The Moore-Penrose Pseudoinverse (Math 33A: Laub)

In these notes we give a brief introduction to the Moore-Penrose pseudoinverse, a generalization of the inverse of a matrix. The Moore-Penrose pseudoinverse is defined for **any matrix** and is **unique**. Moreover, as is shown in what follows, it brings great notational and conceptual clarity to the study of solutions to arbitrary systems of linear equations and linear least squares problems.

1 Definition and Characterizations

We consider the case of $A \in \mathbb{R}_r^{m\times n}$. Every $A \in \mathbb{R}_r^{m\times n}$ has a pseudoinverse and, moreover, the pseudoinverse, denoted $A^+ \in \mathbb{R}_r^{n\times m}$, is unique. A purely algebraic characterization of A^+ is given in the next theorem proved by Penrose in 1956.

Theorem: Let $A \in \mathbb{R}_r^{m\times n}$. Then $G = A^+$ if and only if

(P1) $AGA = A$

(P2) $GAG = G$

(P3) $(AG)^T = AG$

(P4) $(GA)^T = GA$

Furthermore, A^+ always exists and is unique.

Note that the above theorem is *not* constructive. But it does provide a checkable criterion, i.e., given a matrix G that purports to be the pseudoinverse of A, one need simply verify the four Penrose conditions (P1)–(P4) above. This verification is often relatively straightforward.

Example: Consider $A = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$. Verify directly that $A^+ = [\frac{1}{5}\ ,\ \frac{2}{5}]$. Note that other left inverses (for example, $A^{-L} = [3\ ,\ -1]$) satisfy properties (P1), (P2), and (P4) but not (P3).

Still another characterization of A^+ is given in the following theorem whose proof can be found on p. 19 in Albert, A., *Regression and the Moore-Penrose Pseudoinverse*, Academic Press, New York, 1972. We refer to this as the "limit definition of the pseudoinverse."

Theorem: Let $A \in \mathbb{R}_r^{m\times n}$. Then

$$A^+ = \lim_{\delta\to 0} (A^TA + \delta^2 I)^{-1} A^T \quad (1)$$

$$= \lim_{\delta\to 0} A^T(AA^T + \delta^2 I)^{-1} \quad (2)$$

2 Examples

Each of the following can be derived or verified by using the above theorems or characterizations.

Example 1: $A^+ = A^T(AA^T)^{-1}$ if A is onto, i.e., has linearly independent rows (A is right invertible)

Example 2: $A^+ = (A^TA)^{-1}A^T$ if A is 1-1, i.e., has linearly independent columns (A is left invertible)

Example 3: For any scalar α,

$$\alpha^+ = \begin{cases} \alpha^{-1} & \text{if } \alpha \neq 0 \\ 0 & \text{if } \alpha = 0 \end{cases}$$

Example 4: For any vector $v \in \mathbb{R}^n$,

$$v^+ = (v^Tv)^+v^T = \begin{cases} \frac{v^T}{v^Tv} & \text{if } v \neq 0 \\ 0 & \text{if } v = 0 \end{cases}$$

Example 5: $\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}^+ = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$
This example was computed via the limit definition of the pseudoinverse.
Example 6: $\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}^+ = \begin{bmatrix} \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} \end{bmatrix}$
This example was computed via the limit definition of the pseudoinverse.

3 Some Properties

Theorem: Let $A \in \mathbb{R}^{m\times n}$ and suppose $U \in \mathbb{R}^{m\times m}$, $V \in \mathbb{R}^{n\times n}$ are orthogonal (M is orthogonal if $M^T = M^{-1}$). Then

$$(UAV)^+ = V^TA^+U^T.$$

Proof: Simply verify that the expression above does indeed satisfy each of the four Penrose conditions.

Theorem: Let $S \in \mathbb{R}^{n\times n}$ be symmetric with $U^TSU = D$, where U is orthogonal and D is diagonal. Then $S^+ = UD^+U^T$ where D^+ is again a diagonal matrix whose diagonal elements are determined according to Example 3.

Theorem: For all $A \in \mathbb{R}^{m\times n}$,

1. $A^+ = (A^TA)^+A^T = A^T(AA^T)^+$
2. $(A^T)^+ = (A^+)^T$

Both of the above two results can be proved using the limit definition of the pseudoinverse. The proof of the first result is not particularly easy nor does it have the virtue of being especially illuminating. The interested reader can consult the proof in Albert, p. 27. The proof of the second result is as follows:

$$\begin{aligned}
(A^T)^+ &= \lim_{\delta \to 0} (AA^T + \delta^2 I)^{-1} A \\
&= \lim_{\delta \to 0} [A^T (AA^T + \delta^2 I)^{-1}]^T \\
&= [\lim_{\delta \to 0} A^T (AA^T + \delta^2 I)^{-1}]^T \\
&= (A^+)^T
\end{aligned}$$

Note now that by combining the last two theorems we can, in theory at least, compute the Moore-Penrose pseudoinverse of any matrix (since AA^T and $A^T A$ are symmetric). Alternatively, we could compute the pseudoinverse by first computing the SVD of A as $A = U\Sigma V^T$ and then by the first theorem of this section $A^+ = V\Sigma^+ U^T$ where $\Sigma^+ = \begin{bmatrix} S^{-1} & 0 \\ 0 & 0 \end{bmatrix}$. This is the way it's done in MATLAB; the command is called `mpp`.

Additional useful properties of pseudoinverses:

1. $(A^+)^+ = A$
2. $(A^T A)^+ = A^+ (A^T)^+$, $(AA^T)^+ = (A^T)^+ A^+$
3. $\mathcal{R}(A^+) = \mathcal{R}(A^T) = \mathcal{R}(A^+ A) = \mathcal{R}(A^T A)$
4. $\mathcal{N}(A^+) = \mathcal{N}(AA^+) = \mathcal{N}((AA^T)^+) = \mathcal{N}(AA^T) = \mathcal{N}(A^T)$
5. If A is normal then $A^k A^+ = A^+ A^k$ for all $k > 0$, and $(A^k)^+ = (A^+)^k$ for all $k > 0$.

Note: Recall that $A \in \mathbb{R}^{n \times n}$ is *normal* if $AA^T = A^T A$. Thus if A is symmetric, skew-symmetric, or orthogonal, for example, it is normal. However, a matrix can be none of the preceding but still be normal such as

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

4 Applications to the Solution of Arbitrary Linear Systems

The first theorem is fundamental to using pseudoinverses effectively for studying the solution of arbitrary systems of linear equations.

Theorem: Suppose $A \in \mathbb{R}^{m\times n}$, $b \in \mathbb{R}^m$. Then $\mathcal{R}(b) \subseteq \mathcal{R}(A)$ if and only if $AA^+b = b$.

Proof: Suppose $\mathcal{R}(b) \subseteq \mathcal{R}(A)$. Take arbitrary $\gamma \in \mathbb{R}$ so that $\gamma b \in \mathcal{R}(b) \subseteq \mathcal{R}(A)$. Then there exists a vector $v \in \mathbb{R}^n$ such that $Av = \gamma b$. Thus we have

$$\gamma b = Av = AA^+Av = AA^+\gamma b$$

where one of the Penrose properties is used above. Since $\gamma \in \mathbb{R}$ was arbitrary, we have shown that $b = AA^+b$. To prove the converse, assume now that $AA^+b = b$. Then it is clear that $b \in \mathcal{R}(b)$ and hence

$$b = AA^+b \in \mathcal{R}(A)\ .$$

We close with some of the principal results concerning existence and uniqueness of solutions to the general matrix linear system $Ax = b$, i.e., the solution of m equations in n unknowns.

Theorem: **(Existence)** The linear system

$$Ax = b\ ;\quad A \in \mathbb{R}^{m\times n},\ b \in \mathbb{R}^m \tag{3}$$

has a solution if and only if $\mathcal{R}(b) \subseteq \mathcal{R}(A)$; equivalently, there is a solution to these m equations in n unknowns if and only if $AA^+b = b$.

Proof: The subspace inclusion criterion follows essentially from the definition of the range of a matrix. The matrix criterion is from the previous theorem.

Theorem: **(Solution)** Let $A \in \mathbb{R}^{m\times n}$, $B \in \mathbb{R}^m$ and suppose that $AA^+b = b$. Then any vector of the form

$$x = A^+b + (I - A^+A)y \quad \text{where } y \in \mathbb{R}^n \text{ is arbitrary} \tag{4}$$

is a solution of

$$Ax = b. \tag{5}$$

Furthermore, all solutions of (5) are of this form.

Proof: To verify that (4) is a solution, pre-multiply by A:

$$\begin{aligned} Ax &= AA^+b + A(I - A^+A)y \\ &= b + (A - AA^+A)y \quad \text{by hypothesis} \\ &= b \quad \text{since } AA^+A = A \text{ by the first Penrose condition.} \end{aligned}$$

That all solutions are of this form can be seen as follows. Let z be an arbitrary solution of (5), i.e., $Az = b$. Then we can write

$$\begin{aligned} z &\equiv A^+Az + (I - A^+A)z \\ &= A^+b + (I - A^+A)z \end{aligned}$$

and this is clearly of the form (4).

Remark: When A is square and nonsingular, $A^+ = A^{-1}$ and so $(I - A^+A) = 0$. Thus, there is no "arbitrary" component, leaving only the unique solution $x = A^{-1}b$.

Theorem: **(Uniqueness)** A solution of the linear equation

$$Ax = b \; ; \quad A \in \mathbb{R}^{m \times n}, \;\; B \in \mathbb{R}^m \tag{6}$$

is unique if and only if $A^+A = I$; equivalently, there is a unique solution if and only if $\mathcal{N}(A) = 0$.

Proof: The first equivalence is immediate from the form of the general solution in (4). The second follows by noting that the $n \times n$ matrix $A^+A = I$ only if $r = n$ where $r = \text{rank}(A)$ (recall $r \leq n$). But $\text{rank}(A) = n$ if and only if A is 1-1 or $\mathcal{N}(A) = 0$.

EXERCISES:

1. Use the limit definition of the pseudoinverse to compute the pseudoinverse of $\begin{bmatrix} 1 & 1 \\ 2 & 2 \end{bmatrix}$.
2. If $x, y \in \mathbb{R}^n$, show that $(xy^T)^+ = (x^Tx)^+(y^Ty)^+yx^T$.
3. For $A \in \mathbb{R}^{m \times n}$, prove that $\mathcal{R}(A) = \mathcal{R}(AA^T)$ using only definitions and elementary properties of the Moore-Penrose pseudoinverse.
4. For $A \in \mathbb{R}^{m \times n}$, prove that $\mathcal{R}(A^+) = \mathcal{R}(A^T)$.