1.4 Minimum Principles

Notes

1E If A is positive definite, the quadratic $P(x) = \frac{1}{2}x^TAx - x^Tb$ is minimized at the point where $Ax=b$. The minimum value is

$$P(A^{-1}b) = -\frac{1}{2}b^TA^{-1}b$$

Proof: Suppose x is the solution to $Ax=b$ and let y be any point.

$$\begin{aligned}
P(y) - P(x) &= \tfrac{1}{2}y^TAy - y^Tb - \tfrac{1}{2}x^TAx + x^Tb \\
&= \tfrac{1}{2}y^TAy - y^TAx - \tfrac{1}{2}x^TAx + x^TAx \\
&= \tfrac{1}{2}y^TAy - y^TAx + \tfrac{1}{2}x^TAx \\
&= \tfrac{1}{2}y^TAy - \tfrac{1}{2}y^TAx - \tfrac{1}{2}y^TAx + \tfrac{1}{2}x^TAx \\
&= \tfrac{1}{2}(y^TAy - y^TAx - y^TAx + x^TAx) \\
&= \tfrac{1}{2}(y^TAy - x^TAy - y^TAx + x^TAx) \\
&= \tfrac{1}{2}((y^T - x^T)Ay - (y^T - x^T)Ax) \\
&= \tfrac{1}{2}((y-x)^TAy + (y-x)^TA(-x)) \\
&= \tfrac{1}{2}(y-x)^TA(y-x)
\end{aligned}$$

Use: $y^TAx = y^TA^Tx = x^TAy$

$P(y) - P(x) = \frac{1}{2}(y-x)^TA(y-x) \geq 0$ with equality iff $y-x=0$ since A is positive definite. Conclude that $x = A^{-1}b$ is the unique minimizer of P and

$$\begin{aligned}
P(x_{min}) = P(A^{-1}b) &= \tfrac{1}{2}(A^{-1}b)^TAA^{-1}b - (A^{-1}b)^Tb \\
&= \tfrac{1}{2}b^T(A^{-1})^Tb - b^T(A^{-1})^Tb \\
&= \tfrac{1}{2}b^TA^{-1}b - b^TA^{-1}b \\
&= -\tfrac{1}{2}b^TA^{-1}b
\end{aligned}$$

Use: $I = AA^{-1} = A^TA^{-1} \rightarrow (A^T)^{-1} = A^{-1}$

Alternatively,

$$\tfrac{1}{2}(x - A^{-1}b)^TA(x - A^{-1}b) - \tfrac{1}{2}b^TA^{-1}b$$

$-\frac{1}{2}b^TA^{-1}b$ constant wrt x. Writing $P(x)$ in this way shows $P(x)$ minimized when $x = A^{-1}b$ and $P_{min} = -\frac{1}{2}b^TA^{-1}b$.

$$= \tfrac{1}{2}x^TAx - \tfrac{1}{2}b^T(A^{-1})^TAx - \tfrac{1}{2}x^TAA^{-1}b + \tfrac{1}{2}b^T(A^{-1})^TAA^{-1}b - \tfrac{1}{2}b^TA^{-1}b$$

$$= \tfrac{1}{2}x^TAx - \tfrac{1}{2}b^T(A^{-1})^Tb - \tfrac{1}{2}x^Tb + 0 = \tfrac{1}{2}x^TAx - \tfrac{1}{2}x^Tb - \tfrac{1}{2}x^Tb = \tfrac{1}{2}x^TAx - x^Tb = P(x)$$

Consider now the case that A is not assumed to be symmetric positive definite. The coefficient matrix for a physical problem often gets assembled as A^TCA. The matrices A^TA and A^TCA are always symmetric (when C is). We want to know when they are positive definite.

<u>1F</u> (i) If A has linearly independent columns — it can be square or rectangular — then the product A^TA is positive definite.

(ii) If C is symmetric positive definite, so is the triple product A^TCA.

Note that if A is $m \times n$, the columns of A can only be independent if $n \leq m$. If $n > m$ we have no hope of independence since the number of independent rows is the same as the number of independent columns by the fundamental theorem of linear algebra.

Proof (1F): Suppose the columns of A are linearly independent.

$x^TA^TAx = (Ax)^T(Ax) = \|Ax\|_2^2 \geqslant 0$ with equality iff $Ax = 0$. Since the columns of A are independent, $Ax = 0$ iff $x = 0$. Thus x^TA^TAx is positive except when $x = 0$. Conclude A^TA is positive definite.

Suppose C is positive definite and A has linearly independent columns.

$x^TA^TCAx = (Ax)^TC(Ax) \geqslant 0$ with equality iff $Ax = 0$ iff $x = 0$.

Therefore A^TCA is positive definite.

<u>Least Squares Solution of $Ax = b$</u>

Suppose A is $m \times n$ with $m > n$. The problem $Ax = b$ is an overdetermined system of m equations in n unknowns. The vectors b that can be solved for form the n-dimensional subspace of m-dimensional space. This subspace is called the <u>column space</u> of A. $Ax = b$ has a solution iff b is in the column space of A. With $n < m$ that is unlikely.

In general there will be an error $e = b - Ax$. We emphasize that the components e_i of e are the 'vertical' distances between each component of b and Ax, not the shortest distances.

To minimize error is equivalent to minimizing $\|Ax - b\|^2 = (Ax - b)^T(Ax - b)$ if we measure a vector in the most common way.

The question is which x will minimize $\|Ax - b\|^2$. The answer is given in 1G, which we prove using 1E.

<u>1G</u> The x that minimizes $\|Ax-b\|^2$ is the solution to the <u>normal equations</u>:

$$A^TAx = A^Tb$$

This vector $x = (A^TA)^{-1}A^Tb$ is the least squares solution to $Ax=b$.

Proof: We should assume A has linearly independent columns since it is assumed $Ax=b$ is overdetermined and b is not in the column space of A. Removing any dependent columns and reassigning A doesn't change this. Then A^TA is positive definite by 1F. It follows that A^TA is invertible since $A^TAx=0 \rightarrow x^TA^TAx = 0 \rightarrow x=0$ shows that if x is in the null space of A, then $x=0$. In other words, the null space of A^TA is trivial.

The error $e=b-Ax$ is minimized when $\|Ax-b\|^2$ is minimized.

$$\|Ax-b\|^2 = (Ax-b)^T(Ax-b) = (x^TA^T-b^T)(Ax-b) = x^TA^TAx - x^TA^Tb - b^TAx + b^Tb$$

But $\|Ax-b\|^2$ is minimized when $\frac{1}{2}\|Ax-b\|^2$ is minimized and $x^TA^Tb = b^TAx$ since both are scalars so $x^TA^Tb = (x^TA^Tb)^T = b^TAx$. Finally note that since b^Tb is constant wrt x, it does not affect our choice of x in the minimization and should therefore be ignored in the minimization.

Thus we want to find the x that minimizes $\frac{1}{2}x^TA^TAx - x^TA^Tb$. Recall from 1E that the solution x of $Ax=b$ minimizes $P(x) = \frac{1}{2}x^TAx - x^Tb$. Replace the matrix A by the matrix A^TA and the vector b by the vector A^Tb. Then 1E applies here since A^TA is positive definite. This tells us that the x that minimizes $\frac{1}{2}x^TA^TAx - x^TA^Tb$ is the solution to $A^TAx = A^Tb$.

$\therefore x = (A^TA)^{-1}A^Tb$ minimizes the error $e = b - Ax$