Generalizing the inverse to non-invertible matrices

We know that for $A \in K^{n\times n}$, if $|A| \neq 0$ then every system of equations $A\mathbf{x} = \mathbf{b}$ has a unique solution, and the solution can be obtained az $\mathbf{x} = A^{-1}\mathbf{b}$. But there may be a unique solution even if the matrix is not a square matrix but has independent columns.

Can we generalize the inverse for singular or rectangular matrices? What we want is an inverse A^+ for every real matrix such that

- If $A\mathbf{x} = \mathbf{b}$ has a unique solution then it is $\mathbf{x} = A^+\mathbf{b}$.
- If $A\mathbf{x} = \mathbf{b}$ is consistent but has more than one solutions, then $A^+\mathbf{b}$ is one of the solutions; let it be the one closest to the origin (i.e. for which $|\mathbf{x}|$ is minimal)
- If $A\mathbf{x} = \mathbf{b}$ is inconsistent then $A^+\mathbf{b}$ should be a best approximate solution, that is, a solution of the normal equations $A^TA\mathbf{x} = A^T\mathbf{b}$ (and if there are more, then the one for which $|\mathbf{x}|$ is minimal).

We shall see that such a generalized inverse always exists.

The Moore–Penrose inverse

Def. For $A \in \mathbb{R}^{m\times n}$, the matrix $A^+ \in \mathbb{R}^{n\times m}$ is the Moore–Penrose inverse, or in other words, the **pseudoinverse** of A if
(1) $A = AA^+A$,
(2) $A^+ = A^+AA^+$,
(3) AA^+ is symmetric,
(4) A^+A is symmetric.

Theorem. If A^+ is a pseudoinverse of A, then for any system of equations $A\mathbf{x} = \mathbf{b}$, the vector $A^+\mathbf{b}$ is the unique (best approximate) solution of the system for which $|\mathbf{x}|$ is the smallest possible.

Proof. It is enough to show that $\mathbf{x} = A^+\mathbf{b}$ is the solution of the normal equations $A^TA\mathbf{x} = A^T\mathbf{b}$ with minimal $|\mathbf{x}|$.
It is indeed a solution:
$A^TA(A^+\mathbf{b}) = A^T(AA^+)\mathbf{b} \overset{(3)}{=} A^T(AA^+)^T\mathbf{b} = (AA^+A)^T\mathbf{b} \overset{(1)}{=} A^T\mathbf{b}$.

The smallest solution:
If $\mathbf{y}$ is another solution then $\mathbf{y} = A^+\mathbf{b} + \mathbf{h}$, where $\mathbf{h}$ is a solution of the homogeneous system, i.e. $A^TA\mathbf{h} = \mathbf{0}$, thus $0 = \mathbf{h}^TA^TA\mathbf{h} = |A\mathbf{h}|^2 \Rightarrow A\mathbf{h} = \mathbf{0}$.
On the other hand, $A^+\mathbf{b} = (A^+AA^+)\mathbf{b} \overset{(4)}{=} (A^+A)^TA^+\mathbf{b} = A^T(A^+)^TA^+\mathbf{b} = A^T\mathbf{c}$ for $\mathbf{c} = (A^+)^TA^+\mathbf{b}$
so $\langle A^+\mathbf{b}, \mathbf{h} \rangle = (A^T\mathbf{c})^T\mathbf{h} = \mathbf{c}^TA\mathbf{h} = \mathbf{0}$, and
$|\mathbf{y}|^2 = \langle A^+\mathbf{b} + \mathbf{h},\ A^+\mathbf{b} + \mathbf{h} \rangle = |A^+\mathbf{b}|^2 + |\mathbf{h}|^2 \geq |A^+\mathbf{b}|^2$, so indeed, the length of $A^+\mathbf{b}$ is minimal. This also shows that all the other solutions have strictly greater length, so the smallest best approximate solution is unique if A^+ exists. $\square$

Existence of the pseudoinverse for matrices of full rank

Lemma. Spse $A \in \mathbb{R}^{m\times n}$ and $\operatorname{rank}(A) = r$.
Then $\operatorname{rank}(A^TA) = r$, A^TA is symmetric, and all its eigenvalues are non-negative.

Proof. $A^TA \in \mathbb{R}^{n\times n}$.
$\operatorname{Ker} A = \operatorname{Ker} A^TA$: The $\subseteq$ inclusion is obvious, and $\supseteq$ is also true because $A^TA\mathbf{x} = \mathbf{0} \Rightarrow 0 = \mathbf{x}^TA^TA\mathbf{x} = |A\mathbf{x}|^2 \Rightarrow A\mathbf{x} = \mathbf{0}$.
So by the Dimension Theorem, $\operatorname{rank}(A) = n - \dim\operatorname{Ker} A = n - \dim\operatorname{Ker} A^TA = \operatorname{rank}(A^TA)$.
$(A^TA)^T = A^T(A^T)^T = A^TA$, so A^TA is symmetric.
If λ is an eigenvalue of A^TA with eigenvector $\mathbf{v} \neq \mathbf{0}$, then $A^TA\mathbf{v} = \lambda\mathbf{v}$ gives $0 \le |A\mathbf{v}|^2 = \mathbf{v}^TA^TA\mathbf{v} = \mathbf{v}^T\lambda\mathbf{v} = \lambda|\mathbf{v}|^2$, and here $|\mathbf{v}|^2 > 0$, so $\lambda \ge 0$.

Exercise. Determine the rank and the eigenvalues of A^TA and AA^T for

$$A = \begin{bmatrix} 1 & 2 & -1 \\ 0 & 1 & 1 \end{bmatrix}.$$

Now let's see how we can construct the pseudoinverse. Notice first that if it exists, it is unique, since for every i, the vector $A^+\mathbf{e}_i$ is the unique smallest, best approximate solution of $A\mathbf{x} = \mathbf{e}_i$, so $A^+ = A^+I = A^+[\mathbf{e}_1 \ldots \mathbf{e}_m] = [A^+\mathbf{e}_1 \ldots A^+\mathbf{e}_m]$ is also unique.

Def. We call a matrix $A \in K^{m\times n}$ a matrix of **full rank** if $\operatorname{rank} A = \min\{m, n\}$, that is, the largest possible rank for a matrix of this size.

Theorem. Let $A \in \mathbb{R}^{m\times n}$ be a matrix of full rank.
(1) If $\operatorname{rank} A = n$ then A^TA is invertible, and $A^+ = (A^TA)^{-1}A^T$. In this case, A^+ is a left inverse: $A^+A = I$.
(2) If $\operatorname{rank} A = m$ then AA^T is invertible, and $A^+ = A^T(AA^T)^{-1}$. In this case, A^+ is a right inverse: $AA^+ = I$.

Proof. (1): Let $B = (A^TA)^{-1}A^T$. Then
$BA = (A^TA)^{-1}A^TA = I_n$ is symmetric,
and $AB = A(A^TA)^{-1}A^T$ is also symmetric:
$(AB)^T = (A(A^TA)^{-1}A^T)^T = A((A^TA)^{-1})^TA^T = A(A^TA)^{-1}A^T = AB$.
Furthermore $ABA = AI = A$ and $BAB = IB = B$.
So $B = A^+$.
(2): Apply part (1) to $C = A^T$.

Exercise. Calculate the pseudoinverse of $A = \begin{bmatrix} 1 & 2 & 1 \\ 2 & -1 & 1 \end{bmatrix}$.

Solution. A is of full row rank.

$$AA^T = \begin{bmatrix} 1 & 2 & 1 \\ 2 & -1 & 1 \end{bmatrix}\begin{bmatrix} 1 & 2 \\ 2 & -1 \\ 1 & 1 \end{bmatrix} = \begin{bmatrix} 6 & 1 \\ 1 & 6 \end{bmatrix}, \quad (AA^T)^{-1} = \frac{1}{35}\begin{bmatrix} 6 & -1 \\ -1 & 6 \end{bmatrix}$$

$$A^+ = A^T(AA^T)^{-1} = \begin{bmatrix} 1 & 2 \\ 2 & -1 \\ 1 & 1 \end{bmatrix} \frac{1}{35} \begin{bmatrix} 6 & -1 \\ -1 & 6 \end{bmatrix} = \frac{1}{35} \begin{bmatrix} 4 & 11 \\ 13 & -8 \\ 5 & 5 \end{bmatrix}.$$

Pseudoinverse for any real matrix

Theorem (Rank factorization). Every matrix $A \in K^{m\times n}$ can be written as the product of two full-rank matrices: if $\operatorname{rank}(A) = r$, then $A = BC$, where $B \in K^{m\times r}$ and $C \in K^{r\times n}$ both have rank r.

Proof. Use Gaussian elimination to calculate the reduced row-echelon form L of the matrix A. Let B consist of the columns of A corresponding to the columns of L containing leading ones, and let C consist of the nonzero rows of L.
Since elementary row operations do not change the linear correspondances between the columns of the matrix, the elements of the $i'th$ column of L tell the coefficients of the linear combination of the columns of B resulting in the i'th column of A. Thus $A = BC$, and it is clear from the row echelon form that both B and C have rank r.

Exercise. Calculate the rank factorization of the matrix

$$A = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 2 \\ 1 & 1 & 3 \end{bmatrix}$$

Solution.

$$A \mapsto \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 2 \\ 0 & 1 & 2 \end{bmatrix} \mapsto \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 2 \\ 0 & 0 & 0 \end{bmatrix} \Rightarrow B = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 1 \end{bmatrix}, \; C = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 2 \end{bmatrix}$$

Theorem. If $A \in \mathbb{R}^{m\times n}$ and $A = BC$ is a rank factorization of A then $A^+ = C^+B^+$.

Proof. We shall use that $B^+B = I$ and $CC^+ = I$ according to the theorem about the pseudoinverses of full-rank matrices. We show that $A^+ := C^+B^+$ indeed satisfies the four conditions for the pseudoinverse.
$AA^+A = BCC^+B^+BC = BCC^+IC = BCC^+C = BC$.
$A^+AA^+ = C^+B^+BCC^+B^+ = C^+B^+BIB^+ = C^+B^+BB^+ = C^+B^+ = A^+$.
$AA^+ = BCC^+B^+ = BIB^+ = BB^+$ is symmetric because B^+ is a pseudoinverse.
$A^+A = C^+B^+BC = C^+IC = C^+C$ is symmetric because C^+ is a pseudoinverse.

Exercise. Calculate the pseudoinverse of the matrix A in the previous exercise. Find the optimal solution of $A\mathbf{x} = \mathbf{b}$ for $\mathbf{b} = (1,0,1)^T$ and $\mathbf{b} = (1,0,2)^T$.

Solution. $A = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 2 \\ 1 & 1 & 3 \end{bmatrix} = BC = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 2 \end{bmatrix}.$

$$B = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 1 \end{bmatrix}, \quad B^T B = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 1 \end{bmatrix} = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix},$$

$$B^+ = (B^T B)^{-1} B^T = \frac{1}{3} \begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix} \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \end{bmatrix} = \frac{1}{3} \begin{bmatrix} 2 & -1 & 1 \\ -1 & 2 & 1 \end{bmatrix}$$

$$C = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 2 \end{bmatrix}, \quad CC^T = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 2 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 2 \end{bmatrix} = \begin{bmatrix} 2 & 2 \\ 2 & 5 \end{bmatrix},$$

$$C^+ = C^T (CC^T)^{-1} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 2 \end{bmatrix} \frac{1}{6} \begin{bmatrix} 5 & -2 \\ -2 & 2 \end{bmatrix} = \frac{1}{6} \begin{bmatrix} 5 & -2 \\ -2 & 2 \\ 1 & 2 \end{bmatrix}.$$

$$A^+ = C^+ B^+ = \frac{1}{6} \begin{bmatrix} 5 & -2 \\ -2 & 2 \\ 1 & 2 \end{bmatrix} \frac{1}{3} \begin{bmatrix} 2 & -1 & 1 \\ -1 & 2 & 1 \end{bmatrix} = \frac{1}{18} \begin{bmatrix} 12 & -9 & 3 \\ -6 & 6 & 0 \\ 0 & 3 & 3 \end{bmatrix}$$

$$A^+ = \frac{1}{6} \begin{bmatrix} 4 & -3 & 1 \\ -2 & 2 & 0 \\ 0 & 1 & 1 \end{bmatrix}$$

For $\mathbf{b} = \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}$: $\mathbf{x} = A^+\mathbf{b} = \frac{1}{6} \begin{bmatrix} 5 \\ -2 \\ 1 \end{bmatrix}$, for $\mathbf{b} = \begin{bmatrix} 1 \\ 0 \\ 2 \end{bmatrix}$, $\mathbf{x} = A^+\mathbf{b} = \frac{1}{3} \begin{bmatrix} 3 \\ -1 \\ 1 \end{bmatrix}$.

The first is a solution, the second is only an optimal approximate solution:

$$A\mathbf{x} = \begin{bmatrix} 4/3 \\ 1/3 \\ 5/3 \end{bmatrix} \approx \begin{bmatrix} 1 \\ 0 \\ 2 \end{bmatrix}$$