Applied Linear Algebra in Data Analysis Matrix Inverses

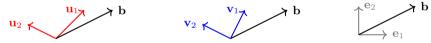
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Representation of vectors in a basis

▶ Consider the vector space \mathbb{R}^n with basis $\{\mathbf{v}_1, \mathbf{v}_2, \dots \mathbf{v}_n\}$. Any vector in $\mathbf{b} \in \mathbb{R}^n$ can be represented as a linear combination of vectors \mathbf{v}_i ,

$$\mathbf{b} = \sum_{i=1}^{n} \mathbf{v}_{i} \mathbf{a}_{i} = \mathbf{V} \mathbf{a}; \ \mathbf{a} \in \mathbb{R}^{n}, \ \mathbf{V} = \begin{bmatrix} \mathbf{v}_{1} & \mathbf{v}_{2} & \dots & \mathbf{v}_{n} \end{bmatrix} \in \mathbb{R}^{n \times n}$$



 $\{\mathbf{v}_1, \mathbf{v}_2\}$, $\{\mathbf{u}_1, \mathbf{u}_2\}$ and $\{\mathbf{e}_1, \mathbf{e}_2\}$ are valid basis for \mathbb{R}^2 , and the presentation for **b** in each one of them is different.

Matrix Inverse

- ▶ Consider the equation $\mathbf{A}\mathbf{x} = \mathbf{y}$, where $\mathbf{A} \in \mathbb{R}^{n \times n}$ and $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$.
- ightharpoonup Let us assume **A** is non-singular \implies columns of **A** represent a basis for \mathbb{R}^n .
- ightharpoonup What does x represent? It is the representation of y in the basis consisting of the columns of A.

$$\mathbf{y} = \mathbf{A}\mathbf{x} = \begin{bmatrix} \mathbf{a}_1 & \mathbf{a}_2 & \dots & \mathbf{a}_n \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \sum_{i=1}^n \mathbf{a}_i x_i$$

$$\implies \mathbf{x} = \mathbf{A}^{-1}\mathbf{y} = \begin{bmatrix} \mathbf{b}_1^\top \\ \mathbf{b}_2^\top \\ \dots \\ \mathbf{b}_n^\top \end{bmatrix} \mathbf{y} = \begin{bmatrix} \mathbf{b}_1^\top \mathbf{y} \\ \mathbf{b}_2^\top \mathbf{y} \\ \dots \\ \mathbf{b}_n^\top \mathbf{y} \end{bmatrix}$$

Matrix Inverse

▶ A^{-1} is a matrix that allows change of basis to the columns of A from the standard basis!

Left Inverse

▶ Consider a rectangular matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$. There exists no inverse \mathbf{A}^{-1} for this matrix.

▶ But, there exist two matrices $\mathbf{B}, \mathbf{C} \in \mathbb{R}^{n \times m}$, such that,

$$\mathbf{C}\mathbf{A} = \mathbf{I}_n \quad \text{or} \quad \mathbf{A}\mathbf{B} = \mathbf{I}_m$$

▶ Both cannot be true for a rectangular matrix, only one can be true when the matrix is full rank.

▶ A rectangular matrix can only have either a left or a right inverse.

Left Inverse

▶ Any non-zero $\mathbf{a} \in \mathbb{R}^{n \times 1}$ is left invertible: $\mathbf{b}\mathbf{a} = 1$, $\mathbf{b} \in \mathbb{R}^{1 \times n}$; $\mathbf{b}^T = \frac{\mathbf{a}}{\|\mathbf{a}\|^2} + \alpha \mathbf{a}^{\perp}$

▶ This can be generalized to $\mathbf{A} \in \mathbb{R}^{m \times n}$, m > n.

$$\left(\mathbf{C} + \hat{\mathbf{C}}\right)\mathbf{A} = \mathbf{I}_m \text{ where } \mathbf{C}, \hat{\mathbf{C}} \in \mathbb{R}^{n \times m}, \ \hat{\mathbf{C}}\mathbf{A} = \mathbf{0}$$

Condition for left inverse of **A** to exist: Colmuns of **A** must be independent. $\longrightarrow rank(\mathbf{A}) = n \longrightarrow \mathbf{A}\mathbf{x} = 0 \implies \mathbf{x} = 0.$

▶ $\mathbf{A}\mathbf{x} = \mathbf{b}$ can be solved, if and only if $\mathbf{A}(\mathbf{C}\mathbf{b}) = \mathbf{b}$, where $\mathbf{C}\mathbf{A} = \mathbf{I}_n$.

Right Inverse

▶ For $\mathbf{A} \in \mathbb{R}^{m \times n}$, n > m with full rank, $\mathbf{AB} = \mathbf{I}_m \longrightarrow \mathbf{B}$ is the right inverse.

▶ Right inverse of **A** exists only if the rows of **A** are independent, i.e. $rank(\mathbf{A}) = m$ $\longrightarrow \mathbf{A}^T \mathbf{x} = \mathbf{0} \implies \mathbf{x} = \mathbf{0}$

ightharpoonup $\mathbf{A}\mathbf{x} = \mathbf{b}$ can be solved for any \mathbf{b} . $\mathbf{x} = \mathbf{B}\mathbf{b} \implies \mathbf{A}(\mathbf{B}\mathbf{b}) = \mathbf{b}$.

ightharpoonup There are an infinite number of $\mathbf{B}\mathbf{s} \implies$ an infinite number of solutions \mathbf{x} .

Pseudo Inverse

▶ Consider a tall matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$ with independent columns. It turns out the Gram matrix $\mathbf{A}^{\top}\mathbf{A} \in \mathbb{R}^{n \times n}$ is invertible. If that is the case then,

$$(\mathbf{A}^{\top}\mathbf{A})^{-1}\mathbf{A}^{\top}\mathbf{A} = \mathbf{I}_n; \quad (\mathbf{A}^{\top}\mathbf{A})^{-1}\mathbf{A}^{\top} \text{ is a left inverse.}$$

 $ightharpoonup \mathbf{A}^{\dagger} = (\mathbf{A}^{\top}\mathbf{A})^{-1} \mathbf{A}^{\top}$ is called the *pseudo inverse* or the *Moore-Penrose inverse*.

► For the case of a fat, wide matrix, we have $\mathbf{A}^{\dagger} = \mathbf{A}^{\top} (\mathbf{A} \mathbf{A}^{\top})^{-1}$.

▶ When **A** is square and invertible, $\mathbf{A}^{\dagger} = \mathbf{A}^{-1}$.

Matrix Inverse and Pseudo Inverse through QR factorization

▶ Consider an invertible, square matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$.

$$\mathbf{A} = \mathbf{Q}\mathbf{R} \implies \mathbf{A}^{-1} = (\mathbf{Q}\mathbf{R})^{-1} = \mathbf{R}^{-1}\mathbf{Q}^{-1} = \mathbf{R}^{-1}\mathbf{Q}^{\top}$$

where, $\mathbf{R}, \mathbf{Q} \in \mathbb{R}^{n \times n}$. **R** is upper triangular, and **Q** is an orthogonal matrix.

In the case of a left invertible rectangular matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$, we can factorize $\mathbf{A} = \mathbf{Q}\mathbf{R}$, with $\mathbf{Q} \in \mathbb{R}^{m \times n}$ and $\mathbf{R} \in \mathbb{R}^{n \times n}$.

$$\mathbf{A}^{\dagger} = \left(\mathbf{A}^{\top}\mathbf{A}\right)^{-1}\mathbf{A}^{\top} = \left(\mathbf{R}^{\top}\mathbf{Q}^{\top}\mathbf{Q}\mathbf{R}\right)^{-1}\mathbf{R}^{\top}\mathbf{Q}^{\top} = \left(\mathbf{R}^{\top}\mathbf{R}\right)^{-1}\mathbf{R}^{\top}\mathbf{Q}^{\top} = \mathbf{R}^{-1}\mathbf{Q}^{\top}$$

Matrix Inverse and Pseudo Inverse through QR factorization

▶ For a right invertible wide, fat matrix, we can find out the pseudo-inverse of \mathbf{A}^{\top} , and then take the transpose of the pseudo-inverse.

$$\mathbf{A}\mathbf{A}^{\dagger} = \mathbf{I} \implies \left(\mathbf{A}^{\dagger}\right)^{\top}\mathbf{A}^{\top} = \left(\mathbf{A}^{\top}\right)^{\dagger}\mathbf{A}^{\top} = \mathbf{I}$$

$$\mathbf{A}^{\top} = \mathbf{Q}\mathbf{R} \implies \left(\mathbf{A}^{\top}\right)^{\dagger} = \mathbf{R}^{-1}\mathbf{Q}^{\top} = \left(\mathbf{A}^{\dagger}\right)^{\top} \implies \mathbf{A}^{\dagger} = \mathbf{Q}\mathbf{R}^{-T}$$

What about when A is not full rank?

▶ There is no left or right inverse for $\mathbf{A} \in \mathbb{R}^{m \times n}$, when $rank(\mathbf{A}) = r < \min(m, n)$.

$$\nexists \mathbf{B} \in \mathbb{R}^{n \times m}, s.t. \mathbf{BA} = \mathbf{I}_n \text{ or } \mathbf{AB} = \mathbf{I}_m$$

▶ **A is tall**: First r columns of **A** are linear independent, then \exists **B** \in $\mathbb{R}^{n \times m}$, s.t.

$$\mathbf{B}\mathbf{A} = egin{bmatrix} \mathbf{I}_r & \mathbf{0} \ \mathbf{0} & \mathbf{0} \end{bmatrix}$$

▶ **A** is fat: First r rows of **A** are linear independent, then \exists **B** \in $\mathbb{R}^{n\times m}$, s.t.

$$\mathbf{AB} = egin{bmatrix} \mathbf{I}_r & \mathbf{0} \ \mathbf{0} & \mathbf{0} \end{bmatrix}$$

What about when A is not full rank?

▶ What if we have a linear system of equations with a non-full rank matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$?

$$Ax = b$$

- ightharpoonup $\mathbf{b} \in \mathcal{C}(\mathbf{A}) \implies$ There are infinitely many solutions to the above equation.
- ▶ $\mathbf{b} \notin \mathcal{C}(\mathbf{A}) \implies$ There is no solution to the above equation. But there are infinitely many solutions $\hat{\mathbf{x}}$ that minimize $\|\mathbf{b} \mathbf{A}\hat{\mathbf{x}}\|_2$.
- ▶ One approach to solve the case where $\mathbf{b} \notin \mathcal{C}(\mathbf{A})$ is to formulate the problem as a regularized least squares problem,

$$\hat{\mathbf{x}} = \arg\min \|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2^2 + \lambda \|\mathbf{x}\|_2^2$$