Quadratic Optimization

This is an important application of the spectral theorem and positive-definiteness.

It is the simplest case of quadratic programming, which is a big subfield of optimization. (So is least squares.)

For an example application, see the Wikipedia page for support-vector machine, an important tool in machine learning that reduces to a quadratic optimization problem. (There are tons of other applications.)

Def: An optimization problem means finding extremal values (minimum & maximum) of a function $f(x_1, \ldots, x_n)$ subject to some constraint on $(x_1, \ldots, x_n)$.

In quadratic optimization, we consider quadratic functions.

Def: A quadratic form in n variables is a function
$q(x_1, \ldots, x_n) =$ sum of terms of the form $a_{ij} x_i x_j$

Eg: $q(x_1, x_2) = \frac{5}{2} x_1^2 + \frac{5}{2} x_2^2 - x_1 x_2$

Non-eg: $q(x_1, x_2) = x_1^2 + x_2^2 + x_1 + x_2$ is not a quadratic form: x_1, x_2 are linear terms.

NB: Thinking of $x=(x_1,\dots,x_n)$ as a vector,

$$q(cx) = q(cx_1,\dots,cx_n) = \sum a_{ij}(cx_i)(cx_j)$$
$$= \sum c^2 a_{ij} x_i x_j = c^2 q(x)$$

$$\boxed{q(cx) = c^2 q(x)}$$

In quadratic optimization, the constraint on $x=(x_1,\dots,x_n)$ is usually $\|x\|=1$, ie $x_1^2+\cdots+x_n^2=1$.

Quadratic Optimization Problem:
Given a quadratic form $q(x)$, find the minimum & maximum values of $q(x)$ subject to $\|x\|=1$.

Eg: $q(x_1,x_2) = 2x_1^2+3x_2^2$

Maximum:

$$q(x_1,x_2) = 2x_1^2+3x_2^2 \le 3x_1^2+3x_2^2$$
$$= 3(x_1^2+x_2^2) = 3\|x\|^2 = 3$$

So the maximum value is 3; it is achieved at $(x_1,x_2) = \pm(0,1)$: $q(0,\pm1)=3$.

Minimum:

$$q(x_1,x_2) = 2x_1^2+3x_2^2 \geq 2x_1^2+2x_2^2$$
$$= 2(x_1^2+x_2^2) = 2\|x\|^2 = 2$$

So the minimum value is 2; it is achieved at $(x_1,x_2) = \pm(1,0)$: $q(\pm 1,0)=2$.

This example is easy because $q(x_1,x_2) = 2x_1^2+3x_2^2$ involves only squares of the coordinates: there is no cross-term x_1x_2

Def: A quadratic form is diagonal if it has the form $q(x_1,\dots,x_n) =$ sum of terms of the form $\lambda_i x_i^2$.

Terms of the form $a_{ij}x_ix_j$ $(i\neq j)$ are cross-terms.

Quadratic Optimization of Diagonal Forms:

Let $q(x) = \sum_i \lambda_i x_i^2$. Order the x_i so that $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$. Then

- The maximum value of $q(x)$ is λ_n.
- The minimum value of $q(x)$ is λ_1.

(subject to $\|x\|=1$).

NB: the λ_i could be negative.

Strategy: To solve a quadratic optimization problem, we want to diagonalize it to get rid of the cross terms.

To do this, we use symmetric matrices!

Fact: Every quadratic form can be written
$$q(x) = x^T S x$$
for a symmetric matrix S.

Eg: $S = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 4 & 5 \\ 3 & 5 & 6 \end{pmatrix}$

$$\leadsto x^T S x = (x_1 \ x_2 \ x_3) \begin{pmatrix} 1 & 2 & 3 \\ 2 & 4 & 5 \\ 3 & 5 & 6 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$$

$$= (x_1 \ x_2 \ x_3) \begin{pmatrix} x_1 + 2x_2 + 3x_3 \\ 2x_1 + 4x_2 + 5x_3 \\ 3x_1 + 5x_2 + 6x_3 \end{pmatrix}$$

$$= x_1^2 + 2x_1x_2 + 3x_1x_3 + 2x_2x_1 + 4x_2^2 + 5x_2x_3 + 3x_3x_1 + 5x_3x_2 + 6x_3^2$$

$$= x_1^2 + 4x_2^2 + 6x_3^2 + 4x_1x_2 + 6x_1x_3 + 10x_2x_3$$

NB: The $(1,2)$ and $(2,1)$ entries contribute to the x_1x_2 coefficient.

Given q, how to get S?

The x_i^2 coefficients go on the diagonal, and half of the x_ix_j coefficient goes in the (i,j) and (j,i) entries.

$$q(x_1,x_2,x_3) = a_{11}x_1^2 + a_{22}x_2^2 + a_{33}x_3^2$$
$$+ a_{12}x_1x_2 + a_{13}x_1x_3 + a_{23}x_2x_3$$
$$\rightsquigarrow \quad S = \begin{pmatrix} a_{11} & a_{12}/2 & a_{13}/2 \\ a_{12}/2 & a_{22} & a_{23}/2 \\ a_{13}/2 & a_{23}/2 & a_{33} \end{pmatrix}$$

NB: q is diagonal $\iff$ S is diagonal: the a_{ij} are the coefficients of the cross-terms.

$$x^T \begin{pmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_n \end{pmatrix} x = \lambda_1 x_1^2 + \lambda_2 x_2^2 + \cdots + \lambda_n x_n^2$$

How does this help quadratic optimization?

Orthogonally diagonalize!

$$q(x) = x^T S x$$

Find a diagonal matrix D and orthogonal matrix Q such that $S = QDQ^T$ $\rightsquigarrow$

$$q(x) = x^T Q D Q^T x$$

Let $x = Qy$: this is a change of variables

$$q(x) = q(Qy) = (Qy)^T Q D Q^T (Qy)$$
$$= y^T \underbrace{Q^T Q}_{I_n} D \underbrace{Q^T Q}_{I_n} y = y^T D y$$

This is now diagonal!

NB: Q is orthogonal $\Rightarrow \|x\| = \|Qy\| = \|y\|$

So $\boxed{\|x\| = 1 \Leftrightarrow \|y\| = 1}$

Eg: Find the minimum & maximum of

$$q(x_1, x_2) = \frac{5}{2}x_1^2 + \frac{5}{2}x_2^2 - x_1 x_2$$ ← cross term ☹

subject to $\|x\| = 1$.

$$q(x) = x^T \begin{pmatrix} 5/2 & -1/2 \\ -1/2 & 5/2 \end{pmatrix} x \rightsquigarrow S = \frac{1}{2}\begin{pmatrix} 5 & -1 \\ -1 & 5 \end{pmatrix}$$

Orthogonally diagonalize: $S = QDQ^T$ for

$$Q = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \quad D = \begin{pmatrix} 2 & 0 \\ 0 & 3 \end{pmatrix}$$

Set $x = Qy$:

$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} y_1 - y_2 \\ y_1 + y_2 \end{pmatrix}$$

$$\begin{cases} x_1 = \frac{1}{\sqrt{2}}(y_1 - y_2) \\ x_2 = \frac{1}{\sqrt{2}}(y_1 + y_2) \end{cases}$$ is a linear change of variables

Then $q(x) = y^T \begin{pmatrix} 2 & 0 \\ 0 & 3 \end{pmatrix} y = 2y_1^2 + 3y_2^2$.

Check:

$$
\begin{aligned}
q(x) &= q\left(\tfrac{1}{\sqrt{2}}(y_1-y_2),\ \tfrac{1}{\sqrt{2}}(y_1+y_2)\right) \\
&= \tfrac{5}{2}\cdot\tfrac{1}{2}(y_1-y_2)^2 + \tfrac{5}{2}\cdot\tfrac{1}{2}(y_1+y_2)^2 - \tfrac{1}{2}(y_1-y_2)(y_1+y_2) \\
&= \tfrac{5}{4}y_1^2 + \tfrac{5}{4}y_2^2 - \cancel{\tfrac{5}{2}y_1y_2} + \tfrac{5}{4}y_1^2 + \tfrac{5}{4}y_2^2 + \cancel{\tfrac{5}{2}y_1y_2} \\
&\qquad - \tfrac{1}{2}y_1^2 + \tfrac{1}{2}y_2^2 \\
&= \tfrac{5}{2}y_1^2 - \tfrac{1}{2}y_1^2 + \tfrac{5}{2}y_2^2 + \tfrac{1}{2}y_2^2 = 2y_1^2 + 3y_2^2 \ \checkmark
\end{aligned}
$$

The maximum value of q subject to $\|x\| = \|y\| = 1$ is 3, achieved at

$$y = (0, \pm 1) \rightsquigarrow x = Qy = \pm\frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ 1 \end{pmatrix}$$

The minimum value of q subject to $\|x\| = \|y\| = 1$ is 2, achieved at

$$y = (\pm 1, 0) \rightsquigarrow x = Qy = \pm\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

NB: The minimum value is the smallest diagonal entry of $D \rightsquigarrow$ smallest eigenvalue.

$Q\begin{pmatrix} \pm 1 \\ 0 \end{pmatrix}$ is $\pm$ the first column of Q

$\rightarrow$ is a unit eigenvector for that eigenvalue.

Likewise for the largest eigenvalue.

Quadratic Optimization:

To find the minimum/maximum of a quadratic form $q(x)$ subject to $\|x\|=1$:

(1) Write $q(x)=x^TSx$ for a symmetric matrix S

(2) Orthogonally diagonalize $S=QDQ^T$ for

$$Q=\underbrace{\begin{pmatrix} | & & | \\ u_1 & \cdots & u_n \\ | & & | \end{pmatrix}}_{\text{eigenvectors}} \qquad D=\underbrace{\begin{pmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_n \end{pmatrix}}_{\text{eigenvalues}}$$

Order the eigenvalues so $\lambda_1 \le \cdots \le \lambda_n$

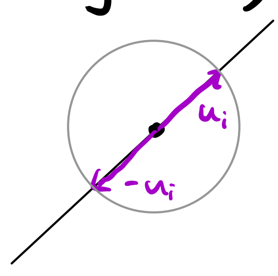
(3) The minimum value of $q(x)$ is the smallest eigenvalue λ_1.

It is achieved for $x=$ any unit λ_1-eigenvector.

The maximum value of $q(x)$ is the largest eigenvalue λ_n.

It is achieved for $x=$ any unit λ_n-eigenvector

NB: If $GM(\lambda_i)=1$ then the only unit λ_i-eigenvectors are $\pm u_i$. (only 2 unit vectors are on any line)



NB: $x=Qy$ diagonalizes q:

$$q(x)=\lambda_1 y_1^2+\cdots+\lambda_n y_n^2$$

Quadratic Optimization Problem, Variant:

Given a quadratic form $q(x)$, find the minimum & maximum values of $\|x\|^2$ subject to $q(x)=1$.

In general this will not work well:

- $q(x_1,x_2) = -x_1^2-2x_2^2$:
  there is no x such that $q(x)=1$!
- $q(x_1,x_2) = x_1^2-x_2^2$:
  there is no maximum $\|x\|^2$ subject to $q(x)=1$:
  $$q\left(C,\sqrt{C^2-1}\right) = 1 \quad \text{for any (huge) } C.$$

Problem: $q(x)$ may be 0 or negative!

Def: A quadratic form is **positive-definite** if $q(x)>0$ for all $x\neq 0$.

NB: If $q(x)=x^TSx$ then q is positive-definite $\iff S$ is positive-definite: this is the positive-energy criterion.

In this case, the problem is equivalent to the previous one.

NB: For q positive-definite,

$$q(x)=1 \iff q\left(\frac{x}{\|x\|}\right)=\frac{1}{\|x\|^2}q(x)=\frac{1}{\|x\|^2}$$

So $\|x\|^2$ minimized/maximized subject to $q(x)=1$

$$\iff q\left(\frac{x}{\|x\|}\right) \text{ is maximized/minimized}$$

Then $\frac{1}{\|x\|^2}$ = maximum/maximum value of $q(u)$ subject to $\|u\|^2=1$. $\left(u=\frac{x}{\|x\|}\right)$

Eg: Extremize $\|x\|^2$ subject to

$$q(x_1,x_2)=\frac{5}{2}x_1^2+\frac{5}{2}x_2^2-x_1x_2=1$$

We know q is maximized at $u_1=\pm\frac{1}{\sqrt{2}}\begin{pmatrix}-1\\1\end{pmatrix}$ with maximum value 3.

$$q(u_1)=3 \Rightarrow q\left(\frac{u_1}{\sqrt{3}}\right)=1$$

The minimum value of $\|x\|^2$ subject to $q(x)=1$ is $1/3$. It is achieved at $\frac{1}{\sqrt{3}}u_1$.

And q is minimized at $u_2=\pm\frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}$ with minimum value 2.

The maximum value of $\|x\|^2$ subject to $q(x)=1$ is $1/2$. It is achieved at $\frac{1}{\sqrt{2}}u_2$.

Quadratic Optimization, Variant:

Given a positive-definite quadratic form q, to find the minimum/maximum values of $\|x\|^2$ subject to $q(x)=1$:

(1) Write $q(x)=x^T S x$ for a symmetric matrix S

(2) Orthogonally diagonalize $S=QDQ^T$ for

$$Q=\underbrace{\begin{pmatrix} | & & | \\ u_1 & \cdots & u_n \\ | & & | \end{pmatrix}}_{\text{eigenvectors}} \qquad D=\underbrace{\begin{pmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_n \end{pmatrix}}_{\text{eigenvalues}}$$

Order the eigenvalues so $\lambda_1 \le \cdots \le \lambda_n$

(3) The minimum value of $\|x\|^2$ is

1/(the largest eigenvalue λ_n.)

It is achieved for

$$x=\frac{\text{any unit } \lambda_n\text{-eigenvector}}{\sqrt{\lambda_n}}$$

The maximum value of $\|x\|^2$ is

1/(the smallest eigenvalue λ_1.)

It is achieved for

$$x=\frac{\text{any unit } \lambda_1\text{-eigenvector}}{\sqrt{\lambda_1}}$$