The 2 by 2 Pseudo Inverse

This is a brief note on the math behind the direct PRESS statistic calculation found in the `RcppDynProg` package.

The actual `C++` code 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 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 which allows us to write the expression as follows.

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

Then if $ad - bc$ is not zero then:

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

And that is what was translated into `C++` code.

Now there is an issue of what to do when $ad - bc$ is zero. For our implementation we apply Tikhonov regularized 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 implementation.

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

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

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

This means, if $ad - bc$ is zero then:

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

Or (using transpose notation), if if $ad - bc$ is zero then:

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

The superscript "top" denoting the transpose operation.

Once we confirm the above relation 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 (or pseudo-inverse) 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 cancelled 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

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

The Moore–Penrose 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.