhonov filter factors given by

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

or equivalently, $f_i(\lambda, L) = \frac{\delta_i^2}{\delta_i^2 + \lambda^2}$

where δ_i are the generalized singular values.

Notice that $f_i(\lambda, L) \approx \begin{cases} 1, & \text{if } \delta_i \gg \lambda \\ 0, & \text{if } \delta_i \ll \lambda \end{cases}$

Proof: For $x_0 = 0$, the solution $x_{\lambda, L}$ is

$$x_{\lambda, L} = (A^T A + \lambda^2 L^T L)^{-1} A^T b$$

Using GSVD of (A, L) we have that

$$A^T A = X^{-T} \begin{bmatrix} S^2 & 0 \\ 0 & I_{n-p} \end{bmatrix} X^{-1} \quad (\text{since } U^T U = I)$$

$$L^T L = X^{-T} \begin{bmatrix} M^2 & 0 \\ 0 & 0 \end{bmatrix} X^{-1}$$

thus

$$A^T A + \lambda^2 L^T L = X^{-T} \begin{bmatrix} S^2 + \lambda^2 M^2 & 0 \\ 0 & I_{n-p} \end{bmatrix} X^{-1}$$

such that

$$(A^T A + \lambda^2 L^T L)^{-1} = X \begin{bmatrix} (S^2 + \lambda^2 M^2)^{-1} & 0 \\ 0 & I_{n-p} \end{bmatrix} X^T$$

and

$$x_{\lambda, L} = X \begin{bmatrix} (S^2 + \lambda^2 M^2)^{-1} & 0 \\ 0 & I_{n-p} \end{bmatrix} X^T X^{-T} \begin{bmatrix} S & 0 \\ 0 & I_{n-p} \end{bmatrix} U^T b$$

$$x_{\lambda, L} = X \begin{bmatrix} (S^2 + \lambda^2 M^2)^{-1} S & 0 \\ 0 & I_{n-p} \end{bmatrix} U^T b$$

Notice that $(S^2 + \lambda^2 M^2)^{-1} S \in \mathbb{R}^{p \times p}$ is a diagonal matrix with the diagonal entries given by

$$\frac{\sigma_i}{\sigma_i^2 + \lambda^2 \mu_i^2}$$

and $U^T b = \begin{bmatrix} u_1^T \cdot b \\ \vdots \\ u_n^T \cdot b \end{bmatrix} \in \mathbb{R}^n$

such that

$$\begin{bmatrix} (S^2 + \lambda^2 M^2)^{-1} S & 0 \\ 0 & I_{n-p} \end{bmatrix} U^T b = \begin{bmatrix} \frac{\sigma_1}{\sigma_1^2 + \lambda^2 \mu_1^2} u_1^T \cdot b \\ \vdots \\ \frac{\sigma_p}{\sigma_p^2 + \lambda^2 \mu_p^2} u_p^T \cdot b \\ u_{p+1}^T \cdot b \\ \vdots \\ u_n^T \cdot b \end{bmatrix}$$

and we obtain

$$x_{\lambda, L} = \sum_{i=1}^p f_i(\lambda, L) \frac{u_i^T \cdot b}{\sigma_i} x_i + \sum_{i=p+1}^n (u_i^T \cdot b) x_i$$

where $f_i(\lambda, L) = \frac{\sigma_i^2}{\sigma_i^2 + \lambda^2 \mu_i^2} = \frac{\sigma_i^2}{\sigma_i^2 + \lambda^2}$