Chap 6. Positive Definite Matrices

6.1 Minima, Maxima, and Saddle Points

Chap 5 established that every symmetric matrix has real eigenvalues. Now we will find a test which will guarantee that all eigenvalues of A are positive, even without computing the eigenvalues of A.

o. The signs of eigenvalues are important in the recognition of a minimum point. Here are two examples.

$$F(x,y) = 7 + 2(x+y)^2 - y\sin y - x^3$$
$$f(x,y) = 2x^2 + 4xy + y^2$$

Does either $F(x,y)$ or $f(x,y)$ have a minimum at $(0,0)$?

Remark 1: The zero-order term $F(0,0)=7$ and $f(0,0)=0$ have no effect on this answer.

Remark 2: The linear terms give a necessary condition. The first derivatives must vanish at $(0,0)$.

$$\frac{\partial F}{\partial x} = 4(x+y) - 3x^2 = 0, \quad \frac{\partial F}{\partial y} = 4(x+y) - y\cos y - \sin y = 0$$
$$\frac{\partial f}{\partial x} = 4x + 4y = 0, \quad \frac{\partial f}{\partial y} = 4x + 2y = 0.$$

Thus $(x,y)=(0,0)$ is a stationary point for both functions.

Remark 3: The second derivatives at $(0,0)$ are decisive.

$$\frac{\partial^2 F}{\partial x^2} = 4 - 6x = 4, \qquad \frac{\partial^2 f}{\partial x^2} = 4$$
$$\frac{\partial^2 F}{\partial x \partial y} = \frac{\partial^2 F}{\partial y \partial x} = 4, \qquad \frac{\partial^2 f}{\partial x \partial y} = \frac{\partial^2 f}{\partial y \partial x} = 4$$
$$\frac{\partial^2 F}{\partial y^2} = 4 + y\sin y - 2\cos y = 2, \qquad \frac{\partial^2 f}{\partial y^2} = 2$$

The two functions behave in exactly the same way near the origin. F has a minimum if and only if f has a minimum. But, we will show that they don't!

[∵ $f(1,-1) = -1$!]

Remark 4: The higher-order term in F have no effect on the question of a local minimum, but they can prevent it from being a global minimum. The term $-x^3$ pulls F toward $-\infty$. For $f(x,y)$, with no higher terms, all the action is at $(0,0)$.

∘ Every quadratic form $f = ax^2 + 2bxy + cy^2$ has a stationary point at the origin, where $\frac{\partial f}{\partial x} = \frac{\partial f}{\partial y} = 0$.
A local minimum would be a global minimum.
If the stationary point of F is at (α, β),

Quadratic part of F $\quad f(x,y) = \frac{x^2}{2}\frac{\partial^2 F}{\partial x^2}(\alpha\beta) + xy\frac{\partial^2 F}{\partial x\partial y}(\alpha\beta) + \frac{y^2}{2}\frac{\partial^2 F}{\partial y^2}(\alpha,\beta)$

This $f(x,y)$ behaves near $(0,0)$ in the same way that $F(x,y)$ behaves near (α,β).

∘ The third derivatives are drawn into the problem when the second derivatives fail to give a definite decision. That happens when the quadratic part is singular. For a true minimum, f is allowed to vanish only at $(0,0)$. When $f(x,y)$ is strictly positive at all other points (the bowl goes up), it is called positive definite.

Figure 6.1 A bowl and a saddle: Definite $A = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$ and indefinite $A = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$.

Definite versus Indefinite : Bowl versus Saddle

What conditions on a, b, and c ensure that the quadratic $f(x,y) = ax^2 + 2bxy + cy^2$ is positive definite?

(i), (ii) If $ax^2 + 2bxy + cy^2$ is positive definite, then necessarily $a>0$ and $c>0$.

pf) Look at $(1,0)$, $f(1,0) = a > 0 \Rightarrow \frac{\partial^2 F}{\partial x^2} > 0$

Look at $(0,1)$, $f(0,1) = c > 0 \Rightarrow \frac{\partial^2 F}{\partial y^2} > 0$ $\lrcorner$

∘ But, the conditions $a>0$ and $c>0$ cannot guarantee that $f(x,y)$ is always positive. The term $2bxy$ can pull the graph below zero.

Ex1:

$f(x,y) = x^2 - 10xy + y^2 \Rightarrow f$ is not positive definite

$f(x,y)$ is positive on the x and y axes.

But, this function is negative on the line $y=x$, because $b=-10$ overwhelms a and c.

Ex2:

Our original $f(x,y) = 2x^2 + 4xy + y^2$ is not positive definite.

Neither F nor f has a minimum at $(0,0)$ because $f(1,-1) = 2-4+1 = -1$.

We now want a necessary and sufficient condition for positive definiteness. The simple technique is to complete the square:

Express $f(x,y)$ using squares: $f = ax^2 + 2bxy + cy^2 = a\left(x + \frac{b}{a}y\right)^2 + \left(c - \frac{b^2}{a}\right)y^2$.

(iii) If $ax^2 + 2bxy + cy^2$ stays positive, then necessarily $\underline{\underline{ac > b^2}}$.

Test for a minimum: The conditions $a>0$ and $ac>b^2$ are just right. They guarantee $c>0$.

$\boxed{6A}$ $ax^2+2bxy+cy^2$ is positive definite if and only if $a>0$ and $ac>b^2$. Any $F(x,y)$ has a minimum at a point where $\partial F/\partial x = \partial F/\partial y = 0$ with

$$\frac{\partial^2 F}{\partial x^2} > 0 \quad \text{and} \quad \left[\frac{\partial^2 F}{\partial x^2}\right]\left[\frac{\partial^2 F}{\partial y^2}\right] > \left[\frac{\partial^2 F}{\partial x \partial y}\right]^2$$

Test for a maximum: Since f has a maximum whenever $-F$ has a minimum, we just reverse the signs of a, b, c. The quadratic form is negative definite if and only if $a<0$ and $ac>b^2$. The same change applies for $F(x,y)$.

Singular case $ac=b^2$:
Positive semidefinite when $a>0$.
Negative semidefinite when $a<0$.
The surface $z=f(x,y)$ degenerates to a valley.

Saddle point $ac<b^2$: This occurs when b dominates a, c.
It also occurs if a and c have opposite signs.
Ex: $f_1 = 2xy$ and $f_2 = x^2-y^2$ have saddle points at $(0,0)$ as $ac-b^2=-1$. These two saddles are practically the same; if we turn one through $45°$, we get the other.
o. These quadractic forms are indefinite, because they can take either sign. We have a stationary point that is neither a maximum nor a minimum. It is called a saddle point.

Higher Dimensions: Linear Algebra

a quadratic $f(x,y)$ comes from a symmetric matrix

$$\mathbf{x}^T A \mathbf{x} \text{ in } \mathbb{R}^2: \quad ax^2+2bxy+cy^2 = \begin{bmatrix} x & y \end{bmatrix}\begin{bmatrix} a & b \\ b & c \end{bmatrix}\begin{bmatrix} x \\ y \end{bmatrix}$$

For any $n\times n$ symmetric matrix A, the product $\mathbf{x}^T A \mathbf{x}$ is a pure quadratic form $f(x_1, \cdots, x_n)$

$$\mathbf{x}^T A \mathbf{x} \text{ in } \mathbb{R}^n: \begin{bmatrix} x_1 & \cdots & x_n \end{bmatrix}\begin{bmatrix} a_{11} & \cdots & a_{1n} \\ & \cdots & \\ a_{n1} & \cdots & a_{nn} \end{bmatrix}\begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} = \sum\sum a_{ij} x_i x_j$$

<u>Ex3</u>: $f = 2x^2+4xy+y^2$ and $A = \begin{bmatrix} 2 & 2 \\ 2 & 1 \end{bmatrix} \rightarrow$ saddle point

<u>Ex4</u>: $f = 2xy$ and $A = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \rightarrow$ saddle point

<u>Ex5</u>: A is 3×3 for $2x_1^2 - 2x_1x_2 + 2x_2^2 - 2x_2x_3 + 2x_3^2$.

$$f = \begin{bmatrix} x_1 & x_2 & x_3 \end{bmatrix}\begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \rightarrow \text{min at } (0,0,0)$$

o. At a stationary point of any function $F(x_1, \cdots, x_n)$, all first derivatives are zero. The second-derivative matrix A has entries $a_{ij} = \partial^2 F/\partial x_i \partial x_j = \partial^2 F/\partial x_j \partial x_i = a_{ji}$. So A is symmetric. Then F has a minimum when the pure quadratic $\mathbf{x}^T A \mathbf{x}$ is positive definite. These second-order terms control F near the stationary point.

Taylor Series: $F(\mathbf{x}) = F(0) + \mathbf{x}^T(\text{grad } F) + \frac{1}{2}\mathbf{x}^T A \mathbf{x} + \begin{pmatrix} \text{higher} \\ \text{order} \\ \text{terms} \end{pmatrix}$.

At a stationary point, grad $F = \left(\frac{\partial F}{\partial x_1}, \cdots, \frac{\partial F}{\partial x_n}\right) = (0, \cdots, 0)$. The second derivatives in $\mathbf{x}^T A \mathbf{x}$ take the graph up or down (or saddle). If the stationary point is at $\mathbf{x}_0$ instead of $\mathbf{0}$, $F(\mathbf{x})$ and all derivatives are computed at $\mathbf{x}_0$. Then $\mathbf{x}$ changes to $\mathbf{x}-\mathbf{x}_0$ on the right-hand side.

6.2 Test for Positive Definiteness

$\boxed{6B}$ Each of the following tests is a necessary and sufficient condition for the real symmetric matrix A to be positive definite

(I) $x^TAx > 0$ for all nonzero real vector x.

(II) all the eigenvalues of A satisfy $\lambda_i > 0$.

(III) all the upper left submatrices of A_k have positive determinants.

(IV) all the pivots (without row exchanges) satisfy $d_i > 0$.

<proof>

(I)⇒(II): $Ax = \lambda x \Rightarrow \overset{>0}{x^TAx} = x^T\lambda x = \lambda\|x\|^2 \Rightarrow \lambda > 0$

(II)⇒(I): Symmetric matrices have a full set of orthonormal eigenvectors (Chap 5). Any $x = c_1x_1 + \cdots + c_nx_n$, Then

$$Ax = c_1Ax_1 + \cdots + c_nAx_n = c_1\lambda_1x_1 + \cdots + c_n\lambda_nx_n$$

$$x^TAx = (c_1x_1^T + \cdots + c_nx_n^T)(c_1\lambda_1x_1 + \cdots + c_n\lambda_nx_n)$$

$$= c_1^2\lambda_1 + \cdots + c_n^2\lambda_n > 0 \quad (\text{if every } \lambda_i > 0)$$

[∵ $x_i^Tx_j = \delta_{ij} = 1$ if $i=j$, 0 if $i \neq j$]

(I)⇒(III): Look at all nonzero vectors x whose last $(n-k)$ components are 0.

$$x^TAx = \begin{bmatrix} x_k^T & 0 \end{bmatrix}\begin{bmatrix} A_k & * \\ * & * \end{bmatrix}\begin{bmatrix} x_k \\ 0 \end{bmatrix} = x_k^TA_kx_k > 0$$

Thus A_k is positive definite. The eigenvalues of A_k (not the same λ_i!) must be positive $\Rightarrow \det(A_k) > 0$.

(III)⇒(IV): The k-th pivot $d_k = \det A_k / \det A_{k-1}$ (Sec 4.4) > 0

(IV)⇒(I):

We are given positive pivots, and must deduce that $x^TAx > 0$, by completing the square (as in the 2x2 case).

To see what happens for symmetric $n \times n$ matrices, we go back to elimination on a symmetric matrix; $A = LDL^T$. (See Example 1 Below). ⇒

Example 1: Positive pivots 2, $\frac{3}{2}$, and $\frac{4}{3}$:

$$A = \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ -\frac{1}{2} & 1 & 0 \\ 0 & -\frac{2}{3} & 1 \end{bmatrix} \begin{bmatrix} 2 & & \\ & \frac{3}{2} & \\ & & \frac{4}{3} \end{bmatrix} \begin{bmatrix} 1 & -\frac{1}{2} & 0 \\ 0 & 1 & -\frac{2}{3} \\ 0 & 0 & 1 \end{bmatrix} = LDL^T$$

We want to split $\mathbf{x}^T A \mathbf{x}$ into $\mathbf{x}^T LDL^T \mathbf{x}$:

If $\mathbf{x} = \begin{bmatrix} u \\ v \\ w \end{bmatrix}$, then $L^T\mathbf{x} = \begin{bmatrix} 1 & -\frac{1}{2} & 0 \\ 0 & 1 & -\frac{2}{3} \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} u \\ v \\ w \end{bmatrix} = \begin{bmatrix} u - \frac{1}{2}v \\ v - \frac{2}{3}w \\ w \end{bmatrix}$

$$\mathbf{x}^T A \mathbf{x} = (L^T\mathbf{x})^T D (L^T\mathbf{x})$$
$$= 2\left(u - \frac{1}{2}v\right)^2 + \frac{3}{2}\left(v - \frac{2}{3}w\right)^2 + \frac{4}{3}w^2 > 0$$

$\therefore$ (IV) $\Rightarrow$ (I). for $\mathbf{x} \neq \mathbf{0}$. ┘

- Every diagonal entry a_{ii} must be positive. However, it is far from sufficient to look only at the diagonal entries.
- The pivots d_i are not to be confused with the eigenvalues. For a typical positive definite matrix, they are two completely different sets of positive numbers.

  In the above 3×3 matrix, the determinant test is easy

  Determinant test: $\det A_1 = 2$, $\det A_2 = 3$, $\det A_3 = 4$

  The pivots are ratios $d_1 = 2$, $d_2 = \frac{3}{2}$, $d_3 = \frac{4}{3}$.

  Ordinarily the eigenvalue test is the longest computation

  Eigenvalue test: $\lambda_1 = 2 - \sqrt{2}$, $\lambda_2 = 2$, $\lambda_3 = 2 + \sqrt{2}$

  Even though it is the hardest to apply to a single matrix, eigenvalues can be the most useful test for theoretical purposes. Each test is enough by itself.

Positive Definite Matrices and Least Squares

$\boxed{6C}$ The symmetric matrix A is positive definite if and only if

(V) There is a matrix R with independent columns s.t. $A = R^T R$.

$\because$ The key is to recognize $x^T A x$ as

$$x^T R^T R x = (Rx)^T (Rx) = \|Rx\|^2 > 0 \quad \text{if } x \neq 0.$$

It remains to find an R for which $A = R^T R$.

① Elimination: $A = LDL^T = (L\sqrt{D})(\sqrt{D}L^T). \Rightarrow R = \sqrt{D}L^T.$

② Eigenvalues: $A = Q\Lambda Q^T = (Q\sqrt{\Lambda})(\sqrt{\Lambda}Q^T). \Rightarrow R = \sqrt{\Lambda}Q^T.$

③ $R = Q\sqrt{\Lambda}Q^T$: the symmetric positive definite square root of A.

There are many other choices.

If we multiply any R by a matrix Q with orthonormal columns

$\Rightarrow (QR)^T(QR) = R^T Q^T Q R = R^T R = A.$

Semidefinite Matrices

$\boxed{6D}$ Each of the following tests is a necessary and sufficient condition for a symmetric matrix A to be positive semidefinite

(I') $x^T A x \geq 0$ for all x (this defines positive semidefinite)

(II') all the eigenvalues of A satisfy $\lambda_i \geq 0$.

(III') No principal submatrices have negative determinants

(IV') No pivots are negative.

(V') There is a matrix R, possibly with dependent columns, such that $A = R^T R$.

- The diagonalization $A = Q\Lambda Q^T$ leads to

$$x^T A x = x^T Q \Lambda Q^T x = y^T \Lambda y.$$

If A has rank r, there are r nonzero λ's and r perfect squares in $y^T \Lambda y = \lambda_1 y_1^2 + \cdots + \lambda_r y_r^2$.

Note: Condition III' applies to all the principal submatrices, not only those in the upper left-hand corner. Otherwise, we could not distinguish between two matrices whose upper left determinants were all zero:

$\begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$: positive semidefinite;

$\begin{bmatrix} 0 & 0 \\ 0 & -1 \end{bmatrix}$: negative semidefinite.

Ex2: $A = \begin{bmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{bmatrix}$: positive semidefinite by all five tests

(I') $x^TAx = (x_1-x_2)^2 + (x_2-x_3)^2 + (x_2-x_3)^2 \geq 0$ (zero if $x_1=x_2=x_3$)

(II') The eigenvalues are $\underline{\lambda_1 = 0}$, $\lambda_2=\lambda_3=3$.

(III') $\det A = 0$ and smaller determinants are positive.

(IV')

$$A = \begin{bmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{bmatrix} \to \begin{bmatrix} 2 & 0 & 0 \\ 0 & \frac{3}{2} & -\frac{3}{2} \\ 0 & -\frac{3}{2} & \frac{3}{2} \end{bmatrix} \to \begin{bmatrix} 2 & 0 & 0 \\ 0 & \frac{3}{2} & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

missing pivot

(V') $A = R^TR$ with dependent columns in R.

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

$(1,1,1)$ in the nullspace.

Remark: The conditions for semidefiniteness could also be deduced from the definiteness conditions by adding εI to give a positive definite matrix: $A+\varepsilon I$, for $\varepsilon>0$. As $\varepsilon \to 0$, the determinants and eigenvalues depend continuously on ε, and they will be positive until the very last moment. At $\varepsilon=0$, they must be nonnegative.

Ellipsoids in n Dimensions

For a positive definite matrix, the equation $\mathbf{x}^T A \mathbf{x} = 1$ describes an ellipse in 2D and an ellipsoid in 3D.

Ellipsoid: $A = \begin{bmatrix} 4 & & \\ & 1 & \\ & & \frac{1}{9} \end{bmatrix}$, $\mathbf{x}^T A \mathbf{x} = 4x_1^2 + x_2^2 + \frac{1}{9}x_3^2 = 1$.

Ex3:

$A = \begin{bmatrix} 5 & 4 \\ 4 & 5 \end{bmatrix}$ and $\mathbf{x}^T A \mathbf{x} = 5u^2 + 8uv + 5v^2 = 1$.

The ellipse is centered at $u = v = 0$, but the axes are not so clear. The axes no longer line up with the coordinate axes. We will show that the axes of the ellipse point toward the eigenvectors of A. Because $A = A^T$, those eigenvectors and axes are orthogonal. The major axis of the ellipse corresponds to the smallest eigenvalue of A.

$\lambda_1 = 1$, $\mathbf{x}_1 = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -1 \end{bmatrix}$; $\lambda_2 = 9$, $\mathbf{x}_2 = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \end{bmatrix}$

New squares: $5u^2 + 8uv + 5v^2 = \left(\frac{u}{\sqrt{2}} - \frac{v}{\sqrt{2}}\right)^2 + 9\left(\frac{u}{\sqrt{2}} + \frac{v}{\sqrt{2}}\right)^2 = 1$

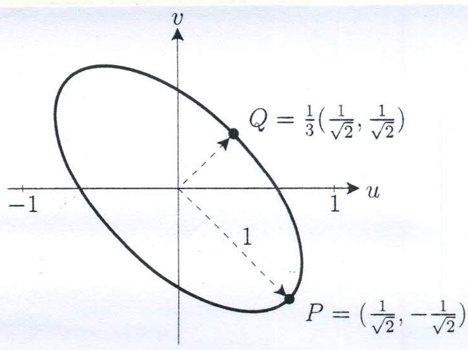

Figure 6.2 The ellipse $x^T A x = 5u^2 + 8uv + 5v^2 = 1$ and its principal axes.

$\boxed{6E}$ Suppose $A = Q\Lambda Q^T$ with $\lambda_i > 0$. Rotating $\mathbf{y} = Q^T\mathbf{x}$,

$\mathbf{x}^T Q \Lambda Q^T \mathbf{x} = 1$, $\mathbf{y}^T \Lambda \mathbf{y} = 1$, $\lambda_1 y_1^2 + \cdots + \lambda_n y_n^2 = 1$.

Its axes have lengths $1/\sqrt{\lambda_1}, \cdots, 1/\sqrt{\lambda_n}$ from the center. In the original $\mathbf{x}$-space, they point along the eigenvectors of A.

6.3 Singular Value Decomposition

- The SVD is closely related to the $Q\Lambda Q^T$ factorization of a positive definite matrix. The eigenvalues are in the diagonal matrix Λ. The eigenvector matrix Q is orthogonal ($Q^TQ = I$) because eigenvectors of a symmetric matrix can be chosen to be orthonormal.
- For most matrices that is not true, and for rectangular matrices it is ridiculous (eigenvalues undefined). But now we allow the Q on the left and the Q^T on the right to be any two orthogonal matrices U and V^T — not necessarily transposes of each other. Then every matrix will split into $A = U\Sigma V^T$.
- The diagonal (but rectangular) matrix Σ has eigenvalues from A^TA, not from A! Those positive entries will be $\sigma_1, \cdots, \sigma_r$ (the singular values of A). They fill the first r places on the main diagonal of Σ — when A has rank r. The rest of Σ is zero.
- With rectangular matrices, the key is almost always to consider A^TA and AA^T.

Singular Value Decomposition:

Any $m\times n$ matrix A can be factored into

$$A = U\Sigma V^T = (\text{orthogonal})(\text{diagonal})(\text{orthogonal})$$

The columns of U ($m\times m$) are eigenvectors of AA^T, and the columns of V ($n\times n$) are eigenvectors of A^TA. The r singular values on the diagonal of Σ ($m\times n$) are the square roots of the nonzero eigenvalues of both AA^T and A^TA.

Remark 1: For positive definite matrices, Σ is Λ and $U\Sigma V^T$ is identical to $Q\Lambda Q^T$. For other symmetric matrices, any negative eigenvalues in Λ become positive in Σ.

Remark 2: U and V give orthonormal bases for all four fundamental subspaces:

$$\begin{bmatrix} \text{first } r \text{ columns of } U : \text{column space of } A \\ \text{last } m-r \text{ columns of } U : \text{left nullspace of } A \\ \text{first } r \text{ columns of } V : \text{row space of } A \\ \text{last } n-r \text{ columns of } V : \text{nullspace of } A \end{bmatrix}$$

Remark 3: The SVD chooses those bases in an extremely special way. They are more than just orthonormal. When A multiplies a column v_j of V, it produces σ_j times a column of U. That comes directly from $AV = U\Sigma$, looked at a column at a time.

Remark 4: Eigenvectors of AA^T and A^TA must go into the columns of U and V:

$$AA^T = (U\Sigma V^T)(V\Sigma^T U^T) = U\Sigma\Sigma^T U^T, \text{ and similarly}$$
$$A^TA = V\Sigma^T\Sigma V^T.$$

U must be the eigenvector matrix for AA^T. The eigenvalue matrix in the middle is $\Sigma\Sigma^T$ — which is $m\times m$ with $\sigma_1^2, \cdots, \sigma_r^2$ on the diagonal. From $A^TA = V\Sigma^T\Sigma V^T$, the V matrix must be the eigenvector matrix for A^TA. The diagonal matrix $\Sigma^T\Sigma$ $(n\times n)$ has the same $\sigma_1^2, \cdots, \sigma_r^2$.

Remark 5: Here is the reason that $Av_j = \sigma_j u_j$.

$$A^TA v_j = \sigma_j^2 v_j \Rightarrow AA^TAv_j = \sigma_j^2 (Av_j) \text{ eigenvector of } AA^T$$
$$\Downarrow$$
$$v_j^T A^TA v_j = \sigma_j^2 v_j^T v_j \Rightarrow \|Av_j\|^2 = \sigma_j^2$$

The unit eigenvector is $Av_j/\sigma_j = u_j$ $\therefore AV = U\Sigma$!

Ex1: A has only one column: rank $r=1$, Σ has only $\sigma_1=3$.

$$\text{SVD}: \quad A=\begin{bmatrix}-1\\2\\2\end{bmatrix}=\begin{bmatrix}-\frac{1}{3}&\frac{2}{3}&\frac{2}{3}\\\frac{2}{3}&-\frac{1}{3}&\frac{2}{3}\\\frac{2}{3}&\frac{2}{3}&-\frac{1}{3}\end{bmatrix}\begin{bmatrix}3\\0\\0\end{bmatrix}\begin{bmatrix}1\end{bmatrix}=U_{3\times3}\Sigma_{3\times1}V^T_{1\times1}$$

A^TA is 1×1, whereas AA^T is 3×3. They both have eigenvalue 9 (whose square root is the 3 in Σ).
The two zero eigenvalues of AA^T leave some freedom for the eigenvectors in the columns 2 and 3 of U. We kept that matrix orthogonal.

Ex2:
Now A has rank 2 and $AA^T=\begin{bmatrix}2&-1\\-1&2\end{bmatrix}$ with $\lambda=3$ and 1.

$$\begin{bmatrix}-1&1&0\\0&-1&1\end{bmatrix}=U\Sigma V^T=\frac{1}{\sqrt{2}}\begin{bmatrix}-1&1\\1&1\end{bmatrix}\begin{bmatrix}\sqrt{3}&0&0\\0&1&0\end{bmatrix}\begin{bmatrix}1&-2&1\\-1&0&1\\1&1&1\end{bmatrix}\begin{matrix}/\sqrt{6}\\/\sqrt{2}\\/\sqrt{3}\end{matrix}$$

The columns of U are left singular vectors (unit eigenvectors of AA^T). The columns of V are right singular vectors (unit eigenvectors of A^TA).

Applications of the SVD

The SVD is terrific for numerically stable computations, because U and V are orthogonal matrices. They never change the length of a vector.

Σ could multiply by a large σ or divide by a small σ, and overflow the computer. But still Σ is as good as possible. The ratio $\sigma_{max}/\sigma_{min}$ is the condition number of an invertible $n\times n$ matrix. The availability of that information is another reason for the popularity of the SVD.

1. Image processing: We want to send a picture containing 1000×1000 color pixels. We may send 10^6 numbers. But it is better to find the essential information and send only that. Suppose we know the SVD. The key is in the singular values (in Σ). Some σ's are significant and others are extremely small. If we keep only 20 of them (throwing away 980), then we send only the corresponding 20 columns of U and V.

$$A = U\Sigma V^T = u_1\sigma_1 v_1^T + u_2\sigma_2 v_2^T + \cdots + u_r\sigma_r v_r^T$$

Any matrix is the sum of r matrices of rank 1. If only 20 terms are kept, we send 20 times 2000 numbers instead of a million (25 to 1 compression). The cost is in the computation of the SVD.

3. Polar decomposition: Every nonzero complex number z is a positive number r times a number $e^{i\theta}$: $z = r \cdot e^{i\theta}$.

If we think of z as a 1×1 matrix, r corresponds to a positive definite matrix and $e^{i\theta}$ corresponds to an orthogonal matrix. The SVD extends this polar factorization to matrices of any size.

[Every real square matrix can be factored into $A = QS$, where Q is orthogonal and S is symmetric positive semidefinite. If A is invertible, then S is positive definite.

Pf

$$A = U\Sigma V^T = (UV^T)(V\Sigma V^T) = QS$$

The factor $S = V\Sigma V^T$ is symmetric and semidefinite (because Σ is). The factor $Q = UV^T$ is an orthogonal matrix (because $Q^TQ = VU^TUV^T = I$).

Ex3: Polar decomposition

$$A = QS: \begin{bmatrix} 1 & -2 \\ 3 & -1 \end{bmatrix} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 3 & -1 \\ -1 & 2 \end{bmatrix}$$

Ex 4: Reverse polar decomposition

$$A = S'Q: \begin{bmatrix} 1 & -2 \\ 3 & -1 \end{bmatrix} = \begin{bmatrix} 2 & 1 \\ 1 & 3 \end{bmatrix} \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$$

Both S and S' are symmetric positive definite because A is invertible.

Application of $A = QS$:

a major use of the polar decomposition is in continuum mechanics (and recently in robotics and of cause in computer graphics!) In any deformation, it is important to separate stretching from rotation. The orthogonal matrix Q is a rotation, and possibly a reflection. The material feels no strain. The symmetric matrix S has eigenvalues $\sigma_1, \cdots, \sigma_r$, which are the stretching (or compression) factors. The diagonalization that displays those eigenvalues is the natural choice of axes - called principal axes. It is S that requires work on the material, and stores up elastic energy.

$S^2 = A^TA$ is symmetric positive definite when A is invertible. S is the symmetric positive definite square root of A^TA, and $Q = AS^{-1}$. In the reverse order $A = S'Q$, the matrix S' is the symmetric positive definite square root of AA^T.

4. Least squares: $A\mathbf{x}=\mathbf{b}$ has two possible difficulties.

① With dependent rows, $A\mathbf{x}=\mathbf{b}$ may have no solution. That happens when $\mathbf{b}$ is outside the column space of A. Instead of $A\mathbf{x}=\mathbf{b}$, we solve $A^TA\hat{\mathbf{x}}=A^T\mathbf{b}$.

② But if A has dependent columns, this $\hat{\mathbf{x}}$ will not be unique. (any vector in the nullspace could be added to $\hat{\mathbf{x}}$.) We have to choose a particular solution of $A^TA\hat{\mathbf{x}}=A^T\mathbf{b}$, and we choose the shortest.

> The optimal solution of $A\mathbf{x}=\mathbf{b}$ is the minimum length solution of $A^TA\hat{\mathbf{x}}=A^T\mathbf{b}$.

That minimum length solution will be called $\mathbf{x}^+$. It is our preferred choice as the best solution to $A\mathbf{x}=\mathbf{b}$ (which had no solution), and also to $A^TA\hat{\mathbf{x}}=A^T\mathbf{b}$ (which had too many).

Ex 5:

$A\hat{\mathbf{x}}=\mathbf{p}$ is
$$\begin{bmatrix}\sigma_1 & 0 & 0 & 0\\ 0 & \sigma_2 & 0 & 0\\ 0 & 0 & 0 & 0\end{bmatrix}\begin{bmatrix}\hat{x}_1\\ \hat{x}_2\\ \hat{x}_3\\ \hat{x}_4\end{bmatrix}=\begin{bmatrix}b_1\\ b_2\\ 0\end{bmatrix}$$

In the column space, the closest point to $\mathbf{b}=(b_1,b_2,b_3)^T$ is $\mathbf{p}=(b_1,b_2,0)^T$. Solving the first two equations,

$\hat{x}_1=b_1/\sigma_1$ and $\hat{x}_2=b_2/\sigma_2$

Now we face the second difficulty. To make $\hat{\mathbf{x}}$ as short as possible, we choose $\hat{x}_3=\hat{x}_4=0$. The minimum length solution is $\mathbf{x}^+$:

A^+ is pseudoinverse : $\mathbf{x}^+=\begin{bmatrix}b_1/\sigma_1\\ b_2/\sigma_2\\ 0\\ 0\end{bmatrix}=\begin{bmatrix}1/\sigma_1 & 0 & 0\\ 0 & 1/\sigma_2 & 0\\ 0 & 0 & 0\\ 0 & 0 & 0\end{bmatrix}\begin{bmatrix}b_1\\ b_2\\ b_3\end{bmatrix}$

$\mathbf{x}^+=A^+\mathbf{b}$ is the shortest

$$\Sigma = \overbrace{\begin{bmatrix} \sigma_1 & & & \\ & \ddots & & \\ & & \sigma_r & \\ & & & \end{bmatrix}}^{n} \Big\} m \qquad \Sigma^+ = \overbrace{\begin{bmatrix} 1/\sigma_1 & & & \\ & \ddots & & \\ & & 1/\sigma_r & \\ & & & \end{bmatrix}}^{m} \Big\} n \qquad \Sigma^+ b = \begin{bmatrix} b_1/\sigma_1 \\ \vdots \\ b_r/\sigma_r \\ \\ \end{bmatrix}.$$

The shortest solution x^+ is always in the row space of A.
Any vector $\hat{x}$ can be split into a row space component x_r and a nullspace component : $\hat{x} = x_r + x_n$.

① The row space component also solves $A^TAx_r = A^Tb$. ($\because Ax_n = 0$)

② The components are orthogonal:

$\|\hat{x}\|^2 = \|x_r\|^2 + \|x_n\|^2$, so $\hat{x}$ is shortest when $x_n = 0$

③ all solutions of $A^TA\hat{x} = A^Tb$ have the same x_r.
That vector is x^+.

Every p in the column space comes from one and only one vector x_r in the row space. all we are doing is to choose that vector, $x^+ = x_r$, as the best solution to $Ax = b$.

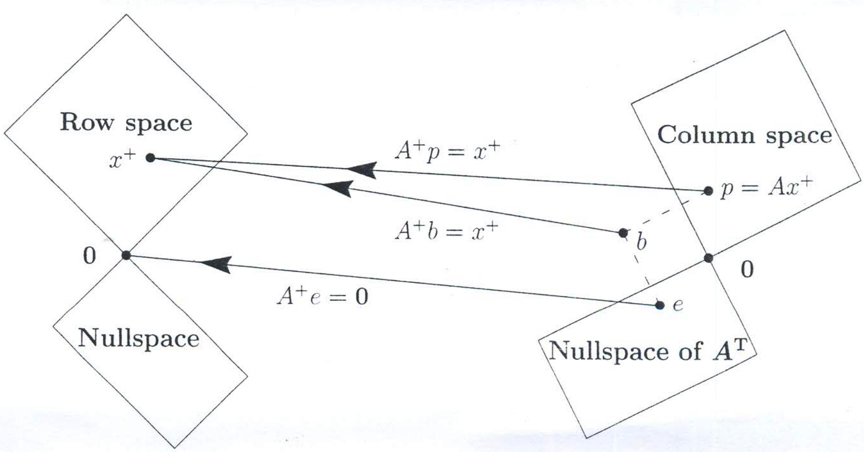

Figure 6.3 The pseudoinverse A^+ inverts A where it can on the column space.

Ex 6: $A\mathbb{x} = \mathbb{b}$ is $-x_1+2x_2+2x_3=18$, a whole plane of solutions. The shortest solution is in the row space of $A=[-1,2,2]$, $\mathbb{x}^+=(-2,4,4)$ which satisfies the equation $A\mathbb{x}^+=18$. There are longer solutions like $(-2,5,3)$, $(-2,7,1)$, or $(-6,3,3)$, but they all have nonzero components from the nullspace. The matrix that produces $\mathbb{x}^+$ from $\mathbb{b}=[18]$ is the pseudoinverse A^+.

$$A^+ = \begin{bmatrix} -1 & 2 & 2 \end{bmatrix}^+ = \begin{bmatrix} -\frac{1}{9} \\ \frac{2}{9} \\ \frac{2}{9} \end{bmatrix} \quad \text{and} \quad A^+[18] = \begin{bmatrix} -2 \\ 4 \\ 4 \end{bmatrix}. \tag{6}$$

The row space of A is the column space of A^+. Here is a formula for A^+:

$$\textbf{If } A = U\Sigma V^{\mathrm{T}} \textbf{ (the SVD), then its pseudoinverse is } A^+ = V\Sigma^+U^{\mathrm{T}}. \tag{7}$$

Example 6 had $\sigma = 3$—the square root of the eigenvalue of $AA^{\mathrm{T}} = [9]$. Here it is again with Σ and Σ^+:

$$A = \begin{bmatrix} -1 & 2 & 2 \end{bmatrix} = U\Sigma V^{\mathrm{T}} = \begin{bmatrix} 1 \end{bmatrix} \begin{bmatrix} 3 & 0 & 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{3} & \frac{2}{3} & \frac{2}{3} \\ \frac{2}{3} & -\frac{1}{3} & \frac{2}{3} \\ \frac{2}{3} & \frac{2}{3} & -\frac{1}{3} \end{bmatrix}$$

$$V\Sigma^+U^{\mathrm{T}} = \begin{bmatrix} -\frac{1}{3} & \frac{2}{3} & \frac{2}{3} \\ \frac{2}{3} & -\frac{1}{3} & \frac{2}{3} \\ \frac{2}{3} & \frac{2}{3} & -\frac{1}{3} \end{bmatrix} \begin{bmatrix} \frac{1}{3} \\ 0 \\ 0 \end{bmatrix} \begin{bmatrix} 1 \end{bmatrix} = \begin{bmatrix} -\frac{1}{9} \\ \frac{2}{9} \\ \frac{2}{9} \end{bmatrix} = A^+.$$

The minimum length least-squares solution is $x^+ = A^+b = V\Sigma^+U^{\mathrm{T}}b$.

<proof> Multiplication by U^{T} leaves lengths unchanged
$\|A\mathbb{x}-\mathbb{b}\| = \|U\Sigma V^{\mathrm{T}}\mathbb{x}-\mathbb{b}\| = \|\Sigma V^{\mathrm{T}}\mathbb{x} - U^{\mathrm{T}}\mathbb{b}\|$
Let $\mathbb{y}=V^{\mathrm{T}}\mathbb{x}=V^{-1}\mathbb{x}$, with $\|V^{-1}\mathbb{x}\|=\|\mathbb{x}\|$. Then minimizing $\|A\mathbb{x}-\mathbb{b}\|$ is the same as minimizing $\|\Sigma\mathbb{y}-U^{\mathrm{T}}\mathbb{b}\|$. Now Σ is diagonal and the best $\mathbb{y}^+=\Sigma^+U^{\mathrm{T}}\mathbb{b}$, so the best $\mathbb{x}^+$ is shortest solution $\mathbb{x}^+=V\mathbb{y}^+=V\Sigma^+U^{\mathrm{T}}\mathbb{b}=A^+\mathbb{b}$.
$V\mathbb{y}^+$ is in the row space, and $A^{\mathrm{T}}A\mathbb{x}^+=A^{\mathrm{T}}\mathbb{b}$ from the SVD.

6.4 Minimum Principles

Our goal is to find the minimum principle that is equivalent to $A\mathbf{x}=\mathbf{b}$, and the minimization equivalent to $A\mathbf{x}=\lambda\mathbf{x}$.
We want to find the "parabola" $P(\mathbf{x})$ whose minimum occurs when $A\mathbf{x}=\mathbf{b}$.

$\boxed{6H}$ If A is symmetric positive definite, then $P(\mathbf{x})=\frac{1}{2}\mathbf{x}^T A\mathbf{x}-\mathbf{x}^T\mathbf{b}$ reaches its minimum at the point where $A\mathbf{x}=\mathbf{b}$. At that point $P_{min}=-\frac{1}{2}\mathbf{b}^T A^{-1}\mathbf{b}$.

<proof> Suppose $A\mathbf{x}=\mathbf{b}$. For any vector $\mathbf{y}$, we show that $P(\mathbf{y})\geq P(\mathbf{x})$

$$\begin{aligned} P(\mathbf{y})-P(\mathbf{x}) &= \tfrac{1}{2}\mathbf{y}^T A\mathbf{y}-\mathbf{y}^T\mathbf{b}-\tfrac{1}{2}\mathbf{x}^T A\mathbf{x}+\mathbf{x}^T\mathbf{b} \\ &= \tfrac{1}{2}\mathbf{y}^T A\mathbf{y}-\mathbf{y}^T A\mathbf{x}+\tfrac{1}{2}\mathbf{x}^T A\mathbf{x} \\ &= \tfrac{1}{2}(\mathbf{y}-\mathbf{x})^T A(\mathbf{y}-\mathbf{x})\geq 0 \text{ and } =0 \text{ only if } \mathbf{y}=\mathbf{x}. \end{aligned}$$

Ex1:

Minimize $P(\mathbf{x})=x_1^2-x_1x_2+x_2^2-b_1x_1-b_2x_2$.

The usual approach is to set the partial derivaties to zero.

$$\begin{cases} \partial P/\partial x_1 = 2x_1-x_2-b_1=0 \\ \partial P/\partial x_2 = -x_1+2x_2-b_2=0 \end{cases} \Rightarrow \begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}=\begin{bmatrix} b_1 \\ b_2 \end{bmatrix}$$

Linear algebra recognizes $P(\mathbf{x})$ as $\frac{1}{2}\mathbf{x}^T A\mathbf{x}-\mathbf{x}^T\mathbf{b}$, and knows that $A\mathbf{x}=\mathbf{b}$ gives the minimum. Substitute $\mathbf{x}=A^{-1}\mathbf{b}$ into $P(\mathbf{x})$:

Minimum value $\underline{P_{min}=\frac{1}{2}(A^{-1}\mathbf{b})^T A(A^{-1}\mathbf{b})-(A^{-1}\mathbf{b})^T\mathbf{b}=-\frac{1}{2}\mathbf{b}^T A^{-1}\mathbf{b}}$.

In applications, $\frac{1}{2}\mathbf{x}^T A\mathbf{x}$ is the internal energy and $-\mathbf{x}^T\mathbf{b}$ is the external work. The total energy $P(\mathbf{x})$ is minimum at $\mathbf{x}=A^{-1}\mathbf{b}$.

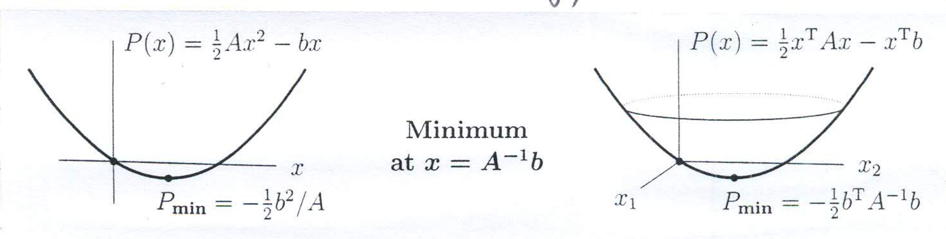

Figure 6.4 The graph of a positive quadratic $P(x)$ is a parabolic bowl.

Minimizing with Constraints

We minimize $P(\mathbb{x})$ subject to the extra requirement $C\mathbb{x}=\mathbb{d}$.
Usually $\mathbb{x}$ can't satisfy n equations $A\mathbb{x}=\mathbb{b}$ and also l extra constraints $C\mathbb{x}=\mathbb{d}$. We need l more unknowns.
The new unknowns $y_1, \cdots, y_l$ are called Lagrange multipliers.
They build the constraint into a function $L(\mathbb{x},\mathbb{y})$.

$$L(\mathbb{x},\mathbb{y}) = P(\mathbb{x}) + \mathbb{y}^T(C\mathbb{x}-\mathbb{d}) = \frac{1}{2}\mathbb{x}^TA\mathbb{x} - \mathbb{x}^T\mathbb{b} + \mathbb{x}^TC^T\mathbb{y} - \mathbb{y}^T\mathbb{d}.$$

$$\begin{array}{l} \text{Constrained} \\ \text{minimization} \end{array} \begin{cases} \partial L/\partial \mathbb{x} = \mathbb{0}: & A\mathbb{x} + C^T\mathbb{y} = \mathbb{b} \\ \partial L/\partial \mathbb{y} = \mathbb{0}: & C\mathbb{x} \qquad\quad = \mathbb{d} \end{cases}$$

The first equations involve $\mathbb{y}$ which tells how much the constrained minimum $P_{C/min}$ (allowing only $\mathbb{x}$ with $C\mathbb{x}=\mathbb{d}$) exceeds the unconstrained P_{min} (allowing all $\mathbb{x}$).

$$P_{C/min} = P_{min} + \frac{1}{2}\mathbb{y}^T(CA^{-1}\mathbb{b}-\mathbb{d}) \geq P_{min} \qquad (5)$$

Ex2:

$P(x_1,x_2) = \frac{1}{2}x_1^2 + \frac{1}{2}x_2^2 \Rightarrow P_{min}=0, \quad n=2, A=I, \mathbb{b}=\mathbb{0}.$
$A\mathbb{x}=\mathbb{b}$ gives $x_1=0$, $x_2=0$.
Now add one constraint $c_1x_1+c_2x_2=d$.

$$L(\mathbb{x},y) = \frac{1}{2}x_1^2 + \frac{1}{2}x_2^2 + y(c_1x_1+c_2x_2-d)$$

$$\begin{cases} \partial L/\partial x_1 = 0: & x_1 + c_1y = 0 \\ \partial L/\partial x_2 = 0: & x_2 + c_2y = 0 \\ \partial L/\partial y = 0: & c_1x_1 + c_2x_2 = d \end{cases} \Rightarrow \begin{array}{l} x_1 = -c_1y \\ x_2 = -c_2y \\ -c_1^2y - c_2^2y = d \end{array}$$

Solution: $y = \dfrac{-d}{c_1^2+c_2^2}$, $x_1 = \dfrac{c_1d}{c_1^2+c_2^2}$, $x_2 = \dfrac{c_2d}{c_1^2+c_2^2}$

The constrained minimum of $P=\frac{1}{2}\mathbb{x}^T\mathbb{x}$ is reached at

$$P_{C/min} = \frac{1}{2}x_1^2 + \frac{1}{2}x_2^2 = \frac{1}{2}\frac{c_1^2d^2+c_2^2d^2}{(c_1^2+c_2^2)^2} = \frac{1}{2}\cdot\frac{d^2}{c_1^2+c_2^2}$$

This equals $-\frac{1}{2}yd$ as predicted in equation (5), since $b=0$ and $P_{min}=0$.

Figure 6.5 shows that the constraint keeps $\mathbf{x}$ on a line $2x_1 - x_2 = 5$. We look for the closest point to $(0,0)$ on this line. The solution is $\mathbf{x} = (2,-1)$. The shortest vector $\mathbf{x}$ is perpendicular to the line.

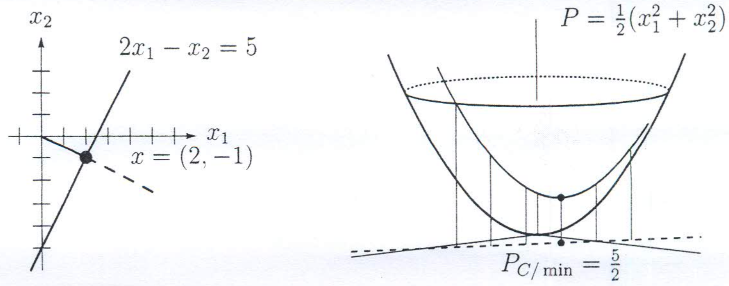

Figure 6.5 Minimizing $\frac{1}{2}\|x\|^2$ for all x on the constraint line $2x_1 - x_2 = 5$.

Least Squares Again

The best $\hat{\mathbf{x}}$ is the vector that minimizes $E^2 = \|A\mathbf{x} - \mathbf{b}\|^2$

Squared Error: $E^2 = (A\mathbf{x}-\mathbf{b})^T(A\mathbf{x}-\mathbf{b}) = \mathbf{x}^TA^TA\mathbf{x} - 2\mathbf{x}^TA^T\mathbf{b} + \mathbf{b}^T\mathbf{b}$.

The minimizing equation changes into the

Least-squares Equation: $A^TA\hat{\mathbf{x}} = A^T\mathbf{b}$

The Rayleigh Quotient

Our second goal is to find a minimization problem equivalent to $A\mathbf{x} = \lambda\mathbf{x}$. That is not so easy. The eigenvalue problem is nonlinear (λ times $\mathbf{x}$). The trick is that we can divide one quadratic by another one:

Rayleigh Quotient: Minimize $R(\mathbf{x}) = \dfrac{\mathbf{x}^TA\mathbf{x}}{\mathbf{x}^T\mathbf{x}}$

[6.2] Rayleigh's Principle: The minimum value of the Rayleigh quotient is the smallest eigenvalue λ_1. $R(x)$ reaches that minimum at the first eigenvector x_1 of A:

Minimum where $Ax_1 = \lambda x_1$: $\quad R(x_1) = \dfrac{x_1^T A x_1}{x_1^T x_1} = \dfrac{x_1^T \lambda_1 x_1}{x_1^T x_1} = \lambda_1$

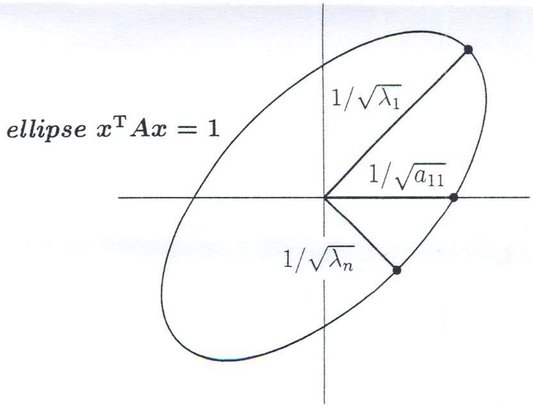

Figure 6.6 The farthest $x = x_1/\sqrt{\lambda_1}$ and the closest $x = x_n/\sqrt{\lambda_n}$ both give $x^T A x = x^T \lambda x = 1$. Those are the major and minor axes of the ellipse.

If we keep $x^T A x = 1$, then $R(x)$ is a minimum when $x^T x = \|x\|^2$ is the largest. We look for the point on the ellipsoid $x^T A x = 1$ farthest from the origin. The largest axis points along the first eigenvector. So $R(x)$ is minimum at x_1.

algebraically, we can diagonalize $A = Q\Lambda Q^T$ and set $x = Qy$,

$$R(x) = \frac{(Qy)^T A (Qy)}{(Qy)^T (Qy)} = \frac{y^T \Lambda y}{y^T y} = \frac{\lambda_1 y_1^2 + \cdots + \lambda_n y_n^2}{y_1^2 + \cdots + y_n^2}$$

The minimum of R is λ_1 at the point where $y_1 = 1$, $y_2 = \cdots = y_n = 0$:

at all points: $\lambda_1 (y_1^2 + \cdots + y_n^2) \leq (\lambda_1 y_1^2 + \cdots + \lambda_n y_n^2)$

The Rayleigh quotient is never below λ_1 and never above λ_n. Its minimum is at x_1 and its maximum is at x_n:

Maximum where $Ax_n = \lambda_n x_n$: $\quad R(x_n) = \dfrac{x_n^T A x_n}{x_n^T x_n} = \dfrac{x_n^T \lambda_n x_n}{x_n^T x_n} = \lambda_n$