

## 1.4 Minimum Principles

### Notes

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

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

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

$$\begin{aligned} P(y) - P(x) &= \frac{1}{2}y^T A y - y^T b - \frac{1}{2}x^T A x + x^T b \\ &= \frac{1}{2}y^T A y - y^T A x - \frac{1}{2}x^T A x + x^T A x \\ &= \frac{1}{2}y^T A y - y^T A x + \frac{1}{2}x^T A x \\ &= \frac{1}{2}y^T A y - \frac{1}{2}y^T A x - \frac{1}{2}y^T A x + \frac{1}{2}x^T A x \\ &= \frac{1}{2}(y^T A y - y^T A x - y^T A x + x^T A x) \\ &= \frac{1}{2}(y^T A y - x^T A y - y^T A x + x^T A x) \\ &= \frac{1}{2}((y^T - x^T)A y - (y^T - x^T)A x) \\ &= \frac{1}{2}((y-x)^T A y + (y-x)^T A(-x)) \\ &= \frac{1}{2}(y-x)^T A(y-x) \end{aligned}$$

Use:  $y^T A x = y^T A^T x = x^T A y$

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

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

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

Alternatively,

$$\begin{aligned} \frac{1}{2}(x-A^{-1}b)^T A(x-A^{-1}b) - \frac{1}{2}b^T A^{-1}b &\quad \leftarrow -\frac{1}{2}b^T A^{-1}b \text{ constant wrt } x. \text{ Writing } P(x) \text{ in this way shows } P(x) \text{ minimized when } x = A^{-1}b \text{ and } P_{\min} = -\frac{1}{2}b^T A^{-1}b. \\ &= \frac{1}{2}x^T A x - \frac{1}{2}b^T (A^{-1})^T A x - \frac{1}{2}x^T A A^{-1}b + \frac{1}{2}b^T (A^{-1})^T A A^{-1}b - \frac{1}{2}b^T A^{-1}b \\ &= \frac{1}{2}x^T A x - \frac{1}{2}b^T (A^{-1})^T b - \frac{1}{2}x^T b + 0 = \frac{1}{2}x^T A x - \frac{1}{2}x^T b - \frac{1}{2}x^T b = \frac{1}{2}x^T A x - x^T b = P(x) \end{aligned}$$

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.

1F (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.

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

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

$x^T A^T C A x = (Ax)^T C (Ax) \geq 0$  with equality iff  $Ax = 0$  iff  $x = 0$ .

Therefore  $A^T C A$  is positive definite.

### Least Squares Solution of $Ax = b$

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 column space 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.

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

$$A^T A x = A^T b$$

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

Proof: For this section it is assumed that the columns of  $A$  are independent. Then  $A^T A$  is positive definite by 1F. It follows that  $A^T A$  is invertible since

$A^T A x = 0 \rightarrow x^T A^T A x = 0 \rightarrow x = 0$  shows that if  $x$  is in the null space of  $A$ , then  $x = 0$ . In other words, the null space of  $A^T A$  is trivial.

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

$$\|Ax - b\|^2 = (Ax - b)^T (Ax - b) = (x^T A^T - b^T)(Ax - b) = x^T A^T A x - x^T A^T b - b^T A x + b^T b$$

But  $\|Ax - b\|^2$  is minimized when  $\frac{1}{2} \|Ax - b\|^2$  is minimized and  $x^T A^T b = b^T A x$  since both are scalars so  $x^T A^T b = (x^T A^T b)^T = b^T A x$ . Finally note that since  $b^T b$  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  $\frac{1}{2} x^T A^T A x - x^T A^T b$ . Recall from 1E that the solution  $x$  of  $Ax = b$  minimizes  $P(x) = \frac{1}{2} x^T A x - x^T b$ . Replace the matrix  $A$  by the matrix  $A^T A$  and the vector  $b$  by the vector  $A^T b$ . Then 1E applies here since  $A^T A$  is positive definite. This tells us that the  $x$  that minimizes  $\frac{1}{2} x^T A^T A x - x^T A^T b$  is the solution to  $A^T A x = A^T b$ .

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

We could call the error minimizing point  $p = (A^T A)^{-1} A^T b$  for 'projection' since  $Ap$  is the closest point to  $b$  in the column space of  $A$ . Note

$$A^T e = A^T(b - Ap) = A^T b - A^T A p = 0$$

The inner (dot) product of  $e$  with each column of  $A$  is zero by this calculation — the error is orthogonal to the column space of  $A$  when we choose  $x = p$ , the projection of  $b$  onto the column space of  $A$ .

The takeaway from this section is simple:

If  $Ax = b$  has no solution, multiply by  $A^T$  and solve  $A^T A x = A^T b$

## Linear Regression

1H Given measurements  $b_1, \dots, b_m$  at times  $t_1, \dots, t_m$ , the line  $y = \alpha t + \beta$  which minimizes error  $\|b - At\|^2$  is determined by

$$A^T A x = A^T b \quad \text{or} \quad \begin{bmatrix} m & \sum t_i \\ \sum t_i & \sum t_i^2 \end{bmatrix} \begin{bmatrix} \beta \\ \alpha \end{bmatrix} = \begin{bmatrix} \sum b_i \\ \sum t_i b_i \end{bmatrix}$$

The best line is  $y = \bar{b} + \alpha(t - \bar{t})$  with  $\alpha = \frac{\sum (t_i - \bar{t}) b_i}{\sum (t_i - \bar{t})^2}$

Proof: The previous section explains how to set up a system that will minimize the error in describing the relationship between the  $t_i$  and  $b_i$  using a line  $y = Ct + D$ . First write out the system we want to solve

$$\begin{array}{l} \beta + \alpha t_1 = b_1 \\ \beta + \alpha t_2 = b_2 \\ \vdots \\ \beta + \alpha t_m = b_m \end{array} \rightarrow \begin{bmatrix} 1 & t_1 \\ 1 & t_2 \\ \vdots & \vdots \\ 1 & t_m \end{bmatrix} \begin{bmatrix} \beta \\ \alpha \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{bmatrix} \rightarrow Ax = b$$

(A)      (x)      (b)

If  $Ax = b$  has a solution this is fine - it means all the  $b_i$  lie along a line and error  $e = 0$ . But in the case we mainly want to consider, the measurements will not be perfectly linear and  $Ax = b$  has no solution:

Solve  $A^T A x = A^T b$  for  $x$

Unless  $t_1 = t_2 = \dots = t_m$  the columns of  $A$  are independent,  $A^T A$  is positive definite and thus a unique solution  $x = (A^T A)^{-1} A^T b$  can be found.\*

$$A^T A x = \begin{bmatrix} 1 & 1 & \dots & 1 \\ t_1 & t_2 & \dots & t_m \end{bmatrix} \begin{bmatrix} 1 & t_1 \\ 1 & t_2 \\ \vdots & \vdots \\ 1 & t_m \end{bmatrix} \begin{bmatrix} \beta \\ \alpha \end{bmatrix} = \begin{bmatrix} 1 & 1 & \dots & 1 \\ t_1 & t_2 & \dots & t_m \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{bmatrix} = A^T b$$

$$A^T A x = \begin{bmatrix} m & \sum t_i \\ \sum t_i & \sum t_i^2 \end{bmatrix} \begin{bmatrix} \beta \\ \alpha \end{bmatrix} = \begin{bmatrix} \sum b_i \\ \sum b_i t_i \end{bmatrix} = A^T b$$

This shows that to find the  $\alpha, \beta$  such that the error in fitting  $y = \alpha t + \beta$  to  $b$  is minimized by solving this  $2 \times 2$  system. Use either the formula for the inverse of a  $2 \times 2$  matrix or use Gaussian elimination. We use the second approach next to find  $x = \begin{bmatrix} \beta \\ \alpha \end{bmatrix}$ .

\* If the columns of  $A$  were dependent we would need to use a pseudoinverse.

$$\begin{aligned}
 \left[ \begin{array}{cc|c} m & \sum t_i & \sum b_i \\ \sum t_i & \sum t_i^2 & \sum t_i b_i \end{array} \right] &\sim \left[ \begin{array}{cc|c} 1 & \bar{t} & \bar{b} \\ 0 & \frac{1}{m} \sum t_i^2 & \frac{1}{m} \sum t_i b_i \end{array} \right] \\
 &\sim \left[ \begin{array}{cc|c} 1 & \bar{t} & \bar{b} \\ 0 & \frac{1}{m} \sum t_i^2 - \bar{t}^2 & \frac{1}{m} \sum t_i b_i - \bar{b} \bar{t} \end{array} \right] \\
 &\sim \left[ \begin{array}{cc|c} 1 & \bar{t} & \bar{b} \\ 0 & 1 & \alpha \end{array} \right] \quad (\alpha \text{ simplified below}) \\
 &\sim \left[ \begin{array}{cc|c} 1 & 0 & \beta \\ 0 & 1 & \alpha \end{array} \right] \quad (\beta = \bar{b} - \alpha \bar{t} \text{ simplified below})
 \end{aligned}$$

$$\begin{aligned}
 \alpha &= \frac{\frac{1}{m} \sum t_i b_i - \bar{b} \bar{t}}{\frac{1}{m} \sum t_i^2 - \bar{t}^2} = \frac{\sum t_i b_i - \frac{1}{m} \sum b_i \sum t_i}{\sum t_i^2 - \frac{1}{m} \sum t_i \sum t_i} = \frac{\sum t_i b_i - \sum \bar{t} b_i}{\sum t_i^2 - \sum \bar{t} t_i} = \frac{\sum (t_i - \bar{t}) b_i}{\sum (t_i^2 - \bar{t} t_i)} \\
 &= \frac{\sum (t_i - \bar{t}) b_i}{\sum (t_i^2 - 2\bar{t} t_i + \bar{t}^2) + \sum (\bar{t} t_i - \bar{t}^2)} = \frac{\sum (t_i - \bar{t}) b_i}{\sum (t_i - \bar{t})^2 + \sum (\bar{t} t_i) - \bar{t}^2} = \frac{\sum (t_i - \bar{t}) b_i}{\sum (t_i - \bar{t})^2 + \bar{t}^2 - \bar{t}^2}
 \end{aligned}$$

$$\alpha = \frac{\sum (t_i - \bar{t}) b_i}{\sum (t_i - \bar{t})^2}$$

or

$$\alpha = \frac{\frac{1}{m} \sum t_i b_i - \bar{b} \bar{t}}{\frac{1}{m} \sum t_i^2 - \bar{t}^2} = \frac{\sum t_i b_i - m \bar{b} \bar{t}}{\sum t_i^2 - m \bar{t}^2}$$

$$\beta = \bar{b} - \alpha \bar{t} = \bar{b} - \frac{\bar{t} \sum t_i b_i - m \bar{b} \bar{t}^2}{\sum t_i^2 - m \bar{t}^2} = \frac{\bar{b} \sum t_i^2 - m \bar{b} \bar{t}^2 - \bar{t} \sum t_i b_i + m \bar{b} \bar{t}^2}{\sum t_i^2 - m \bar{t}^2}$$

$$\beta = \frac{\bar{b} \sum t_i^2 - \bar{t} \sum t_i b_i}{\sum t_i^2 - m \bar{t}^2}$$

The line of best fit is  $y = \alpha t + \beta$  with

$$\alpha = \frac{\sum (t_i - \bar{t}) b_i}{\sum (t_i - \bar{t})^2} = \frac{\sum t_i b_i - m \bar{b} \bar{t}}{\sum t_i^2 - m \bar{t}^2} \quad \beta = \frac{\bar{b} \sum t_i^2 - \bar{t} \sum t_i b_i}{\sum t_i^2 - m \bar{t}^2}$$

Alternatively we could write this using  $\beta = \bar{b} - \alpha \bar{t}$  as

$$y = \alpha t + \bar{b} - \alpha \bar{t} = \bar{b} + \alpha(t - \bar{t}) \text{ with } \alpha = \frac{\sum (t_i - \bar{t}) b_i}{\sum (t_i - \bar{t})^2} = \frac{\sum t_i b_i - m \bar{b} \bar{t}}{\sum t_i^2 - m \bar{t}^2}$$

## Exercises

1.4.2 What equations determine the minimizing  $x$  for

(i)  $P = \frac{1}{2}x^T Ax - x^T b$  ?

By 1E,

$P$  is minimized at the point  $x$  where  $Ax = b$ .

The minimum value is  $P(A^{-1}b) = -\frac{1}{2}b^T A^{-1}b$ .

(ii)  $P = \frac{1}{2}x^T A^T Ax - x^T A^T b$  ?

Replacing  $A$  with  $A^T A$  and  $b$  with  $A^T b$  in 1E,

$P$  is minimized by the point  $x$  where  $A^T A x = A^T b$ .

The minimum value is  $P((A^T A)^{-1} A^T b) = -\frac{1}{2}b^T A(A^T A)^{-1} A^T b = -\frac{1}{2}b^T b$

(iii)  $E = \|Ax - b\|^2$  ?

$$E = \|Ax - b\|^2 = (Ax - b)^T (Ax - b) = x^T A^T Ax - x^T A^T b - b^T A x + b^T b$$

$$= x^T A^T Ax - 2x^T A^T b + b^T b \quad (x^T A^T b = b^T A x \text{ since they are scalars})$$

Since  $b^T b$  does not depend on  $x$ , minimizing  $x^T A^T Ax - 2x^T A^T b + b^T b$  is equivalent to minimizing  $x^T A^T Ax - 2x^T A^T b$ . But then minimizing  $x^T A^T Ax - 2x^T A^T b$  is equivalent to minimizing  $\frac{1}{2}x^T A^T A x - x^T A^T b$ , which is  $P$  of part (ii). Therefore:

$E$  is minimized by the point  $x$  where  $A^T A x = A^T b$

The minimum value is  $E((A^T A)^{-1} A^T b) = 0$

Check:  $E((A^T A)^{-1} A^T b) = b^T A(A^T A)^{-1 T} A^T A(A^T A)^{-1} A^T b - 2b^T A(A^T A)^{-1 T} A^T b + b^T b$   
 $= b^T A(A^T A)^{-1} A^T b - 2b^T A(A^T A)^{-1} A^T b + b^T b$   
 $= b^T A A^{-1} A^{-1 T} A^T b - 2b^T A A^{-1} A^{-1 T} A^T b + b^T b$   
 $= b^T b - 2b^T b + b^T b = 0$

Alternatively, reverse the logic of the previous paragraph, applied to the minimum  $P$  of part (ii), to find:

$$\min_x E = 2(-\frac{1}{2}b^T b) + b^T b = -b^T b + b^T b = 0$$

1.4.4 Find the best least squares solution to

$$Ax = \begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix} = \begin{bmatrix} 0 \\ 4 \\ 2 \end{bmatrix} = b$$

By 1H, the best line is  $y = \bar{b} + \alpha(t - \bar{t})$  with  $\alpha = \frac{\sum (t_i - \bar{t})b_i}{\sum (t_i - \bar{t})^2}$ .

$$\bar{b} = (0+4+2)/3 = 2, \quad \bar{t} = (1+2+3)/3 = 2$$

$$\alpha = \frac{\sum (t_i - \bar{t})b_i}{\sum (t_i - \bar{t})^2} = \frac{(1-2) \cdot 0 + (2-2) \cdot 4 + (3-2) \cdot 2}{(1-2)^2 + (2-2)^2 + (3-2)^2} = 1$$

The best least squares solution is  $y = t$  ( $C = 0, D = 1$ )

1.4.7 For the measurements  $b = 0, 3, 12$  at times  $t = 0, 1, 2$ , find

(i) the best horizontal line  $y = C$

$$Ax = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \begin{bmatrix} C \end{bmatrix} = \begin{bmatrix} 0 \\ 3 \\ 12 \end{bmatrix} = b \rightarrow A^T A x = 3C = 15 = A^T b \rightarrow \underline{y = 5}$$

(ii) the best straight line  $y = Ct + D$

$$Ax = \begin{bmatrix} 1 & 0 \\ 1 & 1 \\ 1 & 2 \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix} = \begin{bmatrix} 0 \\ 3 \\ 12 \end{bmatrix} = b \rightarrow A^T A x = \begin{bmatrix} 3 & 3 \\ 3 & 5 \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix} = \begin{bmatrix} 15 \\ 27 \end{bmatrix} = A^T b$$

$$\rightarrow x = \begin{bmatrix} 1 \\ 6 \end{bmatrix} \quad \underline{y = 6t - 1}$$

(iii) the best parabola  $y = C + Dt + Et^2$

$$Ax = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 1 \\ 1 & 2 & 4 \end{bmatrix} \begin{bmatrix} C \\ D \\ E \end{bmatrix} = \begin{bmatrix} 0 \\ 3 \\ 12 \end{bmatrix} = b \rightarrow A^T A x = \begin{bmatrix} 3 & 3 & 5 \\ 3 & 5 & 9 \\ 5 & 9 & 17 \end{bmatrix} \begin{bmatrix} C \\ D \\ E \end{bmatrix} = \begin{bmatrix} 15 \\ 27 \\ 51 \end{bmatrix}$$

$$\rightarrow x = \begin{bmatrix} 0 \\ 0 \\ 3 \end{bmatrix} \quad \underline{y = 3t^2}$$

1.4.8 Multiple regression fits two-dimensional data by a plane  $y = C + Dt + Ez$ . For the data below, write down the 4 equations in the 3 unknowns  $C, D, E$ . What is the least squares solution from the normal equations?

	$z=0$	$z=1$	System:
$t=0$	$b_1=2$	$b_2=2$	$2 = C$
$t=1$	$b_3=1$	$b_4=5$	$2 = C + E$ $1 = C + D$ $5 = C + D + E$

$$A \begin{bmatrix} 1 & 0 & 0 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \\ 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} C \\ D \\ E \end{bmatrix} = \begin{bmatrix} 2 \\ 2 \\ 1 \\ 5 \end{bmatrix} \rightarrow A^T A \begin{bmatrix} 4 & 2 & 2 \\ 2 & 2 & 1 \\ 2 & 1 & 2 \end{bmatrix} \begin{bmatrix} x \\ C \\ D \\ E \end{bmatrix} = A^T b \begin{bmatrix} 10 \\ 6 \\ 7 \end{bmatrix} \rightarrow x = \begin{bmatrix} 1 \\ 1 \\ 2 \end{bmatrix}$$

$$\underline{y = 1 + t + 2z}$$

1.4.9 For a matrix  $A$  with more columns than rows the matrix  $A^T A$  is not positive definite. Why is it impossible for the columns of  $A^T A$  to be independent?

Compute  $A^T A$  for the following  $A$  matrices and check that  $A^T A$  is singular.

$$A = \begin{bmatrix} 1 & 1 & 0 \\ 2 & 2 & 1 \end{bmatrix} \quad A = \begin{bmatrix} 1 & 2 \end{bmatrix}$$

If  $A$  has more columns than rows, the columns must be dependent. The columns of  $A$  are dependent iff  $\exists x \neq 0$  s.t.  $Ax = 0$ . But this means  $\exists x \neq 0$  s.t.  $A^T A x = A^T 0 = 0$ , which is the case iff  $A^T A$  is singular iff the columns of  $A^T A$  are dependent.

Also, each column of  $A^T A$  is a linear combination of the columns of  $A^T$ , with coefficients given by one of the columns of  $A$ . Since this column of  $A$  could be written as a linear combination of the other columns of  $A$ , so could any column of  $A^T A$  be written as a linear combination of the other columns.

$$A^T A = \begin{bmatrix} 1 & 2 \\ 1 & 2 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 & 0 \\ 2 & 2 & 1 \end{bmatrix} = \begin{bmatrix} 5 & 5 & 2 \\ 5 & 5 & 2 \\ 2 & 2 & 1 \end{bmatrix} \text{ is singular (column 1 = column 2)}$$

$$A^T A = \begin{bmatrix} 1 \\ 2 \end{bmatrix} \begin{bmatrix} 1 & 2 \end{bmatrix} = \begin{bmatrix} 1 & 2 \\ 2 & 4 \end{bmatrix} \text{ is singular (column 2 = 2 · column 1)}$$