

- Unconstrained minimization

$$\begin{aligned} \min f(x), \\ x \in \mathbb{R}^n. \end{aligned}$$

- First order necessary optimality condition:

$$\nabla f(x) = \begin{pmatrix} \frac{\partial f(x)}{\partial x_1} \\ \frac{\partial f(x)}{\partial x_2} \\ \vdots \\ \frac{\partial f(x)}{\partial x_n} \end{pmatrix} = 0.$$

- Point x^* : $\nabla f(x^*) = 0$ is called a *stationary* point.

UNCONSTRAINED QUADRATIC OPTIMIZATION

- Unconstrained quadratic optimization: objective function is quadratic,
no constraints

$$\min_{x \in \mathbb{R}^n} \{f(x) = x^\top Qx + c^\top x\},$$

$$Q = \begin{pmatrix} q_{11} & q_{12} & \cdots & q_{1n} \\ q_{21} & q_{22} & \cdots & q_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ q_{n1} & q_{n2} & \cdots & q_{nn} \end{pmatrix} \in \mathbb{R}^{n \times n}, \quad c = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{pmatrix} \in \mathbb{R}^n,$$

Q assumed to be symmetric: $q_{ij} = q_{ji}$, otherwise you may set

$$Q \leftarrow \frac{1}{2}(Q + Q^\top).$$

(The latter means the following: $x^\top Qx = \frac{1}{2}x^\top (Q + Q^\top)x$ and

$Q + Q^\top$ is always symmetric).

- Unconstrained quadratic optimization: objective function is quadratic,
no constraints

$$\min_{x \in \mathbb{R}^n} \{f(x) = x^\top Qx + c^\top x\},$$

- Extracting Q and c :

Example 1. $f(x_1, x_2) = x_1^2 - x_2^2 - 4x_1 + 6x_2 \Rightarrow Q = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, c = \begin{pmatrix} -4 \\ 6 \end{pmatrix};$

$$f(x) = \underbrace{\begin{pmatrix} x_1 & x_2 \end{pmatrix}}_{x^\top} \underbrace{\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}}_Q \underbrace{\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}}_x + \underbrace{\begin{pmatrix} -4 & 6 \end{pmatrix}}_{c^\top} \underbrace{\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}}_x$$

- Unconstrained quadratic optimization: objective function is quadratic,
no constraints

$$\min_{x \in \mathbb{R}^n} \{f(x) = x^\top Qx + c^\top x\},$$

- Extracting Q and c :

Example 2. $f(x_1, x_2) = 5x_1^2 + 4x_1x_2 + x_2^2 - 16x_1 - 12x_2 \Rightarrow Q = \begin{pmatrix} 5 & 2 \\ 2 & 1 \end{pmatrix}, c = \begin{pmatrix} -16 \\ -12 \end{pmatrix};$

$$f(x) = \underbrace{\begin{pmatrix} x_1 & x_2 \end{pmatrix}}_{x^\top} \underbrace{\begin{pmatrix} 5 & 2 \\ 2 & 1 \end{pmatrix}}_Q \underbrace{\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}}_x + \underbrace{\begin{pmatrix} -16 & -12 \end{pmatrix}}_{c^\top} \underbrace{\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}}_x$$

- Unconstrained quadratic optimization: objective function is quadratic, no constraints

$$\min_{x \in \mathbb{R}^n} \{f(x) = x^T Q x + c^T x\},$$

- Extracting Q and c :

Example 3. $f(x_1, x_2, x_3) = x_1^2 + x_2^2 + 2x_3^2 + x_1x_2 + 2x_1x_3 + 3x_2x_3 - x_1$

$$f(x) = \underbrace{(x_1 \ x_2 \ x_3)}_{x^T} \underbrace{\begin{pmatrix} 1 & \frac{1}{2} & 1 \\ \frac{1}{2} & 1 & \frac{3}{2} \\ 1 & \frac{3}{2} & 2 \end{pmatrix}}_Q \underbrace{\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}}_x + \underbrace{(-1 \ 0 \ 0)}_{c^T} \underbrace{\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}}_x$$

- Unconstrained quadratic optimization: objective function is quadratic,
no constraints

$$\min_{x \in \mathbb{R}^n} \{f(x) = x^\top Qx + c^\top x\},$$

- Eigenstructure: $Q \sim (\Lambda, V)$, $Qv_i = \lambda_i v_i$, $i = 1, \dots, n$.

! Q is symmetric matrix \Rightarrow eigenvalues $\lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n$ are real numbers

$$\Lambda = \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{pmatrix}, \quad V = \begin{pmatrix} \boxed{v_{11}} & \boxed{v_{21}} & \cdots & \boxed{v_{n1}} \\ \boxed{v_{12}} & \boxed{v_{22}} & \cdots & \boxed{v_{n2}} \\ \vdots & \vdots & \vdots & \vdots \\ \boxed{v_{1n}} & \boxed{v_{2n}} & \cdots & \boxed{v_{nn}} \end{pmatrix},$$

\uparrow
 v_1

\uparrow
 v_2

\uparrow
 v_n

Λ - diagonal matrix with eigenvalues on the main diagonal,

V - matrix with eigenvectors v_1, v_2, \dots, v_n as columns.

- Matrix classification
- Q is said to be Positive Definite (PD, $Q \succ 0$) if $x^\top Q x > 0 \forall x \in \mathbb{R}^n, x \neq 0$.
(If Q is symmetric, $Q = Q^\top$, then PD $\sim \lambda_i > 0, i = 1, \dots, n$.)
- Q is said to be Positive SemiDefinite (PSD, $Q \succeq 0$) if $x^\top Q x \geq 0 \forall x \in \mathbb{R}^n$.
(If Q is symmetric, $Q = Q^\top$, then PSD $\sim \lambda_i \geq 0, i = 1, \dots, n$.)
- Q is said to be Negative SemiDefinite (NSD, $Q \preceq 0$) if $x^\top Q x \leq 0 \forall x \in \mathbb{R}^n$.
(If Q is symmetric, $Q = Q^\top$, then NSD $\sim \lambda_i \leq 0, i = 1, \dots, n$.)
- Q is said to be Negative Definite (ND, $Q \prec 0$) if $x^\top Q x < 0 \forall x \in \mathbb{R}^n, x \neq 0$.
(If Q is symmetric, $Q = Q^\top$, then ND $\sim \lambda_i < 0, i = 1, \dots, n$.)
- Otherwise, Q is said to be indefinite.

- Quadratic form: $f(x) = x^T Q x$
- Stationary point: $\nabla f(x) = 2Qx = 0 \Rightarrow x^* = 0$ - trivial!

Example 4. $f(x_1, x_2) = x_1^2 + x_2^2$

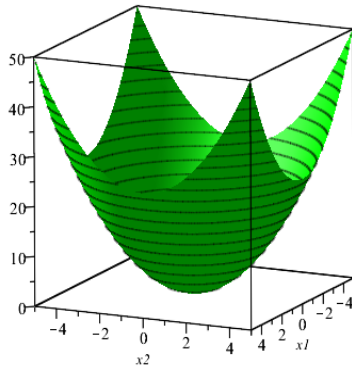
or $f(x_1, x_2) = 0.5x_1^2 + 2x_2^2$

or $f(x_1, x_2) = 5x_1^2 + 0.1x_2^2$

\Downarrow

$$f(x_1, x_2) = \lambda_1 x_1^2 + \lambda_2 x_2^2$$

$\lambda_1 > 0, \lambda_2 > 0 \Rightarrow x^* = 0$ - unique minimum



- Quadratic form: $f(x) = x^T Q x$
- Stationary point: $\nabla f(x) = 2Qx = 0 \Rightarrow x^* = 0$ - trivial!

Example 5. $f(x_1, x_2) = x_1^2$

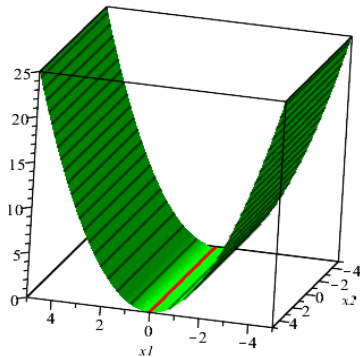
or $f(x_1, x_2) = 0.5x_1^2$

or $f(x_1, x_2) = 0.1x_2^2$

\Downarrow

$$f(x_1, x_2) = \lambda_1 x_1^2 + \lambda_2 x_2^2$$

$$\begin{aligned} \lambda_1 > 0, \lambda_2 &= 0 \\ \lambda_1 &= 0, \lambda_2 > 0 \end{aligned} \Rightarrow x^* = 0 \text{ - nonunique minimum}$$



- Quadratic form: $f(x) = x^T Q x$
- Stationary point: $\nabla f(x) = 2Qx = 0 \Rightarrow x^* = 0$ - trivial!

Example 6. $f(x_1, x_2) = x_1^2 - x_2^2$

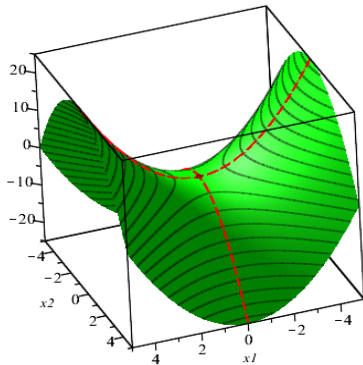
$$\text{or } f(x_1, x_2) = -x_1^2 + 0.5x_1^2$$

$$\text{or } f(x_1, x_2) = 0.1x_1^2 - 8x_2^2$$

\Downarrow

$$f(x_1, x_2) = \lambda_1 x_1^2 + \lambda_2 x_2^2$$

$$\begin{aligned} \lambda_1 > 0, \lambda_2 < 0 \\ \lambda_1 < 0, \lambda_2 > 0 \end{aligned} \Rightarrow x^* = 0 \text{ - saddle point}$$



- Quadratic form: $f(x) = x^T Qx$
- Stationary point: $\nabla f(x) = 2Qx = 0 \Rightarrow x^* = 0$ - trivial!

Example 7. $f(x_1, x_2) = -x_1^2$

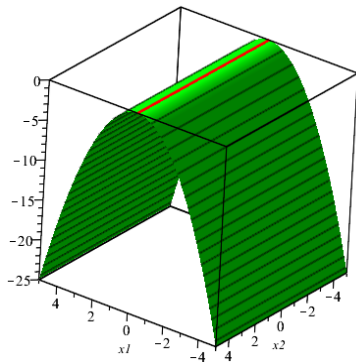
or $f(x_1, x_2) = -0.5x_2^2$

or $f(x_1, x_2) = -100x_1^2$

\Downarrow

$$f(x_1, x_2) = \lambda_1 x_1^2 + \lambda_2 x_2^2$$

$$\begin{aligned} \lambda_1 < 0, \lambda_2 = 0 \\ \lambda_1 = 0, \lambda_2 < 0 \end{aligned} \Rightarrow x^* = 0 \text{ - nonunique maximum}$$



- Quadratic form: $f(x) = x^\top Qx$
- Stationary point: $\nabla f(x) = 2Qx = 0 \Rightarrow x^* = 0$ - trivial!

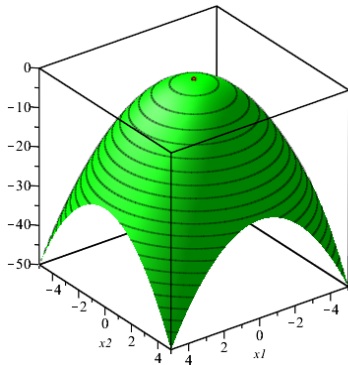
Example 8. $f(x_1, x_2) = -x_1^2 - x_2^2$

or $f(x_1, x_2) = -5x_1^2 - 0.5x_2^2$

or $f(x_1, x_2) = -0.1x_1^2 - 10x_2^2$

$$\Downarrow$$
$$f(x_1, x_2) = \lambda_1 x_1^2 + \lambda_2 x_2^2$$

$\lambda_1 < 0, \lambda_2 < 0 \Rightarrow x^* = 0$ - unique maximum



- Quadratic form: $f(x) = x^\top Qx$

- Stationary point: $\nabla f(x) = 2Qx = 0 \Rightarrow x^* = 0$ - trivial!

- Separable form = Q is diagonal

- $f(x) = \sum_{j=1}^n \lambda_j x_j^2$

$$Q = \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{pmatrix}$$

- .1 $0 < \lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n$ $x^* = 0$ - unique minimum;

- .2 $0 = \lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n$ $x^* = 0$ - nonunique minimum ($\lambda_n > 0$);

- .3 $\lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_k < 0 < \lambda_{k+1} \leq \dots \leq \lambda_n$ $x^* = 0$ - saddle point;

- .4 $\lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n = 0$ $x^* = 0$ - nonunique maximum ($\lambda_1 < 0$);

- .5 $\lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n < 0$ $x^* = 0$ - unique maximum.

- Quadratic form: $f(x) = x^\top Qx$
- Stationary point: $\nabla f(x) = 2Qx = 0 \Rightarrow x^* = 0$ - trivial!

- General case

$$Q = \begin{pmatrix} q_{11} & q_{12} & \cdots & q_{1n} \\ q_{21} & q_{22} & \cdots & q_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ q_{n1} & q_{n2} & \cdots & q_{nn} \end{pmatrix}$$

Example 9. $f(x_1, x_2) = x_1^2 - x_1x_2 + x_2^2$

Nevertheless! $f(x_1, x_2) = \frac{1}{4}(x_1 + x_2)^2 + \frac{3}{4}(-x_1 + x_2)^2 \geq 0$

\Downarrow

$x^* = 0$ is a minimum point, $\nabla f(x) = \begin{pmatrix} 2x_1 - x_2 \\ -x_1 + 2x_2 \end{pmatrix} = 0$.

- Quadratic form: $f(x) = x^\top Qx$
- Stationary point: $\nabla f(x) = 2Qx = 0 \Rightarrow x^* = 0$ - trivial!

- General case

$$Q = \begin{pmatrix} q_{11} & q_{12} & \cdots & q_{1n} \\ q_{21} & q_{22} & \cdots & q_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ q_{n1} & q_{n2} & \cdots & q_{nn} \end{pmatrix}$$

Example 10. $f(x_1, x_2) = -x_1x_2 + x_2^2$

Nevertheless! $f(x_1, x_2) = -0.207(0.924x_1 - 0.383x_2)^2 + 1.207(0.383x_1 + 0.924x_2)^2$

\Downarrow

$$x^* = 0 \text{ is a saddle point, } \nabla f(x) = \begin{pmatrix} -x_2 \\ -x_1 + 2x_2 \end{pmatrix} = 0.$$

- Quadratic form: $f(x) = x^\top Qx$
- Stationary point: $\nabla f(x) = 2Qx = 0 \Rightarrow x^* = 0$ - trivial!

- General case

$$Q = \begin{pmatrix} q_{11} & q_{12} & \cdots & q_{1n} \\ q_{21} & q_{22} & \cdots & q_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ q_{n1} & q_{n2} & \cdots & q_{nn} \end{pmatrix}$$

Example 11. $f(x_1, x_2) = -x_1^2 - x_1x_2 - x_2^2$

Nevertheless! $f(x_1, x_2) = -0.25(x_1 + x_2)^2 - 0.75(-x_1 + x_2)^2$

\Downarrow

$$x^* = 0 \text{ is a maximum point, } \nabla f(x) = \begin{pmatrix} -2x_1 - x_2 \\ -x_1 - 2x_2 \end{pmatrix} = 0.$$

- Quadratic form: $f(x) = x^\top Qx$
- Stationary point: $\nabla f(x) = 2Qx = 0 \Rightarrow x^* = 0$ - trivial!
- Eigenstructure analysis: if $\hat{\lambda}$ and \hat{v} are such that

$$Q\hat{v} = \hat{\lambda}\hat{v}$$

then $\hat{\lambda}$ is called an eigenvalue of matrix Q and

\hat{v} is called an eigenvector of matrix Q .

- In order to find an eigenpair $(\hat{\lambda}, \hat{v})$ one has to solve

$$Qx = \lambda x \Rightarrow (Q - \lambda I)x = 0.$$

- Nontrivial solutions iff (if and only if)

$$\det(Q - \lambda I) = 0.$$

- $\det(Q - \lambda I)$ is a polynomial of the degree n .
- If Q is symmetric then $\det(Q - \lambda I)$ has n real roots (eigenvalues):

$$\lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n.$$

- Unconstrained quadratic optimization: objective function is quadratic,
no constraints

$$\min_{x \in \mathbb{R}^n} \{f(x) = x^T Q x + c^T x\},$$

- Eigenstructure: $Q \sim (\Lambda, V)$, $Q v_i = \lambda_i v_i$, $i = 1, \dots, n$.

! Q is symmetric matrix \Rightarrow eigenvalues $\lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n$ are real numbers

$$\Lambda = \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{pmatrix}, \quad V = \begin{pmatrix} \boxed{v_{11}} & \boxed{v_{21}} & \cdots & \boxed{v_{n1}} \\ \boxed{v_{12}} & \boxed{v_{22}} & \cdots & \boxed{v_{n2}} \\ \vdots & \vdots & \vdots & \vdots \\ \boxed{v_{1n}} & \boxed{v_{2n}} & \cdots & \boxed{v_{nn}} \end{pmatrix},$$

\uparrow
 v_1

\uparrow
 v_2

\uparrow
 v_n

Λ - diagonal matrix with eigenvalues on the main diagonal,

V - matrix with eigenvectors v_1, v_2, \dots, v_n as columns.

- Unconstrained quadratic optimization: objective function is quadratic,
no constraints

$$\min_{x \in \mathbb{R}^n} \{f(x) = x^\top Qx + c^\top x\},$$

- Eigenstructure: $Q \sim (\Lambda, V)$, $Qv_i = \lambda_i v_i$, $i = 1, \dots, n$,

$$QV = V\Lambda \quad (1)$$

Eigenvectors v_1, v_2, \dots, v_n are orthogonal:

$$v_i^\top v_j = \begin{cases} \theta_i, & i = j, \\ 0, & i \neq j \end{cases}, \quad \theta_j = \|v_j\|^2 > 0, \quad \Theta = \begin{pmatrix} \theta_1 & 0 & \dots & 0 \\ 0 & \theta_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \theta_n \end{pmatrix}$$

$$V^\top V = \Theta \quad (2)$$

From (1), (2) \Rightarrow

$$V^\top QV = V^\top V\Lambda = \Theta\Lambda \quad (3)$$

- Unconstrained quadratic optimization: objective function is quadratic,
no constraints

$$\min_{x \in \mathbb{R}^n} \{f(x) = x^\top Qx + c^\top x\},$$

- Inverses matrices:

$$V^\top V = \Theta \quad (2) \Rightarrow V^\top V = \Theta^{\frac{1}{2}} \Theta^{\frac{1}{2}} \Rightarrow \Theta^{-\frac{1}{2}} V^\top V \Theta^{-\frac{1}{2}} = I, \quad (4)$$

$$\Theta^{\frac{1}{2}} = \begin{pmatrix} \sqrt{\theta_1} & 0 & \cdots & 0 \\ 0 & \sqrt{\theta_2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sqrt{\theta_n} \end{pmatrix}, \Theta^{-\frac{1}{2}} = \begin{pmatrix} \frac{1}{\sqrt{\theta_1}} & 0 & \cdots & 0 \\ 0 & \frac{1}{\sqrt{\theta_2}} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \frac{1}{\sqrt{\theta_n}} \end{pmatrix}, I = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{pmatrix}$$

$$\begin{array}{l} \text{From (4) and } (AB)^{-1} = B^{-1}A^{-1} \Rightarrow \left\{ \begin{array}{l} \left(\Theta^{-\frac{1}{2}} V^\top \right)^{-1} = (V^\top)^{-1} \Theta^{\frac{1}{2}} = V \Theta^{-\frac{1}{2}} \Rightarrow (V^\top)^{-1} = V \Theta^{-1}, \quad (5) \\ \left(V \Theta^{-\frac{1}{2}} \right)^{-1} = \Theta^{\frac{1}{2}} V^{-1} = \Theta^{-\frac{1}{2}} V^\top \Rightarrow V^{-1} = \Theta^{-1} V^\top, \quad (6) \end{array} \right. \end{array}$$

- Unconstrained quadratic optimization: objective function is quadratic,
no constraints

$$\min_{x \in \mathbb{R}^n} \{f(x) = x^\top Qx + c^\top x\},$$

- Decomposition of Q :

$$\boxed{\text{From } V^\top QV = \Theta\Lambda \text{ (see (3)), (5), (6))} \Rightarrow Q = \underbrace{V\Theta^{-1}}_{(V^\top)^{-1}} \Theta\Lambda \underbrace{\Theta^{-1}V^\top}_{V^{-1}} = V\Lambda\Theta^{-1}V^\top$$

$$Q = V\Lambda\Theta^{-1}V^\top$$

- Then

$$\boxed{f(x) = x^\top V\Lambda\Theta^{-1}V^\top x + c^\top x} \quad (7)$$

- Variable substitutions: $y = V^\top x \Leftrightarrow x = V\Theta^{-1}y$ (see (5))
- New objective function: $\tilde{f}(y) = y^\top \Lambda\Theta^{-1}y + d^\top y$, $d = \Theta^{-1}V^\top c$.

- Unconstrained quadratic optimization: reduction to the separable problem

$$\begin{array}{ccc}
 \boxed{\min_{x \in \mathbb{R}^n} \{f(x) = x^\top Qx + c^\top x\}} & & \\
 \Downarrow & \Uparrow & \\
 \boxed{x = V\Theta^{-1}y} & & \boxed{y = V^\top x} \\
 \Downarrow & \Uparrow & \\
 \boxed{\min_{y \in \mathbb{R}^n} \{\tilde{f}(y) = y^\top \Lambda \Theta^{-1} y + d^\top y\}} & &
 \end{array}$$

- Advantage: \tilde{f} is a separable function

$$\tilde{f}(y) = \sum_{i=1}^n \left(\frac{\lambda_i}{\theta_i} y_i^2 + d_i y_i \right), \quad d_i = \frac{1}{\theta_i} v_i^\top c \quad (8)$$

- Separable objective:

$$\tilde{f}(y) = \sum_{i=1}^n \left(\frac{\lambda_i}{\theta_i} y_i^2 + d_i y_i \right)$$

- Index sets: $\mathcal{I}^- = \{i : \lambda_i < 0\}$, $\mathcal{I}^0 = \{i : \lambda_i = 0\}$, $\mathcal{I}^+ = \{i : \lambda_i > 0\}$
- Then

$$\tilde{f}(y) = \sum_{i \in \mathcal{I}^-} \left(\frac{\lambda_i}{\theta_i} y_i^2 + d_i y_i \right) + \sum_{i \in \mathcal{I}^0} d_i y_i + \sum_{i \in \mathcal{I}^+} \left(\frac{\lambda_i}{\theta_i} y_i^2 + d_i y_i \right)$$

\Downarrow

$$\tilde{f}(y) = \sum_{i \in \mathcal{I}^- \cup \mathcal{I}^+} \frac{\lambda_i}{\theta_i} \left(y_i + \frac{d_i \theta_i}{2\lambda_i} \right)^2 + \sum_{i \in \mathcal{I}^0} d_i y_i - \frac{1}{4} \sum_{i \in \mathcal{I}^- \cup \mathcal{I}^+} \frac{d_i^2 \theta_i}{\lambda_i} \quad (9)$$