Inverse Problems in Geophysics
Part 4: Singular Value Decomposition

2. MGPY+MGIN

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Recap

Over-determined problems ($N \geq M$)

- least-squares solution model-sided (inverse of $\mathbf{G}^T\mathbf{G}$)
- perfect model resolution (unique model), imperfect data

Under-determined problems ($N < M$)

- least-norm solution data sided (inverse of $\mathbf{G}\mathbf{G}^T$)
- perfect data resolution (all data perfectly fit), imperfect model

The Singular Value Decomposition (SVD)

Splitting an inverse problem into the fundamental ingredients

The Singular Value Decomposition

Any matrix $\mathbf{A}$ can be decomposed into model and data eigenvectors, weighted by singular values:

$$\mathbf{A} = \sum_{i=1}^{r} \sigma_i \mathbf{u}_i \cdot \mathbf{v}_i^T = \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^T$$

with the eigenvalues in $\boldsymbol{\Sigma} = \mathrm{diag}(\sigma_i)$, a set of orthogonal data eigenvectors $\mathbf{U} \in \mathbb{R}^{N\times N}$ with $\mathbf{U}^{-1} = \mathbf{U}^T$, and model eigenvectors $\mathbf{V} \in \mathbb{R}^{M\times M}$ with $\mathbf{V}^{-1} = \mathbf{V}^T$.

Derivation - eigenvalue decomposition

The quadratic matrix $\mathbf{A}$ projects a vector in another direction. Special vectors are eigenvectors who keep their direction

$$\mathbf{A}\mathbf{x} = \lambda\mathbf{x}$$

The solution of the equation $\mathbf{A} - \lambda\mathbf{I} = 0$ leads to eigenvalues λ over the characteristic polynome $\det(\mathbf{A} - \lambda\mathbf{I})$ that correspond to eigenvectors in the matrix $\mathbf{Q}$ by

$$\mathbf{A} = \mathbf{Q}\mathrm{diag}(\lambda_i)\mathbf{Q}^T = \mathbf{Q}\boldsymbol{\Lambda}\mathbf{Q}^T$$

Derivation (2)

We create a symmetric matrix from $\mathbf{G}$ and its transpose

$$\mathbf{A} = \begin{pmatrix} 0 & \mathbf{G} \\ \mathbf{G}^T & 0 \end{pmatrix}$$

It has the eigenvalue decomposition (two coupled eigenvalue problems)

$$\mathbf{A}\mathbf{x}_i = \lambda_i \mathbf{x}_i \quad \text{with} \quad \mathbf{x}_i = \begin{pmatrix} \mathbf{u}_i \\ \mathbf{v}_i \end{pmatrix}$$

$$\Rightarrow \mathbf{G}\mathbf{v} = \lambda \mathbf{u} \quad \text{and} \quad \mathbf{G}^T \mathbf{u} = \lambda \mathbf{v}$$

Derivation (3)

$$\Rightarrow \mathbf{G}\mathbf{v} = \lambda\mathbf{u} \quad \text{and} \quad \mathbf{G}^T\mathbf{u} = \lambda\mathbf{v}$$

Through multiplication with $\mathbf{G}^T$ or $\mathbf{G}$ we obtain

$$\mathbf{G}^T\mathbf{G}\mathbf{v} = \lambda^2\mathbf{v} \quad \text{and} \quad \mathbf{G}\mathbf{G}^T\mathbf{u} = \lambda^2\mathbf{u}$$

i.e. two eigenvalue problems for model space ($\mathbf{v}$) and data space ($\mathbf{u}$)

$$\mathbf{G} = \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^T \quad \text{and} \quad \mathbf{G}^T = \mathbf{V}\boldsymbol{\Sigma}\mathbf{U}^T \quad \text{with} \quad \boldsymbol{\Sigma} = \mathrm{diag}(\lambda_i)$$

Model and Data space

$\mathbf{U} \in \mathbb{R}^{N \times N}$ spans the data space

$\mathbf{V} \in \mathbb{R}^{M \times M}$ spans the model space

$\mathbf{U}$ and $\mathbf{V}$ can be split into a data/model space and a null space

$$\mathbf{U} = [\mathbf{U}_r, \mathbf{U}_0]$$

$$\mathbf{V} = [\mathbf{V}_r, \mathbf{V}_0]$$

Eigenvectors and singular values

The eigenvectors associated with zero singular values ($\sigma_i = 0$) span the null spaces of data and model. The number of non-zero eigenvalues r defines the rank of the matrix which can be abbreviated by

$$\mathbf{A}_r = \sum_{i=1}^{r} \sigma_i \mathbf{u}_i \cdot \mathbf{v}_i^T = \mathbf{U}_r \mathbf{\Sigma}_r \mathbf{V}_r^T$$

where $\mathbf{B}_r$ holds the first r columns of the matrix $\mathbf{B}$.

A matrix can be approximated by choosing the rank by hand.

Operators in terms of SVD

The forward operator $\mathbf{Gm}$ and its adjoint $\mathbf{G}^T$ are written:

$$\mathbf{G} = \mathbf{U}_r \mathbf{\Sigma}_r \mathbf{V}_r^T$$

$$\mathbf{G}^T = \mathbf{V}_r \mathbf{\Sigma}_r \mathbf{U}_r^T$$

$$\mathbf{G}^T\mathbf{G} = \mathbf{V}_r^T \mathbf{\Sigma}_r \mathbf{U}_r^T \mathbf{U}_r \mathbf{\Sigma}_r \mathbf{V}_r = \mathbf{V}_r^T \mathbf{\Sigma}_r^2 \mathbf{V}_r$$

$$\mathbf{G}\mathbf{G}^T = \mathbf{U}_r \mathbf{\Sigma}_r \mathbf{V}_r \mathbf{V}_r^T \mathbf{\Sigma}_r \mathbf{U}_r^T = \mathbf{U}_r \mathbf{\Sigma}_r^2 \mathbf{U}_r^T$$

The generalized inverse

$$\mathbf{G}_r\mathbf{m} = \mathbf{U}_r\mathbf{\Sigma}_r\mathbf{V}_r^T\mathbf{m} = \mathbf{d}$$

$$\mathbf{U}_r^T\mathbf{U}_r\mathbf{\Sigma}_r\mathbf{V}_r^T\mathbf{m} = \mathbf{\Sigma}_r\mathbf{V}_r^T\mathbf{m} = \mathbf{U}_r^T\mathbf{d}$$

$$\mathbf{\Sigma}_r^{-1}\mathbf{\Sigma}_r\mathbf{V}_r^T\mathbf{m} = \mathbf{V}_r^T\mathbf{m} = \mathbf{\Sigma}_r^{-1}\mathbf{U}_r^T\mathbf{d}$$

$$\mathbf{V}_r\mathbf{V}_r^T\mathbf{m} = \mathbf{m} = \mathbf{V}_r\mathbf{\Sigma}_r^{-1}\mathbf{U}_r^T\mathbf{d}$$

$$\Rightarrow \mathbf{m} = \mathbf{G}^\dagger\mathbf{d} \quad \text{with} \quad \mathbf{G}^\dagger = \mathbf{V}_r\mathbf{\Sigma}_r^{-1}\mathbf{U}_r^T$$

The SVD provides a generalized (Moore-Penrose) inverse

Resolution

The model resolution

$$\mathbf{R}^M = \mathbf{G}^\dagger \mathbf{G} = \mathbf{V}_p \mathbf{\Sigma}_p^{-1} \mathbf{U}_p^T \mathbf{U}_p \mathbf{\Sigma}_p \mathbf{V}_p^T = \mathbf{V}_p \mathbf{V}_p^T$$

depends only on the model eigenvectors!

And the data resolution

$$\mathbf{R}^D = \mathbf{G}\mathbf{G}^\dagger = \mathbf{U}_p \mathbf{\Sigma}_p \mathbf{V}_p^T \mathbf{V}_p \mathbf{\Sigma}_p^{-1} \mathbf{U}_p^T = \mathbf{U}_p \mathbf{U}_p^T$$

depends only on the data eigenvectors!

Inverse problem types - classification scheme

The rank r determines the type of the inverse problem

Even-determined

$$M = N = r$$

Over-determined

$$N > r = M$$

Under-determined

$$N = r < M$$

Mixed-determined

$$r < N \quad \text{and} \quad r < M$$

Inverse problem types - Even-determined

$$M = N = r$$

Generalized inverse = normal inverse

$$\mathbf{R}^M = \mathbf{R}^D = \mathbf{I}$$

Inverse problem types - Over-determined

$$N > r = M$$

Generalized inverse = least-squares inverse

$$\mathbf{G}^{\dagger} = (\mathbf{G}^T\mathbf{G})^{-1}\mathbf{G}^T = \mathbf{V}_r\boldsymbol{\Sigma}_r^{-2}\mathbf{V}_r^T\mathbf{V}_r\boldsymbol{\Sigma}_r\mathbf{U}_r^T = \mathbf{V}_r\boldsymbol{\Sigma}_r^{-1}\mathbf{U}_r^T$$

$$\mathbf{R}^M = \mathbf{I} \quad , \quad \mathbf{R}^D \neq \mathbf{I}$$

Inverse problem types - Under-determined

$$N = r < M$$

Generalized inverse = minimum-norm inverse

$$\mathbf{G}^{\dagger} = \mathbf{G}^T(\mathbf{G}\mathbf{G}^T)^{-1} = \mathbf{V}_r\boldsymbol{\Sigma}_r\mathbf{U}_r^T\mathbf{U}_r\boldsymbol{\Sigma}_r^{-2}\mathbf{U}_r^T = \mathbf{V}_r\boldsymbol{\Sigma}_r^{-1}\mathbf{U}_r^T$$

$$\mathbf{R}^M \neq \mathbf{I} \quad , \quad \mathbf{R}^D = \mathbf{I}$$

Inverse problem types - Mixed-determined

$$r < M \quad \text{and} \quad r < M$$

The generalized inverse

$$\mathbf{G}^{\dagger} = \mathbf{V}_r \mathbf{\Sigma}_r^{-1} \mathbf{U}_r^T$$

handles both over-determined and underdetermined model parts.

$$\mathbf{R}^M \neq \mathbf{I} \quad , \quad \mathbf{R}^D \neq \mathbf{I}$$