Inverting Over-Determined Matrices

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Inverting Over-Determined Matrices

Given you know how to invert a square non-singular matrix, how can we invert an over-determined matrix – that is how is a least squares fit done?

Inverting Over-Determined Matrices

Surprisingly, this can be accomplished with a short one-line APL expression.

Even more surprisingly, there is a short (half page) mathematical proof of the validity of this expression by Berthold K. P. Horn:

http://people.csail.mit.edu/bkph/articles/Pseudo_Inverse.pdf

(with an excursion into Matrix Calculus).

Inverting Over-Determined Matrices

Suppose **y = Mx** where **M** is a known **n×m** matrix, **y** is a known **n**-vector and **x** is an unknown **m**-vector. Mathematicians call these “column vectors”.

A least-squares solution minimizes the error term **(y − Mx)**. That is, we want to find **x** that minimizes

$$
\begin{aligned}
\mathbf{f(x)} &= \|\mathbf{y} - \mathbf{Mx}\|^2 \\
&= (\mathbf{y} - \mathbf{Mx})^T (\mathbf{y} - \mathbf{Mx}) \\
&= (\mathbf{y}^T - \mathbf{x}^T\mathbf{M}^T) (\mathbf{y} - \mathbf{Mx}) \\
&= \mathbf{y}^T\mathbf{y} - \mathbf{y}^T\mathbf{Mx} - \mathbf{x}^T\mathbf{M}^T\mathbf{y} + \mathbf{x}^T\mathbf{M}^T\mathbf{Mx}
\end{aligned}
$$

How do we find a minimum of this (matrix!) function?

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Calculus to the rescue!

One of the lessons of calculus is that to solve a minimization problem, we differentiate the function and set the result equal to zero.

Except, how do we differentiate a matrix function?

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Fortunately, differential calculus has been extended to matrices in the form of Matrix Calculus. Here's (almost) everything you need to know about differentiating a matrix function:

	$f(x)$	$f'(x)$
1	Ax	A^T
2	x^TA	A
3	x^TAx	$(A+A^T)x$

For more details, see

http://www.colorado.edu/engineering/cas/courses.d/IFEM.d/IFEM.AppD.d/IFEM.AppD.pdf

Inverting Over-Determined Matrices

0: $\mathbf{f(x) = y^T y - y^T M x - x^T M^T y + x^T M^T M x}$

Differentiating w.r.t. **x** (using the rules of Matrix Calculus) and setting the result equal to zero yields

1: $\mathbf{f'(x) = 0 - (y^T M)^T - M^T y + 2M^T M x = 0}$

2: $\mathbf{-2M^T y + 2M^T M x = 0}$

3: $\mathbf{M^T M x = M^T y}$

4: $\mathbf{x = (M^T M)^{-1} M^T y}$

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(⌹(⍉M)+.×M)+.×⍉M
←→ (⍉M)⌹(⍉M)+.×M
←→ (⍉M)⌹M⌹⍉⌹M
```
(Roy)

	f(x)	f '(x)
1	**Ax**	$\mathbf{A^T}$
2	$\mathbf{x^T A}$	**A**
3	$\mathbf{x^T A x}$	$\mathbf{(A+A^T)x}$