Moore-Pennrose Generalized Inverse

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Disclaimer

This document collects a few facts about how to compute generalized inverses of real-valued matrices in general and in particular how to get to the unique Moore-Pennrose inverse of any matrix A using the singular value decomposition of A. The results shown here are linked to solving systems of linear equations that arise in the context of least squares estimation procedures.

Introduction

What is shown here comes out of a review study of the book (Searle 1971). Chapter 1 of (Searle 1971) reviews many aspect of generalized inverse matrices pointing out that the Moore-Penrose generalized inverse is unique for any given matrix A.

A Generalized Inverse

Definition

We start with the definition of a generlized inverse matrix G for any given matrix A. The definition is given as follows. Given any matrix A, a generalized inverse matrix G of A is defined as

$$AGA = A \tag{1}$$

Computation

One possible solution for G can be computed using the construction of a diagonal form of A. This diagonal form can be computed as

$$PAQ = \Delta = \left[\begin{array}{cc} D_r & 0 \\ 0 & 0 \end{array}\right] \tag{2}$$

where D_r is a diagonal matrix of order r where r is the rank of A. From the above diagonal form (2), we can also see that

$$A = P^{-1}\Delta Q^{-1} \tag{3}$$

The inverse matrices P^{-1} and Q^{-1} exist, because matrices P and Q are matrices of elementary operations. The matrix Δ^- defined as

$$\Delta^- = \left[\begin{array}{cc} D_r^{-1} & 0 \\ 0 & 0 \end{array}\right] \tag{4}$$

is a generalized inverse of Δ satisfying the definition in (1). This is shown by writing the definition in (1) using the matrices Δ and Δ^-, as shown below.

$$\Delta\Delta^{-}\Delta = \begin{bmatrix} D_r & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} D_r^{-1} & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} D_r & 0 \\ 0 & 0 \end{bmatrix} = \Delta$$

One possible instance of the matrix G can be computed as

$$G = Q\Delta^{-}P \tag{5}$$

The matrix G given in (6) is indeed a generalized inverse of A, because according to (1), (3) and (4), we can write

$$AGA = P^{-1}\Delta Q^{-1}Q\Delta^{-}PP^{-1}\Delta Q^{-1} = P^{-1}\Delta\Delta^{-}\Delta Q^{-1} = P^{-1}\Delta Q^{-1} = A \tag{6}$$

The results of (6) and (6) shows us how to come up with a generalized inverse G for any matrix A. Now the question is how to compute such a matrix G efficiently. For that reason it is well worth while to have a closer look at formula (3).

Singular Value Decomposition (SVD)

In (3) the matrix A is decomposed into the product of three matrices P^{-1}, Δ and Q^{-1}. What we know about the three matrices is that the matrix Δ is a diagonal matrix and that matrices P^{-1} and Q^{-1} are invertible. The structure of this decomposition is very similar to the **singular value decomposition** (SVD). The SVD of a matrix A is defined as

$$A = U * D * V^T \tag{7}$$

where D is a diagonal matrix and matrices U and V are orthogonal matrices. Orthogonal matrices are special because their transpose is equal to their inverse, hence $UU^T = U^TU = I$ and $VV^T = V^TV = I$. The diagonal elements in matrix D correspond to the so called singular values of matrix A.

Generalized inverse

When looking at the SVD in (7) and comparing that to the decomposition in (3), we can see that the former decomposition is a special case of the latter one. Hence, we can use the results of the SVD of A to compute the generalized inverse G. As shown in (6), the matrix G is

$$G = Q\Delta^{-}P$$

According to (4) Δ^{-} can be computed by inverting all the non-zero diagnoal elements in Δ and Δ corresponds to the matrix D in the SVD of A. The matrices P and Q can also be taken from the SVD of A. The matrix P^{-1} in (3) corresponds to the matrix U in (7) and similarly the matrix Q^{-1} corresponds to the matrix V^T. Taking into account that matrices U and V are orthogonal, we can write

$$G = Q\Delta^{-}P = VD^{-}U^T \tag{8}$$

Properties

Using the fact that the SVD of any given matrix A is unique, the computed generalized inverse G in (8) should also be unique. The only unique generalized inverse is the Moore-Pennrose inverse which is what we found in (8). This needs to be verified.

An Example

We are given the matrix A as defined by the follwing R-statement.

```r
A <- matrix(data = c(4,1,3, 1,1,1, 2,5,3), nrow = 3)
```

$$A = \begin{bmatrix} 4 & 1 & 2 \\ 1 & 1 & 5 \\ 3 & 1 & 3 \end{bmatrix}$$

We start by the SVD of A

```r
tol = sqrt(.Machine$double.eps)
svd_A <- svd(A)
nz <- svd_A$d > tol * svd_A$d[1]
G = svd_A$v[, nz] %*% (t(svd_A$u[, nz]) / svd_A$d[nz])
```

$$G = \begin{bmatrix} 0.2105 & -0.1447 & 0.0921 \\ 0.0226 & 0.0113 & 0.0188 \\ -0.0752 & 0.2124 & 0.0207 \end{bmatrix}$$

Verifying whether the computed matrix G really is a generalized inverse can be done by

```r
sum( abs(A %*% G %*% A - A) )
```

```
## [1] 8.881784e-15
```

The function `MASS::ginv` does the same computation as above which is much easier than what was shown above.

```r
Ginv <- MASS::ginv(X = A)
```

$$Ginv = \begin{bmatrix} 0.2105 & -0.1447 & 0.0921 \\ 0.0226 & 0.0113 & 0.0188 \\ -0.0752 & 0.2124 & 0.0207 \end{bmatrix}$$

Solving Systems of Linear Equations

The reason why generalized inverses are important, because they play an important role in computing solutions to systems of consistent linear equations. A system of linear equations is consistent when every linear relationship between rows in the coefficient matrix is also present in the right-hand side vector. From this definition, it follows that only consistent equations do have solutions for the vector of unknowns.

Assume, we are given the following system of consistent equations

$$Ax = y$$

We want to find a matrix G for which we can write

$$x = Gy$$

in order to get to the vector x of unknowns. Theorem 1 in (Searle 1971) states that $x = Gy$ is a solution to $Ax = y$, if and only if (iff) $AGA = A$.

The proof given in (Searle 1971) proceeds as follows. If $Ax = y$ is consistent and has solutions $x = Gy$, we consider the equations

$$Ax = a_j$$

where a_j is the j-th column of A. The system $Ax = a_j$ has a solution, namely the null vector with element $x[j] = 1$, hence the system is consistent. Furthermore, since consistent equations $Ax = y$ all have a solution $x = Gy$, we can write

$$x = Ga_j$$

Pre-multiplying both sides of the above equation with A and using the above specification of the system of equations, leads to

$$Ax = AGa_j = a_j$$

This is true for all columns a_j of A and hence $AGA = A$.

Conversely, if $AGA = A$, then $AGAx = Ax$ and when $Ax = y$, then $AGy = y$ and $A(Gy) = y$, hence

$$x = Gy$$

is a solution of $Ax = y$. Because the matrix G is not required to be unique, but is just one possible generalized inverse, the above shown solution for x is also not unique.

Theorem 2 in (Searle 1971) gives all solutions $\tilde{x}$ for $A\tilde{x} = y$ as

$$\tilde{x} = Gy - (GA - I)z$$

for an arbitrary vector z. The proof for this is obtained by pre-multiplying the above equation with A yielding

$$A\tilde{x} = AGy - (AGA - A)z$$

because $AGA = A$ and by Theorem 1 $\tilde{x} = Gy$ is a solution, Theorem 2 holds.

Least Squares

In simple fixed linear models $y = Xb + e$ with $Var(y) = I\sigma^2$, estimates $\hat{b}$ for the unknown parameter vector b are obtained by

$$(X^TX)\hat{b} = X^Ty$$

In general, matrix X does not have full column rank and hence (X^TX) is singular and cannot be inverted. Using the result of Theorem 1 in (Searle 1971), we can still write one solution for $\hat{b}$ as

$$\hat{b} = (X^TX)^-X^Ty$$

(Searle 1971) shows a list of useful properties of generalized inverses of symmatric matrices such as (X^TX)

References

Searle, S.R. 1971. *Linear Models.* Wiley Classics.