Moore-Penrose pseudoinverse

Linear systems with rank-deficient l.h.s.

Linear systems with rank-deficient matrices

Consider

$$\mathbf{A}\vec{x} = \vec{b}$$

with $\mathbf{A} \in \mathbb{R}^{m\times m}$ and $\operatorname{rank} \mathbf{A} < m$.

Use SVD of $\mathbf{A}$: $\mathbf{A} = \mathbf{U\Sigma V}^T$. Recall $\mathbf{A}\vec{v_k} = \sigma_k \vec{u_k}$.

Homogeneous system $\vec{b} = 0$: Any $\vec{v}_k$ with $\sigma_k = 0$ is a solution

Inhomogeneous system $\vec{b} \neq 0$:

- $\vec{b} \notin \operatorname{ran} \mathbf{A}$: no solutions
- $\vec{b} \in \operatorname{ran} \mathbf{A}$: solution is not unique.

Can add an arbitrary vector from the nullspace: if $\mathbf{A}\vec{y} = 0$, $\mathbf{A}(\vec{x} + \vec{y}) = \mathbf{A}\vec{x}$.

Minimum norm solution

Look for the minimum norm solution: Find the solution of $\mathbf{A}\vec{x} = \vec{b}$ with $\|\vec{x}\|_2 \longrightarrow \min.$

if $\mathbf{A}$ were not singular, $\vec{x} = \mathbf{A}^{-1}\vec{b}$,

$$\mathbf{A}^{-1} = \mathbf{V}\ \mathrm{diag}\left[\frac{1}{\sigma_1}, \frac{1}{\sigma_2}, \cdots\right]\ \mathbf{U}^T$$

Minimum norm solution: for zero σ-s, replace $\frac{1}{\sigma}$, with zeros:

$$\mathrm{diag}\left[\frac{1}{\sigma_1}, \frac{1}{\sigma_2}, \cdots, \frac{1}{\sigma_r}, 0, \cdots, 0\right]$$

$\Rightarrow$ Moore-Penrose pseudoinverse

Pseudoinverse

$$\mathbf{A}\vec{x} = \vec{b}$$

A formal solution is $\vec{x} = \mathbf{A}^{-1}\vec{b}$, where

$$\mathbf{A}^{-1}\mathbf{A} = \mathbf{A}\mathbf{A}^{-1} = \mathbf{1}.$$

Pseudoinverse

$\mathbf{A}^P$: Generalization of $\mathbf{A}^{-1}$ (always exists).

1. $\mathbf{A}\mathbf{A}^P\mathbf{A} = \mathbf{A}$

   $\mathbf{A}\mathbf{A}^P \neq \mathbf{1}$, but maps columns of $\mathbf{A}$ onto themselves
2. $\mathbf{A}^P\mathbf{A}\mathbf{A}^P = \mathbf{A}^P$
3. $\left(\mathbf{A}\mathbf{A}^P\right)^T = \left(\mathbf{A}\mathbf{A}^P\right)$
4. $\left(\mathbf{A}^P\mathbf{A}\right)^T = \left(\mathbf{A}^P\mathbf{A}\right)$

Pseudoinverse: examples

- If $\mathbf{A}$ is invertible, then $\mathbf{A}^P = \mathbf{A}^{-1}$
- If $\mathbf{A}$ has full column rank: $\mathbf{A}^T\mathbf{A}$ is invertible. Then

$$\mathbf{A}^P = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T$$

NB: in this case, $\mathbf{A}^P$ is then the *left inverse*, because $\mathbf{A}^P\mathbf{A} = \mathbf{1}$.

Linear least squares and pseudoinverse

LLS problem:

$$\vec{x}_{\mathrm{LS}} = \arg\min_{\vec{x}} \|\mathbf{A}\vec{x} - \vec{b}\|^2$$

A formal solution via the normal equations:

$$\mathbf{A}^T\mathbf{A}\,\vec{x}_{\mathrm{LS}} = \mathbf{A}^T\vec{b} \qquad \Rightarrow \qquad \vec{x}_{\mathrm{LS}} = \mathbf{A}^P\vec{b}$$

Normal equations are

- poorly conditioned
- fail if $\mathbf{A}$ is rank-deficient

Pseudoinverse via SVD

Consider

$$\chi^2 = \|\mathbf{A}\vec{x} - \vec{b}\|^2 \qquad \text{rotate by } \mathbf{U}^T$$

$$= \|\mathbf{U}^T(\mathbf{A}\vec{x} - \vec{b})\|^2 \qquad \text{use } \mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$$

$$= \|\mathbf{\Sigma}\mathbf{V}^T\vec{x} - \mathbf{U}^T\vec{b})\|^2 \qquad \text{define } \vec{y} = \mathbf{V}^T\vec{x}$$

Let $\mathrm{rank}\,\mathbf{A} = r$

$$= \sum_{k=1}^{r}\left(\sigma_k y_k - \vec{u}_k^T\vec{b}\right)^2 + \sum_{k=r+1}^{m}\left(\vec{u}_k^T\vec{b}\right)^2$$

LS solution: zero out the first sum.

Pseudoinverse via SVD

The solution of the LLS problem satisfies

$$y_k = \frac{1}{\sigma_k}\vec{u}_k^T\vec{b}, \qquad\qquad k = 1, \cdots, r$$

Take $y_k = 0$ for $k = r+1, \cdots, m$.

Since $\vec{y} = \mathbf{V}^T\vec{x}$, the LS solution is

$$\vec{x}_{\mathrm{LS}} = \mathbf{V}\Sigma^P\mathbf{U}^T\vec{b} \equiv \mathbf{A}^P\vec{b}$$