Numerical Optimization

Dhyan Laad
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Contents

1 Preliminaries

1.1 Inner Product Spaces

Definition 1.1. Let V be a real vector space. A function $\langle\cdot,\cdot\rangle : V \times V \to \mathbb{R}$ is called a *real inner product* if it satisfies the following properties for $x, y, z \in V$ and $c \in \mathbb{R}$:

(a) $\langle x, y\rangle = \langle y, x\rangle$,

(b) $\langle x + z, y\rangle = \langle x, y\rangle + \langle z, y\rangle$,

(c) $\langle cx, y\rangle = c\langle x, y\rangle$, and

(d) $\langle x, x\rangle \geq 0$ and $\langle x, x\rangle = 0 \Leftrightarrow x = 0$.

The inner product is the generalization of the dot product on Euclidean vector spaces: for $\mathbf{x} = (x_1, x_2, \ldots, x_n)$ and $\mathbf{y} = (y_1, y_2, \ldots, y_n)$ where $x_i, y_i \in \mathbb{R}$ for $i \in 1 : n$,

$$\mathbf{x} \cdot \mathbf{y} = \sum_{i=1}^{n} x_i y_i.$$

It may also be defined on $\mathbb{C}$-spaces, replacing (a) with conjugate symmetry: $\langle x, y\rangle = \overline{\langle y, x\rangle}$, and adding conjugate linearity in the second argument: $\langle x, cy\rangle = \bar{c}\langle x, y\rangle$.

Definition 1.2. Let V be a real vector space and $\langle\cdot,\cdot\rangle$ an inner product. Then, $(V, \langle\cdot,\cdot\rangle)$ is called a *real inner product space*.

For brevity, we may simply state that V is an inner product space, with the notation for the inner product being implicit, and all future inner product spaces map into $\mathbb{R}$ unless stated otherwise.

1.2 Normed Linear Spaces

Definition 1.3. Let V be a real vector space. A function $\|\cdot\| : V \to \mathbb{R}$ is called a *norm* if it satisfies the following properties for $x, y \in V$ and $c \in \mathbb{R}$:

(a) $\|cx\| = |c|\|x\|$,

(b) $\|x\| \geq 0$ and $\|x\| = 0 \Leftrightarrow x = 0$, and

(c) $\|x + y\| \leq \|x\| + \|y\|$.

This last property is referred to as the *triangle inequality*. The norm assigns a notion of length to vectors, and generalizes the standard formula for the length of a vector in a Euclidean vector space: for $\mathbf{x} = (x_1, x_2, \ldots, x_n)^\top$ where $x_i \in \mathbb{R}$ for $i \in 1 : n$.

$$\|\mathbf{x}\| = \left(\sum_{i=1}^{n} x_i^2\right)^{1/2}.$$

Definition 1.4. Let V be a vector space and $\|\cdot\|$ a norm. Then $(V, \|\cdot\|)$ is called a *normed linear space*.

Once again, we may conventionally omit the norm from notation when defining a new normed linear space.

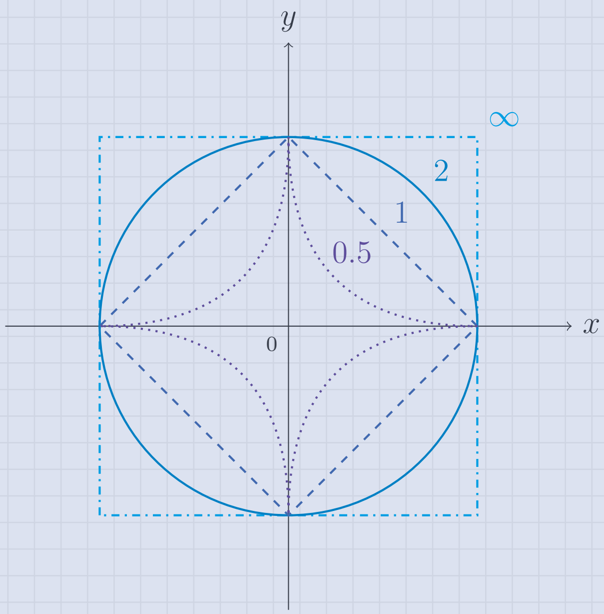
Definition 1.5. Let $p \geq 1$. The *p-norm* (or *ℓ^p-norm*) of a vector $\mathbf{x} = (x_1, x_2, \ldots, x_n)^\top$ where $x_i \in \mathbb{R}$ for $i \in 1 : n$ is

$$\|\mathbf{x}\|_p \coloneqq \left(\sum_{i=1}^{n} |x_i|^p\right)^{1/p}.$$

For $p = 1$, we get the *taxicab* or *Manhattan* norm, for $p = 2$, we get the standard Euclidean norm, and for $p \to \infty$, the p-norm approaches the *infinity* or *maximum* norm:

$$\|\mathbf{x}\|_\infty \coloneqq \max_i |x_i|.$$

For $p \in (0, 1)$, the triangle inequality does not hold, and the resulting functions are called *quasinorms*. Pictured below are unit circles in the 0.5-quasinorm, and p-norms for $p \in \{1, 2, \infty\}$.



Lemma 1.6. *Let V be a normed linear space. Then,*

$$|\|x\| - \|y\|| \leq \|x - y\|$$

for every $x, y \in V$.

Theorem 1.7. *Let $(V, \|\cdot\|)$ be a normed linear space. Then $\|\cdot\| : V \to \mathbb{R}$ is uniformly continuous.*

Proof. Let $\varepsilon > 0$, and choose $\delta = \varepsilon$. If $\|x - y\| < \delta$, then by Lemma 1.6,

$$|\|x\| - \|y\|| \leq \|x - y\| < \delta = \varepsilon.$$

Therefore, $|\|x\| - \|y\|| < \varepsilon$. □

Theorem 1.8. *Every inner product space V is naturally a normed linear space. For $x \in V$ define*

$$\|x\| \coloneqq \sqrt{\langle x, x \rangle}.$$

However, the converse is not always true.

Theorem 1.9. *A normed linear space V is an inner product space iff the norm satisfies the parallelogram law:*

$$\|x + y\|^2 + \|x - y\|^2 = 2(\|x\|^2 + \|y\|^2).$$

The inner product is given by

$$\langle x, y \rangle = \frac{1}{4}\left(\|x + y\|^2 - \|x - y\|^2\right)$$

for all $x, y \in V$.

We now look at a fundamental theorem in linear algebra.

Theorem 1.10 (Cauchy-Schwarz Inequality). *Let V be an inner product space with an induced norm. Then for all $x, y \in V$*

$$|\langle x, y \rangle| \leq \|x\|\|y\|.$$

Proof. We utilize the discriminant of a quadratic equation and the nonnegativity of the norm. Firstly, if $y = 0$, then the inequality holds trivially. For $y \neq 0$, consider the vector $x + ty$ for some $t \in \mathbb{R}$. Then

$$0 \leq \|x + ty\|^2 = \langle x + ty, x + ty \rangle = \|y\|^2 t^2 + 2\langle x, y \rangle t + \|x\|^2.$$

Since the quadratic in t is nonnegative, its discriminant must be nonpositive, giving us

$$4\langle x, y \rangle^2 - 4\|x\|^2\|y\|^2 \leq 0 \Rightarrow |\langle x, y \rangle| \leq \|x\|\|y\|.$$

□

1.3 Eigenvalues and Eigenvectors

Definition 1.11. Let A be a square matrix of order n. Then, λ is said to be an *eigenvalue* of A if there exists nonzero $\mathbf{x} \in \mathbb{R}^n$ such that

$$A\mathbf{x} = \lambda\mathbf{x}.$$

Here, $\mathbf{x}$ is called an *eigenvector* corresponding to λ.

To find the eigenvalues of an arbitrary matrix, consider the following:

$$A\mathbf{x} = \lambda\mathbf{x} \Rightarrow A\mathbf{x} - \lambda\mathbf{x} = \mathbf{0} \Rightarrow (A - \lambda I)\mathbf{x} = \mathbf{0}.$$

Since $\mathbf{x}$ is nonzero, we require the matrix $A - \lambda I$ to be singular. That is,

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

The left side of the equation is a polynomial in λ, and is called the *characteristic polynomial*. Therefore the eigenvalues of a matrix A are the *roots* to its characteristic polynomial.

Theorem 1.12. *Eigenvectors corresponding to distinct eigenvalues are linearly independent.*

Definition 1.13. A square matrix A is said to be diagonalizable if there exists an invertible matrix P such that

$$P^{-1}AP = D$$

where D is a diagonal matrix.

It turns out that in Definition 1.13, the entries of D along the diagonal are the eigenvalues of A, and P contains corresponding eigenvectors in the respective columns of the eigenvalues in D.

1.4 Quadratic Forms

Certain quadratic functions of several variables may be represented using matrices.

Definition 1.14. A *quadratic form* is a homogenous polynomial of degree 2 in multiple variables.

A quadratic form in n variables may be written with a symmetric matrix A of order n and a vector $\mathbf{x} = (x_1, x_2, \ldots, x_n)^\top$ of unknowns:

$$Q(x) = \langle A\mathbf{x}, \mathbf{x}\rangle = \mathbf{x}^\top A\mathbf{x} = \sum_{i=1}^{n} a_{ii}x_i^2 + \sum_{\substack{i=1 \\ i\neq j}}^{n}\sum_{j=1}^{n} a_{ij}x_ix_j$$

where a_{ij} is the (i, j)th entry of A.

Definition 1.15. Let A be a square matrix of order n, and let $p = \langle A\mathbf{x}, \mathbf{x}\rangle$. If for all nonzero $\mathbf{x} \in \mathbb{R}^n$

(a) $p > 0$, then A is said to be *positive definite*,

(b) $p \geq 0$, *positive semidefinite*,

(c) $p < 0$, *negative definite*, and

(d) $p \leq 0$, *negative semidefinite*.

Otherwise, A is said to be *indefinite*.

The definiteness of a matrix may also be realized through its principal minors.

Definition 1.16. Let A be a square matrix of size n. A *principal minor of order k* of A may be computed by the following.

1. Choose any set of k indices $\{i_1, i_2, \ldots, i_k\}$ from $\{1, 2, \ldots, n\}$.
2. Keep the rows and columns corresponding to these indices, creating a $k \times k$ submatrix.
3. Take the determinant of this resulting submatrix to yield a principal minor of order k.

If the first k indices $\{1, 2, \ldots, k\}$ are chosen, then the resulting principal minors called *leading principal minors of order k*.

Theorem 1.17. *A square matrix is*

(a) *positive definite iff all leading principle minors are positive,*

(b) *positive semidefinite iff all principal minors are nonnegative,*

(c) *negative definite iff the kth leading principal minor has the sign of $(-1)^k$, and*

(d) *negative semidefinite iff all principal minors of order k either have the sign of $(-1)^k$ or are 0.*

A matrix that does not fall into the aforementioned categories is indefinite.

We may also characterize definiteness using a matrix's eigenvalues.

Theorem 1.18. *A square matrix of order n with eigenvalues λ_i for $i \in 1:n$ is*

(a) *positive definite iff $\lambda_i > 0$ for all i,*

(b) *positive semidefinite iff $\lambda_i \geq 0$ for all i,*

(c) *negative definite iff $\lambda_i < 0$ for all i, and*

(d) *negative semidefinite iff $\lambda_i \leq 0$ for all i.*

A matrix that does not fall into the aforementioned categories is indefinite.

1.5 Matrix Norms

Definition 1.19. Let $\mathbb{R}^{m\times n}$ denote the set of all matrices of size $m \times n$ with real entries. A function $\|\cdot\| : \mathbb{R}^{m\times n} \to \mathbb{R}$ is called a *real matrix norm* if it satisfies the following properties for $c \in \mathbb{R}$ and $A, B \in \mathbb{R}^{m\times n}$:

(a) $\|A\| \geq 0$ and $\|A\| = 0 \Leftrightarrow A = \mathbf{0}$,

(b) $\|cA\| = |c|\|A\|$,

(c) $\|A + B\| \leq \|A\| + \|B\|$, and

(d) $\|AB\| \leq \|A\|\|B\|$ for $m = n$.

Four of the most widely used ones are detailed below for a square matrix $A = [a_{ij}]_n$.

1-norm. The 1-norm is the *maximum absolute column sum*:

$$\|A\|_1 = \max_{1\leq j\leq n} \sum_{i=1}^{n} |a_{ij}|.$$

∞-norm. The ∞-norm is the *maximum absolute row sum*:

$$\|A\|_\infty = \max_{1\leq i\leq n} \sum_{j=1}^{n} |a_{ij}|.$$

2-norm. The 2-norm is also called the *spectral norm* and is given by

$$\|A\|_2 = \sqrt{\lambda_{\max}(A^\top A)}$$

where $\lambda_{\max}(M)$ is the largest eigenvalue of M.

Frobenius norm. The Frobenius norm is the sum of the squared entries of the matrix:

$$\|A\|_F = \left(\sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij}^2\right)^{1/2} = \sqrt{\operatorname{tr}(A^\top A)}$$

where $\operatorname{tr}(M)$ is the trace of M.

In general, a specific matrix norm can be induced from an existing vector norm by defining

$$\|A\| = \sup_{\mathbf{x}\neq 0} \frac{\|A\mathbf{x}\|}{\|\mathbf{x}\|}.$$

2 Calculus

2.1 Extreme Points

We start by reviewing and defining the concepts of a minimum and maximum from elementary calculus. Let $I = [a, b] \subset \mathbb{R}$ and $f : I \to \mathbb{R}$.

Definition 2.1. $x^* \in I$ is said to be a *local minimum* of f if there exists $\delta > 0$ such that $f(x^*) \leq f(x)$ for all $x \in B(x^*, \delta)$.

Definition 2.2. $x^* \in I$ is said to be a *local maximum* of f if there exists $\delta > 0$ such that $f(x^*) \geq f(x)$ for all $x \in B(x^*, \delta)$.

Definition 2.3. $x^* \in I$ is said to be a *global minimum* of f if $f(x^*) \leq f(x)$ for all $x \in I$.

Definition 2.4. $x^* \in I$ is said to be a *global maximum* of f if $f(x^*) \geq f(x)$ for all $x \in I$.

The definitions for the corresponding strict versions of the maxima and minima may be obtained by simply replacing the inequality with a strict one. The point x^* is called a *minimizer* of *maximizer*.

Theorem 2.5. *Let x^* be a local minimizer of f and let x^* be an interior point of $I = [a, b]$. If f is differentiable at x^*, then $f'(x^*) = 0$.*

Proof. Since x^* is a local minimizer and an interior point of I, there exists $\delta > 0$ such that $f(x^*) \leq f(x)$ for all $x \in B(x^*, \delta)$. For $h > 0$ such that $h < \delta$,

$$f(x^*) \leq f(x^* + h) \quad \text{and} \quad f(x^*) \leq f(x^* + h).$$

We know that f is differentiable at x^*. As such,

$$f'(x^*) = f'_+(x^*) = \lim_{h\to 0^+} \frac{f(x^*+h) - f(x^*)}{h},$$

$$f'(x^*) = f'_-(x^*) = \lim_{h\to 0^+} \frac{f(x^*) - f(x^*-h)}{h}.$$

As such, $f'(x^*) = f'_+(x^*) \geq 0$ and $f'(x^*) = f'_-(x^*) \leq 0$, and therefore $f'(x^*) = 0$. $\square$

An analogous result holds for a maximizer.

Theorem 2.6. *Let x^* be a local maximizer of f and let x^* be an interior point of $I = [a, b]$. If f is differentiable at x^*, then $f'(x^*) = 0$.*

Definition 2.7. Let $f : [a, b] \to \mathbb{R}$, and $x^* \in (a, b)$. If f is differentiable at x^* and $f'(x^*) = 0$, or if f is not differentiable at x^*, it is said to be a *critical point of f*.

Definition 2.8. Let $f : [a, b] \to \mathbb{R}$, and $x^* \in (a, b)$. If f is differentiable at x^* and $f'(x^*) = 0$, then it is said to be a *stationary point of f*.

We now proceed to list out a few preliminary results of use.

Theorem 2.9 (Weierstrass Extreme Value Theorem). *Let S be a compact set, and $f : S \to \mathbb{R}$ be a continuous mapping. Then, f attains a global maximum and a global minimum on S.*

Theorem 2.10 (Closed Point Theorem). *Let S be a nonempty, closed, and convex set in $\mathbb{R}^n$, and $y \notin S$. Then, there exists a unique point $x^* \in S$ such that*

$$\|y - x^*\| \leq \|y - x\|$$

for all $x \in S$. Thus, x^* is the minimizing point iff

$$(y - x^*)^\top (x - x^*) \leq 0$$

for all $x \in S$.

Theorem 2.11 (Taylor's Theorem). *Let $I \subseteq \mathbb{R}$ be an interval, $f : I \to \mathbb{R}$ such that $f \in \mathcal{C}^n(I)$, and $x, x^* \in I$. Let $h = x - x^*$. Then, there exists $\xi \in (0, 1)$ such that*

$$f(x) = f(x^*) + hf^{(1)}(x^*) + \frac{h^2}{2!} f^{(2)}(x^*) + \cdots + \frac{h^{n-1}}{(n-1)!} f^{(n-1)}(x^*) + \frac{h^n}{n!} f^{(n)}(x^* + \xi h).$$

The proofs of the above theorems have been omitted for brevity.

Theorem 2.12. *Let $I \subseteq \mathbb{R}$ be an interval, $f \in \mathcal{C}^2(I)$, and x^* a critical point of f.*

(a) *If $f^{(2)}(x^*) > 0$ for all $x \in I$, then x^* is a global minimizer of f.*

(b) *If $f^{(2)}(x^*) < 0$, for all $x \in I$, then x^* is a global maximizer of f.*

Proof. Let $x \in I$ and $h = x - x^*$. By Taylor's Theorem,

$$f(x) = f(x^*) + hf^{(1)}(x^*) + \frac{h^2}{2} f^{(2)}(x^* + \xi h)$$

for some $\xi \in (0, 1)$. Since x^* is a critical point of f, $f^{(1)}(x^*) = 0$. Therefore,

$$f(x) - f(x^*) = \frac{h^2}{2} f^{(2)}(x^* + \xi h).$$

If $f^{(2)}(x) > 0$ for all $x \in I$, then $f(x) - f(x^*) > 0$ for all $x \neq x^*$, and thus x^* is a global minimizer of f. Similarly, if $f^{(2)}(x) < 0$ for all $x \in I$, then $f(x) - f(x^*) < 0$ for all $x \neq x^*$, and thus x^* is a global maximizer of f. □

2.2 Multivariable Calculus

We first explore differentiability of multivariable functions.

Definition 2.13. Let $\Omega \subseteq \mathbb{R}^n$. A function $f : \Omega \to \mathbb{R}$ is said to be *differentiable at* $x^* \in \Omega$ if the partial derivatives

$$f_{x_i} \equiv \frac{\partial f}{\partial x_i}, \quad i \in \{1, 2, \ldots, n\},$$

exist. Furthermore, the *gradient* of f at x^* is defined as

$$\nabla f(x^*) := \left[\frac{\partial f}{\partial x_1} \; \frac{\partial f}{\partial x_2} \; \ldots \; \frac{\partial f}{\partial x_n}\right]^\top.$$

Definition 2.14. Let $\Omega \subseteq \mathbb{R}^n$. The *Hessian* of a function $f : \Omega \to \mathbb{R}$ at $x^* \in \Omega$ is defined as the square matrix of second-order partial derivatives:

$$H_f(x^*) = \begin{bmatrix} f_{x_1 x_1}(x^*) & f_{x_1 x_2}(x^*) & \ldots & f_{x_1 x_n}(x^*) \\ f_{x_2 x_1}(x^*) & f_{x_2 x_2}(x^*) & \ldots & f_{x_2 x_n}(x^*) \\ \vdots & \vdots & \ddots & \vdots \\ f_{x_n x_1}(x^*) & f_{x_n x_2}(x^*) & \ldots & f_{x_n x_n}(x^*) \end{bmatrix}.$$

If the function f is continuously differentiable at x^*, then the Hessian is symmetric.

Definition 2.15. A vector valued function $f : [a, b] \to \mathbb{R}^n$ is said to be *differentiable at* $x^* \in [a, b]$ if all of its component functions $f_i : [a, b] \to \mathbb{R}$ for $i \in 1 : n$ are differentiable at x^*.

$$f'(x^*) = [f_1'(x^*) \; f_2'(x^*) \; \cdots \; f_n'(x^*)]^\top$$

Now consider two functions:

- $f : \Omega \to [a, b]$, where $\Omega \subseteq \mathbb{R}$.
- $g : [a, b] \to \Omega$.

We are interested in the differentiability of the composition $h = f \circ g : [a, b] \to [a, b]$. The derivative is given by the chain rule:

$$h'(t) = \nabla f(g(t)) g'(t).$$

We may also extend the notion of Taylor series to multivariable functions. For a smooth function $f : \mathbb{R}^2 \to \mathbb{R}$,

$$f(x + h, y + h) = \sum_{k=0}^{\infty} \frac{(h\partial_x + k\partial_y)^k}{k!} f(x, y).$$

Definition 2.16. The *level set* of a function $f : \Omega \to \mathbb{R}$ at $c \in \mathbb{R}$ is defined as

$$L_c = \{x \in \Omega : f(x) = c\}.$$