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Optimization

- Elements of Calculus

- Basics of constrained and unconstrained optimization

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In this lecture, we will talk about methods to find the extrema of a function.
These methods are also useful if you don't have the function

Optimization – the general problem

Optimization

minimize $f(x)$,
subject to $x \in \Omega$

- $x = (x_1, \dots, x_n)$, optimization variables, or decision variables
- $f\colon R^n \to R$, objective function
- Ω, is the constraint set or feasible set, sometimes $\Omega = \{x \in R^n |\ f_i(x) \le b_i$, where $i = 1, \dots, m\}$
- $f_i(x)\ R^n \to R$, where $i = 1, \dots, m$: constraint functions
- x **optimal solution** or **minimizer,** is the smallest value of f among $x = (x_1, \dots, x_n)$, satisfying the constraint

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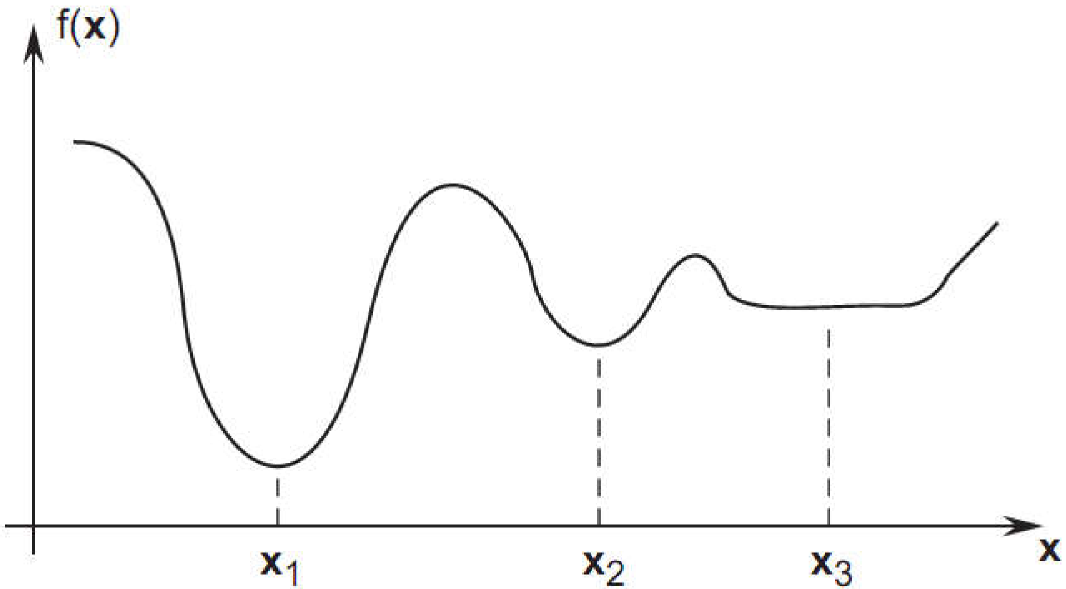
Local minimizer

Definition 6.1 Suppose $f\colon R^n \to R$, is a real-valued function defined on the set $\Omega \subseteq R^n$. A point x is a local minimizer of f over Ω if there exists $\varepsilon > 0$ such that $f(x) \geq f(x^*)$ for all $x \in \Omega$ and $\| x - x^* \| < \varepsilon$. A point x^* is a global minimizer of f over Ω if $f(x) \geq f(x\ )$ for all $x \in \Omega$. omega is the set of contraints



There are many minimisers around x3

Partiel derivatives and the Hessian matrix

Gradient of $f : \mathbb{R}^n \to \mathbb{R}$ is a column vector

$$\nabla f(\boldsymbol{x}) = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \\ \vdots \\ \frac{\partial f}{\partial x_n} \end{bmatrix}$$

First derivative—row vector

$$Df(\boldsymbol{x}) = \nabla f(\boldsymbol{x})^\top = \begin{bmatrix} \frac{\partial f}{\partial x_1} & \cdots & \frac{\partial f}{\partial x_n} \end{bmatrix}$$

$$\begin{aligned} \boldsymbol{F}(\boldsymbol{x}) &= D^2 f(\boldsymbol{x}) = \begin{bmatrix} D\left(\frac{\partial f}{\partial x_1}\right) \\ D\left(\frac{\partial f}{\partial x_2}\right) \\ \vdots \\ D\left(\frac{\partial f}{\partial x_n}\right) \end{bmatrix} \\ &= \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \cdots & \frac{\partial^2 f}{\partial x_n \partial x_1} \\ \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_1 \partial x_n} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix} \end{aligned}$$

Example 6.1 Let $f(x_1, x_2) = 5x_1 + 8x_2 + x_1x_2 - x_1^2 - 2x_2^2$. Then,

$$Df(\boldsymbol{x}) = (\nabla f(\boldsymbol{x}))^\top = \left[\frac{\partial f}{\partial x_1}(\boldsymbol{x}), \frac{\partial f}{\partial x_2}(\boldsymbol{x})\right] = [5 + x_2 - 2x_1, 8 + x_1 - 4x_2]$$

and

$$\boldsymbol{F}(\boldsymbol{x}) = D^2 f(\boldsymbol{x}) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2}(\boldsymbol{x}) & \frac{\partial^2 f}{\partial x_2 \partial x_1}(\boldsymbol{x}) \\ \frac{\partial^2 f}{\partial x_1 \partial x_2}(\boldsymbol{x}) & \frac{\partial^2 f}{\partial x_2^2}(\boldsymbol{x}) \end{bmatrix} = \begin{bmatrix} -2 & 1 \\ 1 & -4 \end{bmatrix}.$$

■

Directional derivatives

The directional derivative of f at $x \in \mathbb{R}^n$ in the direction d is denoted

$$\frac{\partial f(x)}{\partial d}$$

$$\begin{aligned}\frac{\partial f(x)}{\partial d} &= \lim_{\alpha \to 0} \frac{f(x+\alpha d) - f(x)}{\alpha} \\ &= \frac{d}{d\alpha} f(x+\alpha d)\Big|_{\alpha=0} \\ &= \begin{bmatrix} & Df(x) & \end{bmatrix} \begin{bmatrix} \\ d \\ \\ \end{bmatrix}\end{aligned}$$

This is a composition of two functions like f(g(x))

Example 6.2 Define $f : \mathbb{R}^3 \to \mathbb{R}$ by $f(\boldsymbol{x}) = x_1 x_2 x_3$, and let

$$\boldsymbol{d} = \left[\frac{1}{2}, \frac{1}{2}, \frac{1}{\sqrt{2}}\right]^\top .$$

The directional derivative of f in the direction $\boldsymbol{d}$ is

$$\frac{\partial f}{\partial \boldsymbol{d}}(\boldsymbol{x}) = \nabla f(\boldsymbol{x})^\top \boldsymbol{d} = [x_2 x_3, x_1 x_3, x_1 x_2] \begin{bmatrix} 1/2 \\ 1/2 \\ 1/\sqrt{2} \end{bmatrix} = \frac{x_2 x_3 + x_1 x_3 + \sqrt{2} x_1 x_2}{2}.$$

Level sets and contour plots

The *level set* of a function $f : \mathbb{R}^n \to \mathbb{R}$ at level c is the set of points

$$S = \{\boldsymbol{x} : f(\boldsymbol{x}) = c\}.$$

Gradient is always orthogonal to the level set

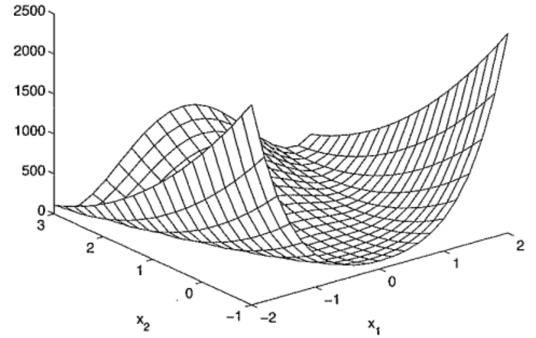
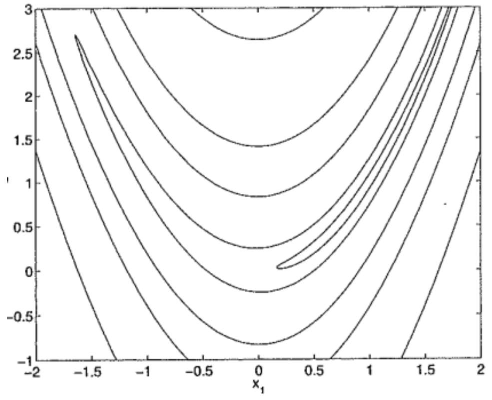


Figure 5.2 Graph of Rosenbrock's function.



$$f(\boldsymbol{x}) = 100(x_2 - x_1^2)^2 + (1 - x_1)^2,$$

MatLab demo: ContoursInMatlab.m

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Exercise on Derivatives

Find a point (x,y) where the gradient parallel to the y-axis for the following function:

Set the x=0 to find the gradient parallel to the y-axis

$$f(x, y) = 3\mathrm{x}^2 \quad 4\mathrm{xy} + 7\mathrm{y}^2$$

In the point you found above, what is the directional derivation in the direction (1,0)?

Feasible directions

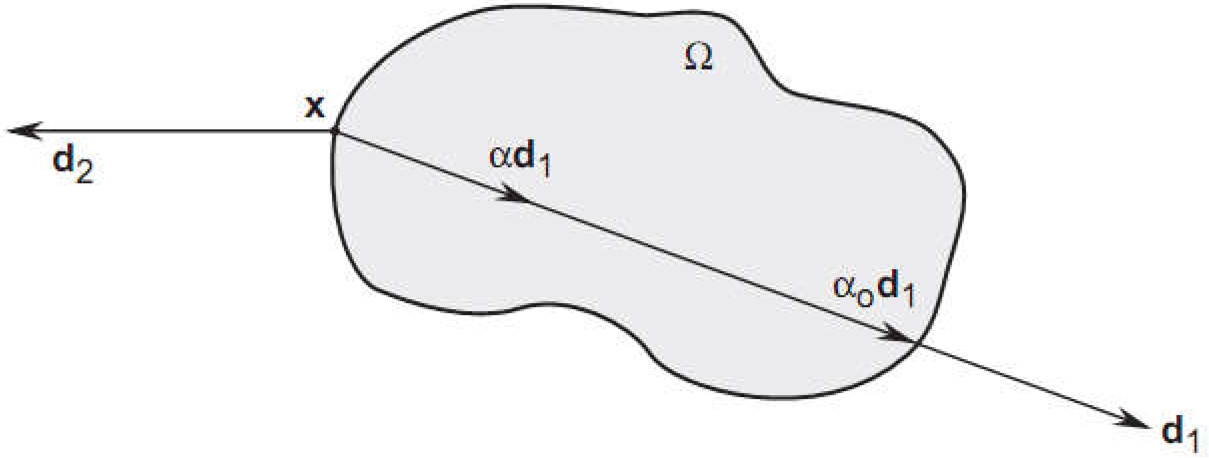
are used in constrained optimisation. A feasible direction is associated with a specific point.

$\boldsymbol{d} \in \mathbb{R}^n$ is a feasible direction at $\boldsymbol{x} \in \Omega$ if there is $\alpha_0 > 0$ such that

$$\boldsymbol{x} + \alpha \boldsymbol{d} \in \Omega \quad \text{for all} \quad \alpha \in [0, \alpha_0]$$

alpha can very small`

In other words, d is a feasible direction at x if x is added to d with a very small value, the resulting point is still within the feasible set.



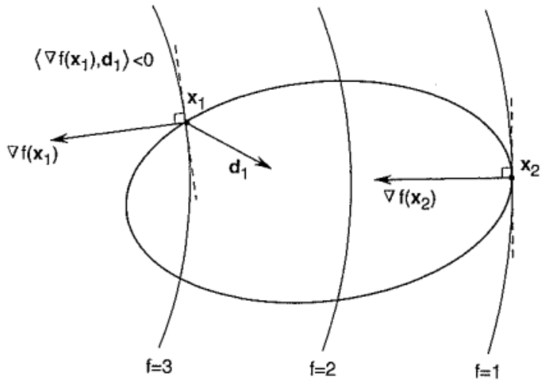
First Order Necessary Condition (FONC)

Theorem 6.1 ***First-Order Necessary Condition (FONC).*** *Let Ω be a subset of $\mathbb{R}^n$ and $f \in \mathcal{C}^1$ a real-valued function on Ω. If $\boldsymbol{x}^*$ is a local minimizer of f over Ω, then for any feasible direction $\boldsymbol{d}$ at $\boldsymbol{x}^*$, we have*

$$\boldsymbol{d}^T \nabla f(\boldsymbol{x}^*) \geq 0.$$

□

This allows us to determine whether a point can be a local minimiser in the case where the point is at the border of the feasible set



Less important

Corollary 6.1 ***Interior Case.*** *Let Ω be a subset of $\mathbb{R}^n$ and $f \in \mathcal{C}^1$ a real-valued function on Ω. If $\boldsymbol{x}^*$ is a local minimizer of f over Ω and if $\boldsymbol{x}^*$ is an interior point of Ω, then*

$$\nabla f(\boldsymbol{x}^*) = \boldsymbol{0}.$$

□

More important

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FONC example (Thm. 6.1)

Example 6.3 Consider the problem

$$\begin{array}{ll} \text{minimize} & x_1^2 + 0.5x_2^2 + 3x_2 + 4.5 \\ \text{subject to} & x_1, x_2 \geq 0. \end{array}$$

a. Is the first-order necessary condition (FONC) for a local minimizer satisfied at $\boldsymbol{x} = [1, 3]^\top$?

b. Is the FONC for a local minimizer satisfied at $\boldsymbol{x} = [0, 3]^\top$?

c. Is the FONC for a local minimizer satisfied at $\boldsymbol{x} = [1, 0]^\top$?

d. Is the FONC for a local minimizer satisfied at $\boldsymbol{x} = [0, 0]^\top$?

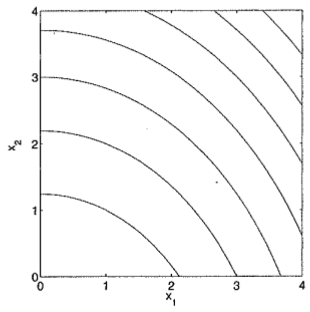

Figure 6.4 Level sets of the function in Example 6.3.

FONC example (Cor. 6.1)

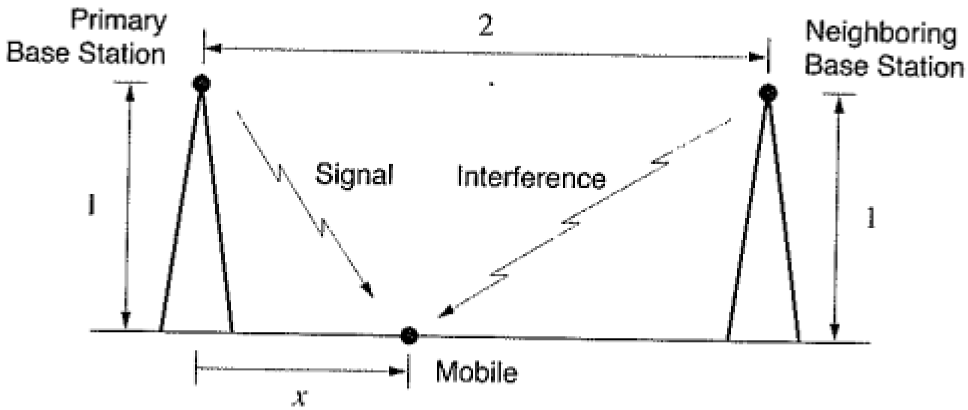

Figure 6.5 Simplified cellular wireless system in Example 6.4.

$$f(x) = \frac{1 + (2 - x)^2}{1 + x^2}.$$

$$\begin{aligned} f'(x) &= \frac{-2(2 - x)(1 + x^2) - 2x(1 + (2 - x)^2)}{(1 + x^2)^2} \\ &= \frac{4(x^2 - 2x - 1)}{(1 + x^2)^2}. \end{aligned}$$

Quadratic forms – using matrices

EXAMPLE 1 Let $\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$. Compute $\mathbf{x}^T A \mathbf{x}$ for the following matrices:

a. $A = \begin{bmatrix} 4 & 0 \\ 0 & 3 \end{bmatrix}$ b. $A = \begin{bmatrix} 3 & -2 \\ -2 & 7 \end{bmatrix}$

a. $\mathbf{x}^T A \mathbf{x} = [\, x_1 \quad x_2 \,] \begin{bmatrix} 4 & 0 \\ 0 & 3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = [\, x_1 \quad x_2 \,] \begin{bmatrix} 4x_1 \\ 3x_2 \end{bmatrix} = 4x_1^2 + 3x_2^2.$

b. There are two -2 entries in A. Watch how they enter the calculations. The $(1, 2)$-entry in A is in boldface type.

$$\begin{aligned} \mathbf{x}^T A \mathbf{x} &= [\, x_1 \quad x_2 \,] \begin{bmatrix} 3 & \mathbf{-2} \\ -2 & 7 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = [\, x_1 \quad x_2 \,] \begin{bmatrix} 3x_1 - \mathbf{2}x_2 \\ -2x_1 + 7x_2 \end{bmatrix} \\ &= x_1(3x_1 - \mathbf{2}x_2) + x_2(-2x_1 + 7x_2) \\ &= 3x_1^2 - \mathbf{2}x_1x_2 - 2x_2x_1 + 7x_2^2 \\ &= 3x_1^2 - 4x_1x_2 + 7x_2^2 \end{aligned}$$

Examples from Lay sec. 7.2

Quadratic forms – using matrices

EXAMPLE 2 For $\mathbf{x}$ in $\mathbb{R}^3$, let $Q(\mathbf{x}) = 5x_1^2 + 3x_2^2 + 2x_3^2 - x_1x_2 + 8x_2x_3$. Write this quadratic form as $\mathbf{x}^TA\mathbf{x}$.

Solution The coefficients of x_1^2, x_2^2, x_3^2 go on the diagonal of A. To make A symmetric, the coefficient of x_ix_j for $i \neq j$ must be split evenly between the (i, j)- and (j, i)-entries in A. The coefficient of x_1x_3 is 0. It is readily checked that

$$Q(\mathbf{x}) = \mathbf{x}^TA\mathbf{x} = [\,x_1 \quad x_2 \quad x_3\,]\begin{bmatrix} 5 & -1/2 & 0 \\ -1/2 & 3 & 4 \\ 0 & 4 & 2 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

Examples from Lay sec. 7.2

Qudratic forms – using matrices

EXAMPLE 3 Let $Q(\mathbf{x}) = x_1^2 - 8x_1x_2 - 5x_2^2$. Compute the value of $Q(\mathbf{x})$ for $\mathbf{x} = \begin{bmatrix} -3 \\ 1 \end{bmatrix}, \begin{bmatrix} 2 \\ -2 \end{bmatrix}$, and $\begin{bmatrix} 1 \\ -3 \end{bmatrix}$.

Solution

$$
\begin{aligned}
Q(-3, 1) &= (-3)^2 - 8(-3)(1) - 5(1)^2 = 28 \\
Q(2, -2) &= (2)^2 - 8(2)(-2) - 5(-2)^2 = 16 \\
Q(1, -3) &= (1)^2 - 8(1)(-3) - 5(-3)^2 = -20
\end{aligned}
$$

In some cases, quadratic forms are easier to use when they have no cross-product terms—that is, when the matrix of the quadratic form is a diagonal matrix. Fortunately, the cross-product term can be eliminated by making a suitable change of variable.

Examples from Lay sec. 7.2

Qudratic forms – change of varibles

EXAMPLE 4 Make a change of variable that transforms the quadratic form in Example 3 into a quadratic form with no cross-product term.

Solution The matrix of the quadratic form in Example 3 is

$$A = \begin{bmatrix} 1 & -4 \\ -4 & -5 \end{bmatrix}$$

The first step is to orthogonally diagonalize A. Its eigenvalues turn out to be $\lambda = 3$ and $\lambda = -7$. Associated unit eigenvectors are

$$\lambda = 3: \begin{bmatrix} 2/\sqrt{5} \\ -1/\sqrt{5} \end{bmatrix}; \qquad \lambda = -7: \begin{bmatrix} 1/\sqrt{5} \\ 2/\sqrt{5} \end{bmatrix}$$

These vectors are automatically orthogonal (because they correspond to distinct eigenvalues) and so provide an orthonormal basis for $\mathbb{R}^2$. Let

$$P = \begin{bmatrix} 2/\sqrt{5} & 1/\sqrt{5} \\ -1/\sqrt{5} & 2/\sqrt{5} \end{bmatrix}, \qquad D = \begin{bmatrix} 3 & 0 \\ 0 & -7 \end{bmatrix}$$

Examples from Lay sec. 7.2

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Qudratic forms – and extremal points

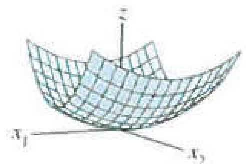
DEFINITION

A quadratic form Q is:

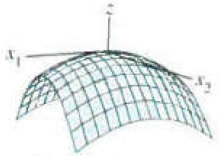
a. **positive definite** if $Q(\mathbf{x}) > 0$ for all $\mathbf{x} \neq \mathbf{0}$,

b. **negative definite** if $Q(\mathbf{x}) < 0$ for all $\mathbf{x} \neq \mathbf{0}$,

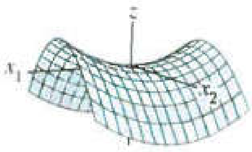
c. **indefinite** if $Q(\mathbf{x})$ assumes both positive and negative values.



Positive definite



Negative definite



Indefinite

THEOREM 5

Quadratic Forms and Eigenvalues

Let A be an $n \times n$ symmetric matrix. Then a quadratic form $\mathbf{x}^T A\mathbf{x}$ is:

a. positive definite if and only if the eigenvalues of A are all positive,

b. negative definite if and only if the eigenvalues of A are all negative, or

c. indefinite if and only if A has both positive and negative eigenvalues.

a. Minimum

b. Maximum

c. No min. No max

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Exercise on Qudratic forms

Classify the quadratic forms in Exercises 9–18. Then make a change of variable, $\mathbf{x} = P\mathbf{y}$, that transforms the quadratic form into one with no cross-product term. Write the new quadratic form. Construct P using the methods of Section 7.1.

9. $3x_1^2 - 4x_1x_2 + 6x_2^2$

10. $9x_1^2 - 8x_1x_2 + 3x_2^2$

11. $2x_1^2 + 10x_1x_2 +$ [illegible]

12. $-5x_1^2 + 4x_1x_2 - 2x_2^2$

13. $x_1^2 - 6x_1x_2 + 9$[illegible]

[illegible] $+ 6x_1x_2$

15. **[M]** $-2x_1^2 - 6$[illegible]$x_1x_2 + 4x_1x_3 + 4x_1x_4 + 6x_3x_4$

16. **[M]** $4x_1^2 + 4$[illegible]$x_3x_4 - 4x_1x_4 + 4x_2x_3$

17. **[M]** $x_1^2 + x_2^2 + x_3^2 + x_4^2$ [illegible] $2x_2x_3 + 9x_3x_4$

18. **[M]** $11x_1^2 - x_2^2 - 12x_1x_2$ [illegible] $2x_3x_4$

Examples from Lay sec. 7.2

Optimization

Theorem 6.2 ***Second-Order Necessary Condition (SONC).*** *Let $\Omega \subset \mathbb{R}^n$, $f \in \mathcal{C}^2$ a function on Ω, $\boldsymbol{x}^*$ a local minimizer of f over Ω, and $\boldsymbol{d}$ a feasible direction at $\boldsymbol{x}^*$. If $\boldsymbol{d}^\top \nabla f(\boldsymbol{x}^*) = 0$, then*

$$\boldsymbol{d}^\top \boldsymbol{F}(\boldsymbol{x}^*)\boldsymbol{d} \geq 0,$$

where $\boldsymbol{F}$ is the Hessian of f. □

Corollary 6.2 ***Interior Case.*** *Let $\boldsymbol{x}^*$ be an interior point of $\Omega \subset \mathbb{R}^n$. If $\boldsymbol{x}^*$ is a local minimizer of $f : \Omega \to \mathbb{R}$, $f \in \mathcal{C}^2$, then*

$$\nabla f(\boldsymbol{x}^*) = \boldsymbol{0},$$

This is important.

and $\boldsymbol{F}(\boldsymbol{x}^*)$ is positive semidefinite ($\boldsymbol{F}(\boldsymbol{x}^*) \geq 0$); that is, for all $\boldsymbol{d} \in \mathbb{R}^n$,

$$\boldsymbol{d}^\top \boldsymbol{F}(\boldsymbol{x}^*)\boldsymbol{d} \geq 0.$$

This is the same as saying that all eigenvalues are positive

□

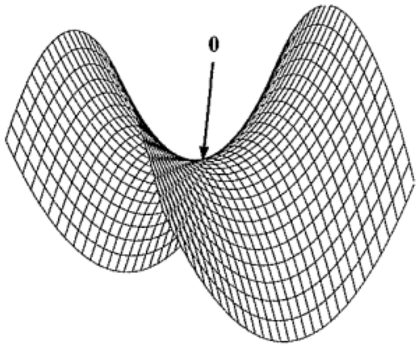
Optimization

Example 6.6 Consider a function of one variable $f(x) = x^3$, $f : \mathbb{R} \to \mathbb{R}$. Because $f'(0) = 0$, and $f''(0) = 0$, the point $x = 0$ satisfies both the FONC and SONC. However, $x = 0$ is not a minimizer (see Figure 6.6). ■

Example 6.7 Consider a function $f : \mathbb{R}^2 \to \mathbb{R}$, where $f(\boldsymbol{x}) = x_1^2 - x_2^2$. The FONC requires that $\nabla f(\boldsymbol{x}) = [2x_1, -2x_2]^\top = \mathbf{0}$. Thus, $\boldsymbol{x} = [0, 0]^\top$ satisfies the FONC. The Hessian matrix of f is

$$\boldsymbol{F}(\boldsymbol{x}) = \begin{bmatrix} 2 & 0 \\ 0 & -2 \end{bmatrix}.$$

Here, the eigenvalues are easy to read off the matrix.



Optimization

Theorem 6.3 ***Second-Order Sufficient Condition (SOSC), Interior Case.*** *Let $f \in \mathcal{C}^2$ be defined on a region in which $\boldsymbol{x}^*$ is an interior point. Suppose that*

1. $\nabla f(\boldsymbol{x}^*) = \boldsymbol{0}$.
2. $\boldsymbol{F}(\boldsymbol{x}^*) > 0$.

Then, $\boldsymbol{x}^*$ is a strict local minimizer of f. □