

Least Squares Pseudoinverse

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Here we calculate a least squares solution for the Moore-Penrose pseudoinverse of an $M \times N$ matrix, A .

The Moore-Penrose pseudoinverse of an $M \times N$ matrix, A , has the property that

$$AA^+A = A \quad (1)$$

Thus, we wish to solve for the matrix A^+ . Restated in terms of the coefficients, A_{ij} , of A , this is equivalent to

$$\sum_{l=1}^N \sum_{k=1}^M A_{il} A_{lk}^+ A_{kj} = A_{ij} \quad (2)$$

The least squares solution to this equation is the solution which minimizes the Total Sum of Squares (TSS), defined by

$$\begin{aligned} \text{TSS} &= \sum_{i=1}^M \sum_{j=1}^N \left(\sum_{l=1}^N \sum_{k=1}^M A_{il} A_{lk}^+ A_{kj} - A_{ij} \right)^2 \\ \text{TSS}_{ij} &= \left(\sum_{l=1}^N \sum_{k=1}^M A_{il} A_{lk}^+ A_{kj} - A_{ij} \right)^2 \end{aligned} \quad (3)$$

The TSS is minimized by differentiating with respect to A_{nm}^+ , setting the result equal to zero, and solving for A_{nm}^+ . This yields $M \times N$ equations in $M \times N$ variables:

$$\begin{aligned} 0 &= \frac{\partial}{\partial A_{nm}^+} \text{TSS}_{ij} = 2 \left(\sum_{l=1}^N \sum_{k=1}^M A_{il} A_{lk}^+ A_{kj} - A_{ij} \right) (A_{in} A_{nm}^+ A_{mj}) \\ A_{ij} &= \sum_{l=1}^N \sum_{k=1}^M A_{il} A_{lk}^+ A_{kj} \\ A_{ij} &= \sum_{l \neq n}^N \sum_{k \neq m}^M A_{il} A_{lk}^+ A_{kj} + A_{in} A_{nm}^+ A_{mj} \\ A_{in} A_{nm}^+ A_{mj} &= A_{ij} - \sum_{l \neq n}^N \sum_{k \neq m}^M A_{il} A_{lk}^+ A_{kj} \\ A_{nm}^+ &= \frac{A_{ij} - \sum_{l \neq n}^N \sum_{k \neq m}^M A_{il} A_{lk}^+ A_{kj}}{A_{in} A_{mj}} \end{aligned} \quad (4)$$

