R401: Statistical and Mathematical Foundations

Lecture 14: Unconstrained Optimization. Static Optimization with Equality Constraints. Lagrange Multipliers

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General Principles and Caveats for the Optimization Module

- Emphasis on practicality over rigour
- Consequently, algorithmic approach and "recipes" rather than proofs
- Also, existence and relevant properties of various objects are often implicitly assumed
- Pathologies and mathematical peculiarities discussed only in special cases

Lecture Contents

Warm-up: Basic Unconstrained Optimization in $\mathbb{R}^1$

Fact 1

For a function $f : \mathbb{R} \to \mathbb{R}$ differentiable at a point x, a necessary condition for a local extreme point (i.e. a maximum or a minimum) at x is

$$f'(x) = 0.$$

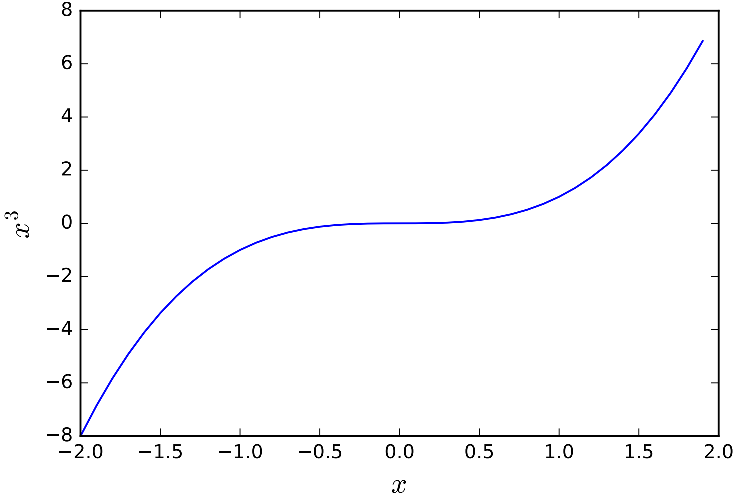
Example 1

If $f(x) = ax^2 + bx + c$, then $f'(x) = 2ax + b$ and the condition $f'(x) = 0$ yields the familiar $x = -\frac{b}{2a}$ (recall your high-school days). Depending on the sign of a, this is a maximum or a minimum (What is the relationship?).

Example 2

If $f(x) = x^3$, then $f'(x) = 3x^2$ and $f'(x) = 0 \Rightarrow x = 0$.
Does the function attain a maximum or a minimum at $x = 0$?

Warm-up: Basic Unconstrained Optimization in $\mathbb{R}^1$



Warm-up: Basic Unconstrained Optimization in $\mathbb{R}^1$

Example 2 (cont.)

The answer is "neither"! The point $x = 0$ is not a local extreme point of $f(x) = x^3$.

This illustrates the pitfalls of using necessary conditions – they supply only candidates that need to be checked further.

The above examples generalize in the following manner:

Fact 2

Let a function f be n times differentiable at a point x and

$$f'(x) = f''(x) = \ldots = f^{(n-1)}(x) = 0, \qquad f^{(n)} \neq 0.$$

1. If n is odd, the point x is not an extreme point of $f(x)$.
2. If n is even and $f^{(n)}(x) > 0$, the point x is a minimum.
3. If n is even and $f^{(n)}(x) < 0$, the point x is a maximum.

Unconstrained Optimization in $\mathbb{R}^n$

Necessary conditions

Fact 3

For a function $f : \mathbb{R}^n \to \mathbb{R}$, differentiable at a point $\mathbf{x}$, a necessary condition for $\mathbf{x}$ to be a local extreme point is

$$f'(\mathbf{x}) = \mathbf{0},$$

where

$$\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}, \; \mathbf{0} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \text{ and } f'(\mathbf{x}) = \begin{pmatrix} \dfrac{\partial f(x_1, \ldots, x_n)}{\partial x_1} \\ \vdots \\ \dfrac{\partial f(x_1, \ldots, x_n)}{\partial x_n} \end{pmatrix}$$

Note: A point where the gradient of a function f vanishes is called a *critical point* or a *stationary point*. This also applies to functions on $\mathbb{R}^1$.

Unconstrained Optimization in $\mathbb{R}^n$

Example 3

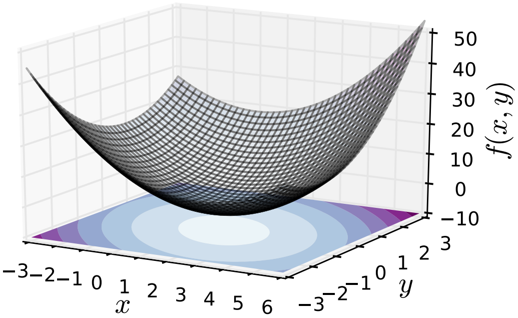
$$f(x,y) = x^2 + 2y^2 - 3x + xy$$

$$\frac{\partial f}{\partial x} = 2x - 3 + y = 0 \quad \Rightarrow \quad x = \frac{3-y}{2}$$

$$\frac{\partial f}{\partial y} = 4y + x = 0 \quad \Rightarrow \quad y = -\frac{x}{4}$$

$$x = \frac{12}{7},\ y = -\frac{3}{7}$$

Unconstrained Optimization in $\mathbb{R}^n$



Unconstrained Optimization in $\mathbb{R}^n$

The necessity of the condition $f'(\mathbf{x}) = \mathbf{0}$ has implications that are similar to the univariate case:

Example 4

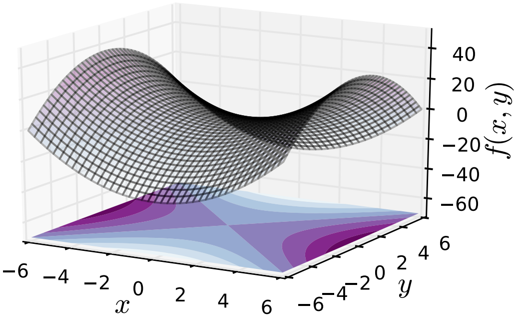
Consider the function $f(x,y) = x^2 - y^2$. The NCs yield the following candidate:

$$\frac{\partial f}{\partial x} = 2x = 0 \quad \Rightarrow \quad x = 0,$$

$$\frac{\partial f}{\partial y} = -2y = 0 \quad \Rightarrow \quad y = 0.$$

Let's look at the graph of the function in a neighbourhood of the point $(0,0)'$.

Unconstrained Optimization in $\mathbb{R}^n$



Unconstrained Optimization in $\mathbb{R}^n$

Example 4 (cont.)

The critical point $\mathbf{x} = (0,0)'$ is an example of a *saddle point*. The function f (obviously) does not attain an extremum at $\mathbf{x}$.

Example 4 illustrates the need to refine the approach for checking candidate points in the n-dimensional case. To this end, we have to review several concepts.

A symmetric square matrix A is called *positive semidefinite* if, for any vector $\mathbf{x}$, we have

$$\mathbf{x}' A\mathbf{x} \geq 0.$$

If the inequality is strict for any non-zero vector $\mathbf{x}$, the matrix is called *positive definite*.
Similarly, a symmetric square matrix A is called *negative semidefinite* if, for any vector $\mathbf{x}$, we have $\mathbf{x}' A\mathbf{x} \leq 0$, and *negative definite* in case of strict inequality for $\mathbf{x} \neq \mathbf{0}$.

Unconstrained Optimization in $\mathbb{R}^n$

Incidentally, for a given square symmetric matrix A, the function $Q(\mathbf{x}) = \mathbf{x}' A\mathbf{x}$ is called a *quadratic form*. Quadratic forms are also referred to as "positive/negative (semi)definite", depending on the properties of the respective matrix.

Recall that, for an $n \times n$ matrix A, a *principal minor* of order k ($1 \leq k \leq n$), denoted by Δ_k, is the determinant of the submatrix obtained by deleting $n - k$ rows of the matrix and the correspondingly numbered columns, e.g.

$$\begin{bmatrix} a_{1,1} & a_{1,2} & a_{1,3} & \cdots & a_{1,n} \\ a_{2,1} & a_{2,2} & a_{2,3} & \cdots & a_{2,n} \\ a_{3,1} & a_{3,2} & a_{3,3} & \cdots & a_{3,n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{n,1} & a_{n,2} & a_{n,3} & \cdots & a_{n,n} \end{bmatrix}$$

Note: The notation Δ_k does not identify a unique principal minor of order k.

Unconstrained Optimization in $\mathbb{R}^n$

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Unconstrained Optimization in $\mathbb{R}^n$

The k-th *leading principal minor* of a matrix A ($1 \leq k \leq n$), denoted by D_k, is the determinant of the submatrix

$$\begin{bmatrix} a_{1,1} & a_{1,2} & \cdots & a_{1,k} \\ a_{2,1} & a_{2,2} & \cdots & a_{2,k} \\ \vdots & \vdots & \ddots & \vdots \\ a_{k,1} & a_{k,2} & \cdots & a_{k,k} \end{bmatrix},$$

i.e. the principal minor obtained by deleting the last $n - k$ rows and columns and, respectively, keeping the first k.

Unconstrained Optimization in $\mathbb{R}^n$

Fact 4 (Sylvester's criterion)

Let A be a symmetric matrix. Then:

1. A is positive definite if and only if $D_k > 0,\ k = 1, \ldots, n$.
2. A is positive semidefinite if and only if $\Delta_k \geq 0$ for all principal minors of order $k = 1, \ldots, n$.
3. A is negative definite if and only if $(-1)^k D_k > 0,\ k = 1, \ldots, n$.
4. A is negative semidefinite if and only if $(-1)^k \Delta_k \geq 0$ for all principal minors of order $k = 1, \ldots, n$.

Note that the necessary and sufficient conditions for "semidefiniteness" involve all principal minors (and hence are cumbersome to check), not just the leading principal minors.

Unconstrained Optimization in $\mathbb{R}^n$

Let a function $f(\mathbf{x}) = f(x_1, \ldots, x_n)$ be twice differentiable. The matrix of second partial derivatives, evaluated at a point $\mathbf{x}$, i.e.

$$\begin{bmatrix} \frac{\partial^2 f(\mathbf{x})}{\partial x_1^2} & \frac{\partial^2 f(\mathbf{x})}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f(\mathbf{x})}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f(\mathbf{x})}{\partial x_2 \partial x_1} & \frac{\partial^2 f(\mathbf{x})}{\partial x_2^2} & \cdots & \frac{\partial^2 f(\mathbf{x})}{\partial x_2 \partial x_n} \\ \cdots & \cdots & \ddots & \cdots \\ \frac{\partial^2 f(\mathbf{x})}{\partial x_n \partial x_1} & \frac{\partial^2 f(\mathbf{x})}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f(\mathbf{x})}{\partial x_n^2} \end{bmatrix}$$

is called the *Hessian (matrix)* of f at $\mathbf{x}$.

Unconstrained Optimization in $\mathbb{R}^n$

- The Hessian is denoted $\mathbf{f}''(\mathbf{x})$.
- The Hessian is symmetric.
- Sometimes the partial derivative $\frac{\partial^2 f(\mathbf{x})}{\partial x_i \partial x_j}$ is written as $f''_{ij}(\mathbf{x})$.
- A leading principal minor of order k of the Hessian is denoted $D_k(\mathbf{x})$.
- An arbitrary principal minor of order k of the Hessian is denoted $\Delta_k(\mathbf{x})$.

Unconstrained Optimization in $\mathbb{R}^n$

Fact 5

Let a (twice) differentiable function $f : \mathbb{R}^n \to \mathbb{R}$ have a critical point at $\mathbf{x}^*$.

1. If the Hessian $\mathbf{f}''(\mathbf{x}^*)$ is positive definite or, equivalently, $D_k(\mathbf{x}^*) > 0,\ k = 1, \ldots, n,$ then $\mathbf{x}^*$ is a *local minimum point.*
2. If the Hessian $\mathbf{f}''(\mathbf{x}^*)$ is negative definite or, equivalently, $(-1)^k D_k(\mathbf{x}^*) > 0,\ k = 1, \ldots, n,$ then $\mathbf{x}^*$ is a *local maximum point.*
3. If $D_n(\mathbf{x}^*) \neq 0$ and neither 1) nor 2) is satisfied, then $\mathbf{x}^*$ is a *saddle point.*

Unconstrained Optimization in $\mathbb{R}^n$

Fact 6

Let a (twice) differentiable function $f : \mathbb{R}^n \to \mathbb{R}$ have an extreme point at $\mathbf{x}^*$.

1. If $\mathbf{x}^*$ is a local minimum point, then the Hessian $\mathbf{f}''(\mathbf{x}^*)$ is positive semidefinite or, equivalently, $\Delta_k(\mathbf{x}^*) \geq 0$ for all principal minors of order $k = 1, \ldots, n$.
2. If $\mathbf{x}^*$ is a local maximum point, then the Hessian $\mathbf{f}''(\mathbf{x}^*)$ is negative semidefinite or, equivalently, $(-1)^k \Delta_k(\mathbf{x}^*) \geq 0$ for all principal minors of order $k = 1, \ldots, n$.