The 2 by 2 Real Pseudo Inverse

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This is a brief note on the math behind the direct PRESS statistic calculation¹ found in the RcppDynProg package².

The actual 'C++' code³ is a bit ugly and intimidating. That is because we are using a verbose scalar notation to represent matrix concepts. In matrix notation we are solving a linear system by inverting a two by two matrix (yes, there are the usual admonitions that one should not invert a matrix to solve a linear system, but for system this small they do not apply). We are in turn inverting the two by two matrix by exploiting the following well know rule.

If ad - bc is not zero then:

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix}^{-1} = \frac{1}{ad - bc} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$$

Throughout a, b, c, and d all real scalars.

This can be re-written as the following general relation.

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix} = (ad - bc) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

The above can be directly checked just by applying the rules for multiplying matrices to the left two matrices. This has a particularly pleasant presentation if we recognize that ad - bc is the determinant of the left matrix and use the traditional vertical bar determinant notation.

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix} = \begin{vmatrix} a & b \\ c & d \end{vmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Now there is an issue of what to do when ad-bc is zero. For our implementation we apply Tikhonov regularized⁴ which (barring the exact numeric coincidence of minus two times the expected value of the independent variable equaling our regularization constant) is going to be non-singular. For our actual application, we could simply switch degenerate situations to the out-of sample mean implementation⁵.

 $^{^1}$ http://www.win-vector.com/blog/2014/09/estimating-generalization-error-with-the-press-statistic/

²https://github.com/WinVector/RcppDynProg

³https://github.com/WinVector/RcppDynProg/blob/master/src/xlin_fits.cpp

 $^{^4}$ https://en.wikipedia.org/wiki/Tikhonov_regularization

 $^{^5 {\}tt https://github.com/WinVector/RcppDynProg/blob/master/src/const_costs.cpp}$

But, for fun, let's play with the math a bit.

There is an additional lesser known algebraic relation for two by two matrices.

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} a & c \\ b & d \end{pmatrix} \begin{pmatrix} a & b \\ c & d \end{pmatrix} = (a^2 + b^2 + c^2 + d^2) \begin{pmatrix} a & b \\ c & d \end{pmatrix} + (ad - bc) \begin{pmatrix} -d & c \\ b & -a \end{pmatrix}$$

Or (using transpose, matrix Frobenius norm, and determinant notation):

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} a & b \\ c & d \end{pmatrix}^{\top} \begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} a & b \\ c & d \end{pmatrix}_{2}^{2} \begin{pmatrix} a & b \\ c & d \end{pmatrix} + \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} -d & c \\ b & -a \end{pmatrix}$$

The superscript "top" denoting the transpose operation, the $||.||_2^2$ denoting sum of squares norm, and the single |.| denoting determinant.

This means, if ad - bc is zero then:

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} a & b \\ c & d \end{pmatrix}^{\top} \begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} a & b \\ c & d \end{pmatrix}_{2}^{2} \begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

Once we [confirm the above relation⁶ we can also confirm that if $a^2 + b^2 + c^2 + d^2$ is not zero, then the following matrix:

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix}^+ = \frac{1}{a^2 + b^2 + c^2 + d^2} \begin{pmatrix} a & c \\ b & d \end{pmatrix}$$

satisfies all of the conditions for being the Moore Penrose inverse 7 (or pseudoinverse) of our original matrix. The superscript-plus denoting the Moore Penrose inverse operation.

Or in transpose notation:

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix}^+ = \frac{1}{a^2 + b^2 + c^2 + d^2} \begin{pmatrix} a & b \\ c & d \end{pmatrix}^\top$$

This is called the pseudo-inverse because it acts like an inverse, even for non-invertible matrices. For the pseudo-inverse we have:

$$AA^+A = A$$

And the above looks a lot like an inverse. We can think of it having almost canceled the A to the left or the A to the right.

For general matrices the situation is much more complicated.

However, for a real 2 by 2 matrix:

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

 $^{^{6} \}texttt{https://github.com/WinVector/RcppDynProg/blob/master/extras/PseudoInverse.ipynb}$

^{'7}https://en.wikipedia.org/wiki/MoorePenrose_inverse

The MoorePenrose inverse is:

when ad - bc is not zero:

$$\frac{1}{ad - bc} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$$

when ad-bc is zero and $a^2+b^2+c^2+d^2$ is not zero:

$$\frac{1}{a^2 + b^2 + c^2 + d^2} \begin{pmatrix} a & c \\ b & d \end{pmatrix}$$

otherwise:

 $\begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$

The wealth of symmetries and relations is really kind of neat.