Another Discussion of Least Squares

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Suppose we are faced with solving the linear system of equations $Ax = b$ where A is not square and the system has no solution. There are many versions of "do the best we can". One version called *Tikhonov Regularization* is as follows. We pick a convenient matrix L (maybe the identity matrix or maybe 0) and find the vector or vectors x that minimize

$$g(x) = \|Ax - b\|^2 + \|Lx\|^2 .$$

In some contexts this is a best fit to for a problem that doesn't have a solution. This note will prove that the equation

$$A^T Ax + L^T Lx = A^T b$$

always has a solution that minimizes $g(x)$ and for many L (for example $L = I$) the solution is unique.

Definition 1. *A C^2 function f defined on all of $\mathbb{R}^n$ is* ***convex*** *if the Hessian matrix $H = [h_{ij}] = [\partial^2_{x_1 x_j} f]$ is positive semidefinite.*

Remark 1. *Sometimes this is taken as a theorem. We will take it as a definition.*

Proposition 1. *Suppose a convex function f has a critical point a. Then $f(x) \geq f(a)$ for all x. If f has a minimum it is attained at a critical point. Hence if a convex function has a minimum it is unique. (The minimum may be attained at more than one point.)*

Proof. The proof that if f has a minimum it is attained at a critical point is easy and will be left out. So suppose a is a critical point. Then by Taylor's theorem

$$f(x) = f(a) + \frac{1}{2}(x - a)^T H(c)(x - a),$$

where $H(c)$ is the Hessian evaluated at some point between x and a. This is Lagrange's form for the remainder. Since $(x - a)^T H(c)(x - a) \geq 0$, $f(x) \geq f(a)$ and f has a minimum at a. □

We compute the directional derivative $D_v g(x)$.

$$g(x+tv) = x^T A^T Ax + 2tv^T A^T Ax + t^2 v^T A^T Av - 2tv^T A^T b - 2x^T A^T b + \|b\|^2 + x^T L^T Lx + 2tv^T L^T Lx + t^2 v^T L^T Lv.$$

Now differentiate with respect to t and set $t = 0$ to get

$$2v^t [A^T Ax - A^T b + L^T Lx] = 0,$$

or

$$(A^T A + L^T L)x = A^T b.$$

This is a generalization of the *normal equations*. Let us denote a solution of this equation by a. It is a critical point of g.

If we compute $g''(0)$ at any point x we get $2v^T(A^TA + L^TL)v$, so the Hessian of g is

$$H = 2(A^TA + L^TL).$$

Since this is a positive semidefinite matrix, g is convex and the critical points (if they exist) are indeed points where g has a *global* minimum.

So we now address a general problem.

Problem 1. *When does a linear equation $Lx = b$ have a solution?*

The answer is the

Theorem 1 (Fredholm Alternative)**.** *1. $Lx = b$ has a solution exactly when b is orthogonal to every vector z that is orthogonal to the column space of L. Hence there is a solution if $z^TL = 0$ implies that $z^Tb = 0$.*

2. Either $Lx = b$ has a solution or there is a vector z so that $z^TA = 0$ and $z^Tb \neq 0$.

These two statements are equivalent. The second statement is the ***alternative*** *version of the theorem. Jim Burke says this is* the Fundamental Theorem of the Alternative

Proof. We use the fact that in finite dimensional vector spaces the orthogonal complement of the orthogonal complement of a subspace W is W. So b is in the column space of L exactly when it is orthogonal to every vector orthogonal to the column space. That is what the theorem says. □

How do we use this result? When does $(A^TA + L^TL)a = A^Tb$ have a solution? Suppose

$$z^TA^TA + z^TL^TL = 0.$$

Then

$$\|Az\|^2 + \|Lz\|^2 = 0.$$

So $Az = 0$ and $Lz = 0$. But then $z^TA^Tb = (Az)^Tb = 0$ so there is always a solution and hence always a minimum.