

Techniques in Optimization and Sampling

(book in progress with improving citations)

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February 17, 2025

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Contents

0.1	Examples	5
1	Introduction	6
1.1	Why non-convex functions can be difficult to optimize	7
1.2	Why is convexity useful? Linear Separability!	7
1.3	Convex problems are everywhere!	11
1.4	Examples of convex sets and functions	13
1.5	Checking convexity	14
1.6	Subgradients	15
1.7	Logconcave functions	15
I	Optimization	18
2	Gradient Descent	19
2.1	Philosophy	19
2.2	Basic Algorithm	19
2.3	Analysis for convex functions	22
2.4	Strongly Convex Functions	24
2.5	Line Search	25
2.6	Generalizing Gradient Descent*	25
2.7	Gradient Flow	28
2.8	Discussion	28
3	Elimination	29
3.1	Cutting Plane Methods	29
3.2	Ellipsoid Method	30
3.3	From Volume to Function Value	32
3.4	Center of Gravity Method	34
3.5	Sphere and Parabola Methods	39
3.6	Lower Bounds	44
4	Reduction	46
4.1	Equivalences between Oracles	46
4.2	Gradient from Evaluation via Finite Difference	49
4.3	Separation via Membership	54
4.4	Composite Problem via Duality	59
5	Geometrization	64
5.1	Norms and Local Metrics	64
5.2	Mirror Descent	64
5.3	Frank-Wolfe	71
5.4	The Newton Method	72
5.5	Interior Point Method for Linear Programs	76
5.6	Interior Point Method for Convex Programs	82

6	Sparsification	88
6.1	Subspace embedding	88
6.2	Leverage Score Sampling	93
6.3	Stochastic Gradient Descent	95
6.4	Coordinate Descent	99
7	Acceleration	101
7.1	Chebyshev Polynomials	101
7.2	Conjugate Gradient	102
7.3	Accelerated Gradient Descent via Plane Search	105
7.4	Accelerated Gradient Descent	106
7.5	Accelerated Coordinate Descent	110
7.6	Accelerated Stochastic Descent	111
II	Sampling	112
8	Gradient-based Sampling	113
8.1	Gradient-based methods: Langevin Dynamics	113
8.2	Langevin Dynamics is Gradient Descent in Density Space*	118
9	Elimination and Reduction	121
9.1	Cutting Plane method for Volume Computation	121
9.2	Optimization from Membership via Sampling	122
10	Geometrization	124
10.1	Basics of Markov chains	124
10.2	Conductance of the Ball Walk	128
10.3	Generating a warm start	135
10.4	Isotropic Transformation	135
10.5	Isoperimetry via localization	136
10.6	Hit-and-Run	140
10.7	Dikin walk	143
10.8	Mixing with Strong Self-Concordance	145
10.9	Hamiltonian Monte Carlo	148
11	Annealing	154
11.1	Simulated Annealing	154
11.2	Volume Computation	155
A	Calculus - Review	162
A.1	Divergence and Integration by Parts	162
A.2	Tips for Computing Gradients	162
A.3	Solving optimization problems by hand	165
B	Notation	167

Preliminaries

Notation

We use $B(x, r)$ to denote the Euclidean (or ℓ_2) ball centered at x with radius r : $\{y : \|y - x\|_2 \leq r\}$. We use $\text{conv}(X)$ to denote the convex hull of X , namely $\text{conv}(X) = \{\sum \alpha_i x_i : \alpha_i \geq 0, \sum \alpha_i = 1, x_i \in X\}$. We use $\langle x, y \rangle$ to denote the ℓ_2 inner product $x^T y$ of x and y . For any two points $x, y \in \mathbb{R}^n$, we view them as column vectors, and use $[x, y]$ to denote $\text{conv}(\{x, y\})$, namely, the line segment between x and y .

We use e_i to denote the coordinate vector whose i -th coordinate is 1 and all other coordinates are 0.

Functions

Definition 0.1. For any $L \geq 0$, a function $f : V \rightarrow W$ is L -Lipschitz if $\|f(x) - f(y)\|_W \leq L \|x - y\|_V$ where the norms $\|\cdot\|_V$ and $\|\cdot\|_W$ are ℓ_2 norms if unspecified.

Definition 0.2. A function $f \in \mathcal{C}^k(\mathbb{R}^n)$ if f is a k -differentiable function and its k^{th} derivative is continuous.

Definition 0.3. A function $f : X \subseteq \mathbb{R}^n \rightarrow \mathbb{R}$ is called lower semi-continuous at a point $x_0 \in X$ if for every real $y < f(x_0)$ there exists a neighborhood U of x_0 such that $f(x) > y$ for all $x \in U$. Equivalently, f is lower semi-continuous at x_0 iff

$$\liminf_{x \rightarrow x_0} f(x) \geq f(x_0).$$

The function is lower semi-continuous if it is so at every point in its domain. The definition of upper semi-continuous is analogous with the inequalities reversed and \liminf replaced by \limsup .

Theorem 0.4 (Taylor's Remainder Theorem). *For any $g \in \mathcal{C}^{k+1}(\mathbb{R})$, and any x and y , there is a $\zeta \in [x, y]$ such that*

$$g(y) = \sum_{j=0}^k g^{(j)}(x) \frac{(y-x)^j}{j!} + g^{(k+1)}(\zeta) \frac{(y-x)^{k+1}}{(k+1)!}.$$

Definition 0.5. The *convolution* of two functions $f, g : \mathbb{R}^n \rightarrow \mathbb{R}$ is defined as $h(x) = \int_{\mathbb{R}^n} f(z)g(x-z) dz$.

Linear Algebra

Definition 0.6. A real symmetric matrix A is positive semi-definite (PSD) if $x^T A x \geq 0$ for all $x \in \mathbb{R}^n$. Equivalently, a real symmetric matrix with all nonnegative eigenvalues is PSD. We write $A \succeq 0$ if A is PSD and $A \succeq B$ if $A - B$ is PSD.

Definition 0.7. For any matrix A , we define its trace, $\text{tr} A = \sum A_{ii}$, Frobenius norm, $\|A\|_F^2 = \text{tr}(A^T A) = \sum_{i,j} A_{ij}^2$, and operator norm, $\|A\|_{\text{op}} = \sup_{\|x\|_2=1} \|Ax\|_2$. Note that $x^T A x = \text{tr}(A x x^T)$ and in general, $\text{tr}(AB) = \text{tr}(BA)$.

For symmetric A , we have $\text{tr} A = \sum_i \lambda_i$, $\|A\|_F^2 = \sum_i \lambda_i^2$ and $\|A\|_{\text{op}} = \max_i |\lambda_i|$ where λ_i are the eigenvalues of A .

For a vector x , $\|x\|_A = \sqrt{x^T A x}$; for a matrix B ,

$$\|B\|_A = \sup_x \frac{\|Bx\|_A}{\|x\|_A}.$$

Lemma 0.8 (Sherman-Morrison-Woodbury). For matrix $A \in \mathbb{R}^{n \times n}$ and vectors $u, v \in \mathbb{R}^n$, we have

$$(A + uv^\top)^{-1} = A^{-1} - \frac{A^{-1}uv^\top A^{-1}}{1 + u^\top A v}.$$

For matrices $U, V \in \mathbb{R}^{n \times k}$, we have

$$(A + UV^\top)^{-1} = A^{-1} - A^{-1}U(I + V^\top A^{-1}U)^{-1}V^\top A^{-1}.$$

Probability

Definition 0.9. The Total Variation (TV) or ℓ_1 -distance between two distributions with measures ρ, ν with support Ω is

$$d_{TV}(\rho, \nu) = \frac{1}{2} \int_{\Omega} |\rho(x) - \nu(x)| dx = \sup_{S \subset \Omega} |\rho(S) - \nu(S)| = \sup_{S \subset \Omega} \rho(S) - \nu(S).$$

The following “distances” are not symmetric.

Definition 0.10. The KL-divergence of a density ρ with respect to another density ν , also known as relative entropy of ρ with respect to ν , is

$$d_{KL}(\rho \| \nu) = \int \rho(x) \log \frac{\rho(x)}{\nu(x)} dx.$$

Definition 0.11. The χ -squared distance of a densities ρ with respect to another density ν is defined as

$$\chi^2(\rho, \nu) = \mathbf{E}_{\nu} \left(\left(\frac{\rho(x)}{\nu(x)} - 1 \right)^2 \right) = \mathbf{E}_{\rho} \left(\frac{\rho(x)}{\nu(x)} \right) - 1.$$

Definition 0.12. The Wassestein p -distance between two probability measures ρ, ν over a metric space M is defined as

$$W_p(\rho, \nu) = \left(\inf_{\gamma \in \Gamma(\rho, \nu)} \mathbf{E}_{x, y \sim \gamma} (d(x, y)^p) \right)^{1/p}$$

where $\Gamma(\rho, \nu)$ is the set of all couplings of ρ and ν (joint probability measures with support $M \times M$ whose marginals are ρ and ν).

Definition 0.13. For μ, ν probability measures in \mathbb{R}^n , the f -divergence of μ towards ν with $\mu \ll \nu$ is defined as, for a convex function $f : \mathbb{R}_+ \rightarrow \mathbb{R}$ with $f(1) = 0$ and $f'(\infty) = \infty$,

$$D_f(\mu \| \nu) := \int f \left(\frac{d\mu}{d\nu} \right) d\nu.$$

For $q \in (1, \infty)$, the d_{KL} -divergence and χ^q -divergence correspond to $f(x) = x \log x$ and $x^q - 1$, respectively. The q -Rényi divergence is defined as

$$\mathcal{R}_q(\mu \| \nu) := \frac{1}{q-1} \log (\chi^q(\mu \| \nu) + 1).$$

The Rényi-infinity divergence is defined as

$$\mathcal{R}_{\infty}(\mu \| \nu) := \log \operatorname{ess\,sup}_{\mu} \frac{d\mu}{d\nu}.$$

Fact 0.14. $d_{KL} = \lim_{q \downarrow 1} \mathcal{R}_q \leq \mathcal{R}_q \leq \mathcal{R}_{q'} \leq \mathcal{R}_{\infty}$ for $1 \leq q \leq q'$ and $2 \|\cdot\|^2 \leq d_{KL} \leq \mathcal{R}_2 = \log(\chi^2 + 1) \leq \chi^2$.

We refer readers to [72] for other basic properties of Rényi-divergence.

Definition 0.15. The *marginal* of a distribution in \mathbb{R}^n with density ν in the span of a k -dimensional subspace V is defined as

$$g(x) = \int_{y \in V^\perp} \nu(x, y) dy$$

for any $x \in V$.

Note that the marginal is a convolution of the density with the indicator function of the subspace.

Definition 0.16. A distribution D with support contained in \mathbb{R}^n is said to be **isotropic** if $\mathbf{E}_D(x) = 0$ and $\mathbf{E}_D(xx^\top) = I$.

Geometry

Definition 0.17. We denote the unit Euclidean ball as $B^n = \{x : \|x\|_2 \leq 1\}$. More generally, we define the ℓ_p -norm ball of radius r centered at z as $B_p^n(z, r) = \{x : \|x - z\|_p \leq r\}$.

Definition 0.18. The *Minkowski sum* of two sets $A, B \subset \mathbb{R}^n$ is defined as $A + B = \{x + y : x \in A, y \in B\}$.

■ 0.1 Examples

Here is a list of problems we want to cover with general techniques:

- linear system, SDD, M matrices, directed Laplacian, multi-commodity flow, totally unimodular matrices (what other linear systems?)
- logistic regression, other regressions, ℓ_p regression, convex regression
- linear program < quadratic program < second order cone program < semidefinite program < conic program < convex program
 - Example: John ellipsoid, minimum enclosing ball, geometric programming, matrix scaling.
- Shortest Path, maximum flow, min-cost flow
 - Example: Transportation
- Markov Decision Processes
- matroid intersection, submodular minimization
- Analogous sampling problems in all of the above

Chapter 1

Introduction

In this book, we will study two topics involving convexity, namely optimization and sampling. Given a multivariate, real-valued function f ,

1. How quickly can we find a point that (approximately) minimizes f ?
2. How fast can we sample a point (approximately) according to the distribution with density defined by f , i.e., proportional to e^{-f} ?

Optimization problems appear naturally across mathematics, the sciences and engineering for a variety of theoretical and practical reasons. Their study over centuries has been extremely fruitful. Sampling is motivated by the question of choosing a representative point or subset (rather than an extremal point). Instead of a feasible set, we have a distribution which assigns probabilities to subsets. The goal is to sample a point from such a target distribution, i.e., the output point should lie in a given subset with probability equal to the probability of the set in the target distribution. These problems are quite closely connected, e.g., sampling can be used to find near-optimal points. They are intractable in full generality, and have exponential (in dimension) complexity even under smoothness assumptions as we note presently.

Convexity and its extensions are a current frontier of tractable, i.e., polynomial-time, computation. The assumption of convexity induces structure in instances that makes them amenable to efficient algorithms. For example, any local minimum of a convex function is a global minimum. Convexity is maintained by natural operations such as intersection (for sets) and addition (for functions). Perhaps less obvious, but also crucial, is that convex sets can be approximated by ellipsoids in various ways.

We will learn several techniques that lead us to polynomial-time algorithms for both problems and (nearly) linear-time algorithms in some cases, e.g., when f is close to a quadratic function.

Although convex optimization has been formally studied since the 19th century¹ with many tight results emerging, there are still basic open problems. Here is an example:

Open Problem. Given an $n \times n$ random 0/1 matrix A with $O(n)$ nonzero entries and a 0/1 vector b , can we solve $Ax = b$ in $o(n^2)$ time?

Computing the volume is an ancient problem, the early Egyptians and Greeks developed formulas for specific shapes of interest. Unlike convex optimization, even computing the volume of a convex body is intractable, as we will see later. Nevertheless, there are efficient randomized algorithms that can estimate the volume of convex bodies to arbitrary accuracy in time polynomial in the dimension and the desired accuracy. This extends to efficient algorithms for integrating *logconcave* functions, i.e., functions of the form e^{-f} where f is convex. The core ingredient is sampling in high dimension. Sampling and volume computation will be the motivating problems for the second part of this book. Again, many basic problems remain open. To illustrate:

Open Problem. Given a polytope defined by $\{x : Ax \leq b\}$, can we estimate its volume to within a constant factor in nearly linear time?

¹Augustin-Louis Cauchy introduced gradient descent in 1847.

■ 1.1 Why non-convex functions can be difficult to optimize

We first note that optimizing general functions can be difficult. Consider the function

$$f(x) = \begin{cases} 1 & \text{if } x \neq x^* \\ 0 & \text{if } x = x^* \end{cases}$$

and suppose that we can only access the function by querying the function value at any point. This function f always returns 1 unless we know x^* . Hence, no algorithm can find x^* (the adversary simply reports 0 for all queries, and can do so for a countably infinite number of queries).

This function is difficult to optimize, and not merely because of its discontinuity. Similar functions can be constructed that are continuous. Consider the function $f : B(0_n, 1) \rightarrow \mathbb{R}$ defined by

$$f(x) = \min(\|x - x^*\|_2, \epsilon) \quad (1.1)$$

where $B(0_n, 1)$ is the unit ball centered at the origin, 0_n . This function is 1-Lipschitz, i.e., for any x, y , we have $|f(x) - f(y)| \leq \|x - y\|_2$, and unless we query $f(x)$ with x that is ϵ -close to x^* , it will always return ϵ . Since the region where f is not ϵ has volume $\frac{1}{\epsilon^n}$ times the volume of the unit ball, one can show that it takes $\Omega(\frac{1}{\epsilon^n})$ calls to f for any algorithm to find x^* . The following exercise asks you to prove that this bound is tight.



Figure 1.1: Optimizing general 1-Lipschitz functions

Exercise 1.1. Show that if f is 1-Lipschitz on $B(0_n, 1)$, we can find x^* such that $f(x^*) - \min_x f(x) \leq \epsilon$ by evaluating $f(x)$ at $O(\frac{1}{\epsilon^n})$ points.

Thus $O(1/\epsilon^n)$ is the best possible bound for optimizing general 1-Lipschitz functions. Similar constructions can also be made for infinitely differentiable functions. We note that it is easy to find local minima for all the functions above. In Section 2.2, we will show that it is easy to find an approximate local minimum of a continuously differentiable function.

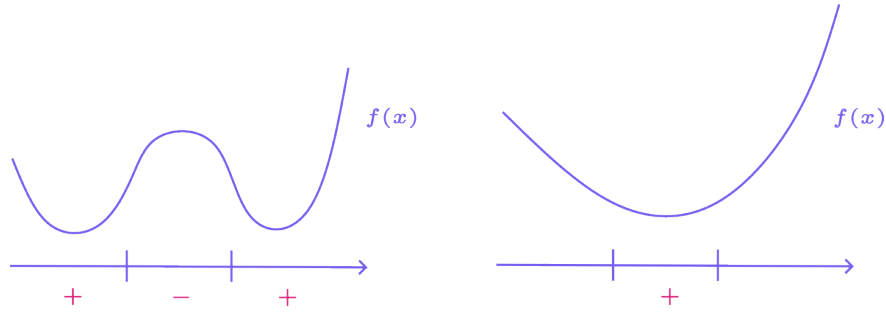
■ 1.2 Why is convexity useful? Linear Separability!

In the previous section, we saw that general functions are difficult to optimize because we can only find the minimum via exhaustive search. Now we define convex sets, convex functions and convex problems (see Fig. 1.3). One benefit of convexity is that it enables “binary search”. We will see that for convex functions, local minima are global minima, and (later in this book), in fact we can solve convex optimization problems in polynomial time.

Definition 1.2. A set $K \subseteq \mathbb{R}^n$ is *convex* if for every pair of points $x, y \in K$, we have $[x, y] \subseteq K$, where $[x, y] = \{(1-t)x + ty : t \in [0, 1]\}$ is the one-dimensional interval from x to y .

Definition 1.3. A function $f : \mathbb{R}^n \rightarrow \mathbb{R} \cup \{+\infty\}$ is *convex* if for every $t \in [0, 1]$, we have

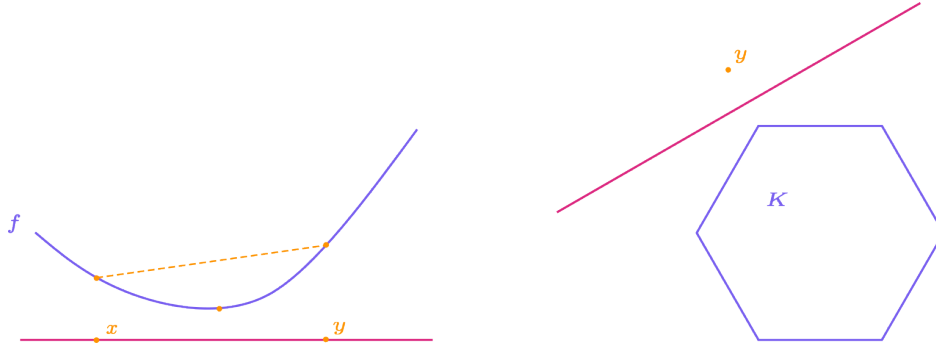
$$f(tx + (1-t)y) \leq tf(x) + (1-t)f(y).$$

**Figure 1.2:** Non-Convex Function; Convex Function

Exercise 1.4. Suppose we have a function $f : \mathbb{R}^n \rightarrow \mathbb{R} \cup \{+\infty\}$ that has the property that for every $x, y \in \mathbb{R}^n$,

$$f\left(\frac{x+y}{2}\right) \leq \frac{1}{2}(f(x) + f(y)).$$

Show that this implies f is convex.

**Figure 1.3:** Convex function; Convex set

Definition 1.5. An optimization problem $\min_{x \in K} f(x)$ is convex if K and f are convex.

Any point not in a convex set can be separated by a hyperplane from the set. We will see in Chapter 3 that separating hyperplanes allow us to do binary search to find a point in a convex set. This is the basis of all polynomial-time algorithms for optimizing general convex functions. We will explore these binary search algorithms in Chapter 3. The following notions will be used routinely. A *halfspace* in \mathbb{R}^n is defined as the set $\{x : \langle a, x \rangle \geq b\}$ for some $a \in \mathbb{R}^n, b \in \mathbb{R}$. A *polyhedron* is the intersection of halfspaces. A *polytope* is the convex hull of a set of points.

Theorem 1.6 (Hyperplane separation theorem). *Let K be a nonempty closed convex set in \mathbb{R}^n and $y \notin K$. There is a non-zero $\theta \in \mathbb{R}^n$ such that*

$$\langle \theta, y \rangle > \max_{x \in K} \langle \theta, x \rangle.$$

Proof. Let x^* be a point in K closest to y , namely $x^* \in \arg \min_{x \in K} \|x - y\|_2^2$ (such a minimizer always exists for closed convex sets and is unique; this is sometimes called Hilbert's projection theorem but can be proved directly for this setting). Using convexity of K , for any $x \in K$ and any $0 < t \leq 1$, we have that $(1-t)x^* + tx \in K$ and hence

$$\|y - (1-t)x^* - tx\|_2^2 \geq \min_{x \in K} \|y - x\|_2^2 = \|y - x^*\|_2^2.$$

Expanding the LHS, we have

$$\begin{aligned}\|y - (1-t)x^* - tx\|_2^2 &= \|y - x^* + t(x^* - x)\|_2^2 \\ &= \|y - x^*\|_2^2 + 2t \langle y - x^*, x^* - x \rangle + t^2 \|x^* - x\|_2^2.\end{aligned}$$

Canceling the term $\|y - x^*\|_2^2$ and dividing both sides by t ,

$$2 \langle y - x^*, x^* - x \rangle + t \|x^* - x\|_2^2 \geq 0.$$

Taking $t \rightarrow 0^+$, we have that

$$\langle y - x^*, x^* - x \rangle \geq 0 \text{ for all } x \in K. \quad (1.2)$$

Taking $\theta = y - x^*$ and using (1.2), for all $x \in K$, we have that

$$\begin{aligned}\langle \theta, y - x \rangle &= \langle \theta, y - x^* \rangle + \langle y - x^*, x^* - x \rangle \\ &= \|\theta\|^2 + \langle y - x^*, x^* - x \rangle \\ &> 0\end{aligned}$$

where we used that $y \notin K$ and hence $\|\theta\|^2 > 0$. \square

Theorem 1.6 shows that a polyhedron (a finite intersection of halfspaces) is essentially as general as a convex set.



Figure 1.4: Convex set with separating hyperplane

Corollary 1.7. Any closed convex set K can be written as the intersection of halfspaces as follows

$$K = \bigcap_{\theta \in \mathbb{R}^n} \left\{ x : \langle \theta, x \rangle \leq \max_{y \in K} \langle \theta, y \rangle \right\}.$$

In other words, any closed convex set is the limit of a sequence of polyhedra.

Proof. Let $L \stackrel{\text{def}}{=} \bigcap_{\theta \in \mathbb{R}^n} \{x : \langle \theta, x \rangle \leq \max_{y \in K} \langle \theta, y \rangle\}$. Since $K \subseteq \{x : \langle \theta, x \rangle \leq \max_{y \in K} \langle \theta, y \rangle\}$, we have $K \subseteq L$.

For any $x \notin K$, Theorem 1.6 shows that there is a θ such that $\theta^\top x > \max_{y \in K} \theta^\top y$. Hence, we have $x \notin L$ and hence $L \subseteq K$. \square

This shows that convex optimization is related to linear programs (optimize linear functions over polytopes) as follows:

$$\min_{x \in K} f(x) = \min_{(x,y) \in \{x \in K, y \in \mathbb{R} : y \geq f(x)\}} y$$

where the set $\{x \in K, y \in \mathbb{R} : y \geq f(x)\}$ then can be approximated by intersection of halfspaces, namely $\{A \binom{x}{y} \leq b\}$ for some matrix $A \in \mathbb{R}^{m \times (n+1)}$ and vector $b \in \mathbb{R}^m$ with $m \rightarrow +\infty$.

Exercise 1.8. Let $A, B \subset \mathbb{R}^n$ be nonempty disjoint closed convex sets. Then there exists a vector $v \in \mathbb{R}^n$ such that $\sup_{x \in A} v^\top x \leq \inf_{x \in B} v^\top x$. Show strict inequality if the sets are also bounded.

Similar to convex sets, we have a separation theorem similar to Theorem 1.6 for convex functions. In Chapter 3, we will see that this allows us to use binary search to minimize convex functions.



Figure 1.5: First-order condition for convexity of a function

Theorem 1.9. Let $f \in \mathcal{C}^1(\mathbb{R}^n)$ be convex. Then,

$$f(y) \geq f(x) + \nabla f(x)^\top (y - x) \text{ for all } x, y \in \mathbb{R}^n \quad (1.3)$$

Later in this chapter we will see that the above condition is in fact an equivalent definition of convexity.

Proof. Fix any $x, y \in \mathbb{R}^n$. Let $g(t) = f((1-t)x + ty)$. Since f is convex, it is convex along every line, in particular over the segment $[x, y]$, and so g is convex over $[0, 1]$. Then, we have

$$g(t) \leq (1-t)g(0) + tg(1)$$

which implies that

$$g(1) \geq g(0) + \frac{g(1) - g(0)}{1 - 0}.$$

Taking $t \rightarrow 0^+$, we have that $g(1) \geq g(0) + g'(0)$. In other words, using the chain rule for derivatives, we have $g'(0) = \langle \nabla f(x), y - x \rangle$ and hence

$$f(y) \geq f(x) + \langle \nabla f(x), y - x \rangle.$$

□

This theorem shows that $\nabla f(x) = 0$ (local minimum) implies x is a global minimum.

Theorem 1.10 (Optimality condition for unconstrained problems). Let $f \in \mathcal{C}^1(\mathbb{R}^n)$ be convex. Then, $x \in \mathbb{R}^n$ is a minimizer of $f(x)$ if and only if $\nabla f(x) = 0$.

Proof. If $\nabla f(x) \neq 0$, then

$$f(x - \varepsilon \nabla f(x)) = f(x) - \varepsilon \|\nabla f(x)\|_2^2 + O(\varepsilon^2) \|\nabla f(x)\|_2^2 < f(x)$$

for small enough ε . Hence, such a point cannot be the minimizer.

On the other hand, if $\nabla f(x) = 0$, Theorem 1.9 shows that

$$f(y) \geq f(x) + \nabla f(x)^\top (y - x) = f(x) \text{ for all } y.$$

□

We note that the proof above is in fact a constructive proof. If x is not a minimum, it suggests a point that has better function value. This will be the discussion of an upcoming section. For continuous convex functions, there is a weaker notion of gradient called sub-differential, which is a set instead of a vector. Both theorems above hold with gradients replaced by sub-differentials.

■ 1.3 Convex problems are everywhere!

In this section, we give a few examples of convex problems to illustrate the wide applicability of convex optimization.

■ 1.3.1 Minimum Cost Flow Problem (Computer Science)

The min cost flow problem has lots of applications such as route planning, airline scheduling, image segmentation, recommendation systems, etc. In this problem, there is a graph $G = (V, E)$ with $m = |E|$ and $n = |V|$. Each edge $e \in E$ has capacity $u_e > 0$ and cost c_e . The problem is to minimize the total cost of sending d amount of flow from a source vertex $s \in V$ to a sink vertex $t \in V$. To imagine this less abstractly, imagine we want to match every person to the best flight for them. Then we can have a source node s connected to a node for each person with $u_e = 1$ for all such e . Further, we take t to be connected to a node for each flight, with u_e being the number of people that can fit on that flight. Then, all the remaining edges will be from people nodes to flight nodes. For any such e , $u_e = 1$ and c_e is proportional to how good that flight is for that person (does it get them where they need to go at the time they need to go?) with 0 representing a perfect flight and ∞ representing a flight they would not take even if given the option for free. Then we can calculate the min-cost flow to find the best allocation of people to flights.

Formally, the problem can be written as an optimization problem $\min_{f \in \mathbb{R}^{|E|}} \sum_{e \in E} c_e \cdot f_e$ subject to the constraints:

- Capacity constraints: $0 \leq f_e \leq u_e$ for all $e \in E$.
- Flow conservation: $\sum_{e \text{ enters } v} f_e = \sum_{e \text{ leaves } v} f_e$ for all $v \in V \setminus \{s, t\}$.
- Demand: $\sum_{e \text{ enters } t} f_e = \sum_{e \text{ leaves } s} f_e = d$.

To check this is a convex problem, we note that the objective function is a linear function $c^\top f$ which is convex. The domain is the intersection of three sets (the three sets of equations above). The first set is a scaled hypercube, the second and last set is a linear subspace. All of them are convex and so is their intersection. Therefore, this is a convex problem.

■ 1.3.2 Linear Programs (Operation Research/Economics)

Consider the diet problem: find a cheapest diet plan that satisfies the nutrients requirements. Formally, suppose there are n different foods and m different nutrients. The food i has unit cost c_i , a_{1i} unit of nutrient 1, a_{2i} unit of nutrient 2, \dots . Furthermore, every day we need b_j unit of the nutrient j . Then, the problem is simply find an assignment x such that

$$\min_{x \geq 0, Ax \geq b} c^\top x$$

where $c \in \mathbb{R}^n$ is the cost vector, $b \in \mathbb{R}^m$ is the intake requirement vector and $A \in \mathbb{R}^{m \times n}$ is the matrix of nutrients contents of each food².

²Unfortunately, Nobel Laureate Stigler showed that [69] the optimal meal is evaporated milk, cabbage, dried navy beans, and beef liver.

Both the diet problem and the minimum cost flow problem can be reformulated into the form

$$\min_{Ax=b, x \geq 0} c^\top x \quad (1.4)$$

for some vectors c, b and some matrix A . These problems are called linear programs and have many applications in resource allocation. Special cases of linear programs are also of great interest; for example the diet problem is a packing/covering LP.

Exercise 1.11. Show how the minimum cost flow problem and the diet problem can be written in the form (1.4). Also, show that (1.4) is a convex problem.

■ 1.3.3 Logistic regression (from Machine Learning)

Consider the problem of predicting the likelihood of getting diabetes in the future. Suppose we have collected many examples $\{(x_i, y_i)\}_{i=1}^n$ where $x_i \in \mathbb{R}^d$ represents the features of a person and $y_i \in \{\pm 1\}$ represents whether that person gets diabetes. For example, the feature vector can be (age, weight, height, BMI, fasting glucose level, ...). The features in the vector may be redundant and the purpose of extra variables is to make linear functions expressive enough to be able to classify. In particular, we assume that there is a vector θ such that for most i , we have $\langle x^i, \theta \rangle < 0$ if $y_i = 1$ and $\langle x^i, \theta \rangle > 0$ if $y_i = -1$. The error of the vector θ is

$$\frac{1}{n} \sum_{i=1}^n 1_{y_i \langle x^i, \theta \rangle > 0}.$$

This function is not convex in θ . More generally, one considers the objective function (to be minimized over θ)

$$R(\theta) = \frac{1}{n} \sum_{i=1}^n f(y_i \langle x^i, \theta \rangle) + \lambda \|\theta\|_1 \quad (1.5)$$

where f is some function such that $f(z)$ is large when z is positive and large and $f(z) = 0$ when z is highly negative, and $\lambda \|\theta\|_1$ is a *regularization* term to make sure θ is bounded. One popular function is $f(z) = \log(1 + e^z)$, and this problem is called logistic regression. In the section 1.5, we prove that the function (1.5) is indeed convex when $f(z) = \log(1 + e^z)$.

■ 1.3.4 Minimal Surface (Physics)

A surface $M \subset \mathbb{R}^3$ is a minimal surface if it has the minimum surface area among all surfaces with the same boundary. These surfaces appear naturally and have been studied extensively not just for \mathbb{R}^3 but also for different manifolds. For simplicity, we consider the case that the surface is parameterized by

$$M = \{(x, y, f(x, y)) : 0 \leq x \leq 1, 0 \leq y \leq 1\}.$$

In this case, f is a minimal surface if

$$f = \operatorname{argmin}_{\text{feasible } g} \text{SurfaceArea}(g)$$

where we say g is feasible if $g(x, y) = f(x, y)$ for all x, y on the boundary of $[0, 1]^2$. One natural question (called Plateau's problem) is to find a minimal surface with a given boundary. For this particular case we consider, we can simply use convex optimization. Note that the constraint (g is feasible) is exactly a linear subspace on the space of functions on $[0, 1]^2$. Furthermore, the objective is convex by using the fact that

$$\text{SurfaceArea}(f) = \int_0^1 \int_0^1 \sqrt{1 + \left(\frac{\partial f(x, y)}{\partial x}\right)^2 + \left(\frac{\partial f(x, y)}{\partial y}\right)^2} dx dy.$$

Exercise 1.12. Show that surface area is convex by using the definition.

Calculus of variations is an area of mathematics that studies optimization in function spaces and there are many common theorems between this and convex optimization.

■ 1.4 Examples of convex sets and functions

There are many important convex sets and here we only list some that appear in this course. One of the most important classes of convex functions comes from convex sets.

Definition 1.13. For a convex set K , we define the indicator function of K by

$$\delta_K(x) = \begin{cases} 0 & \text{if } x \in K \\ +\infty & \text{otherwise} \end{cases}.$$

We can also construct convex sets by convex functions. We let the domain $\text{dom} f \stackrel{\text{def}}{=} \{x \in \mathbb{R}^n : f(x) < +\infty\}$. The definition of a convex function shows that $\text{dom} f$ is a convex set if f is a convex function. Alternatively, by looking at the set of points above the graph of the function, we obtain a convex set called an epigraph.

Definition 1.14. The *epigraph* of $f : \mathbb{R}^n \rightarrow \mathbb{R}$ is $\text{epi} f \stackrel{\text{def}}{=} \{(x, t) \in \mathbb{R}^n \times \mathbb{R} : t \geq f(x)\}$.

A function f is convex if and only if $\text{epi} f$ is a convex set.

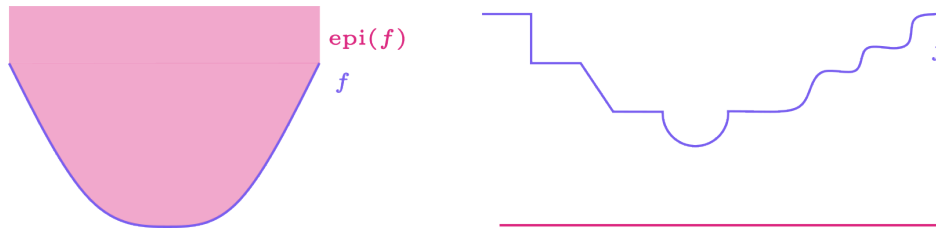


Figure 1.6: Epigraph of f ; quasiconvex function

This characterization shows that $\min_x f(x)$ is the same as $\min_{(x,t) \in \text{epi} f} t$. Therefore, convex optimization is the same as optimizing a linear function over a convex set. Another important feature of a convex set is the following.

Fact 1.15. Any level set $\{x \in \mathbb{R}^n : f(x) \leq t\}$ of a convex function f is convex.

In particular, this shows that the set of minimizers is connected. Therefore, any local minimum is a global minimum. We note that the converse of the fact above is not true. A function is *quasiconvex* if every level set is convex. Equivalently, a function $f : \mathbb{R}^n \rightarrow \mathbb{R}$ is quasiconvex if for every $x, y \in \mathbb{R}^n$ and $t \in [0, 1]$,

$$f((1-t)x + ty) \leq \max f(x), f(y).$$

For example, Fig. 1.6 shows a function that is quasiconvex but not convex.

Finally, we note that many operations preserve convexity. Here is an example.

Exercise 1.16. For a matrix A , vector b , positive scalars $t_1, t_2 \geq 0$, and convex functions f_1 and f_2 , the function $g(x) = t_1 f_1(Ax + b) + t_2 f_2(x)$ is convex.

Here are some convex sets and functions. In Section 1.5, we illustrate how to check convexity.

Example. Convex sets: polyhedron $\{x : Ax \leq b\}$, polytope $\text{conv}(\{v_1, \dots, v_m\})$ with $v_1, \dots, v_m \in \mathbb{R}^n$, ellipsoid $\{x : x^\top A x \leq 1\}$ with $A \succeq 0$, positive semidefinite cone $\{X \in \mathbb{R}^{n \times n} : X \succeq 0\}$, norm ball $\{x : \|x\|_p \leq 1\}$ for all $p \geq 1$.

Example. Convex functions: x , $\max(x, 0)$, e^x , $|x|^a$ for $a \geq 1$, $-\log(x)$, $x \log x$, $\|x\|_p$ for $p \geq 1$, $(x, y) \rightarrow \frac{x^2}{y}$ (for $y > 0$), $A \rightarrow -\log \det A$ over PSD matrices A , $(x, Y) \rightarrow x^\top Y^{-1} x$ (for $Y \succ 0$), $\log \sum_i e^{x_i}$, $(\prod_i^n x_i)^{\frac{1}{n}}$.

Exercise 1.17. Show that the above sets and functions are all convex.

Exercise 1.18. Show that the intersection of convex sets is convex; show that for convex functions, f, g , the function $h(x) = \max f(x), g(x)$ is also convex.

■ 1.5 Checking convexity

It is often cumbersome to check if a function is convex via (1.3). The major benefit of that definition is that it works for non-differentiable functions and infinite dimensional spaces. However, when a function is twice differentiable, one can check the convexity by simply checking if the Hessian is positive semi-definite. (Recall the definition of $A \succeq 0$ in 0.6.)

To show this, we first prove the following second-order Taylor theorem. A useful idea here is to note that a function is convex if and only if its restriction to any one-dimensional line is convex, and to define a suitable one-dimensional function.

Theorem 1.19. *For any $f \in \mathcal{C}^2(\mathbb{R}^n)$, and any $x, y \in \mathbb{R}^n$, there is a $z \in [x, y]$ s.t.*

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

Proof. Let $g(t) = f((1 - t)x + ty)$. Taylor expansion (Theorem 0.4) shows that

$$g(1) = g(0) + g'(0) + \frac{1}{2} g''(\zeta)$$

where $\zeta \in [0, 1]$. To see the result, note that $g(0) = f(x)$, $g(1) = f(y)$, $g'(0) = \nabla f(x)^\top (y - x)$ and $g''(\zeta) = (y - x)^\top \nabla^2 f((1 - \zeta)x + \zeta y)(y - x)$. \square

Now, we show that f is convex if and only if $\nabla^2 f(x) \succeq 0$ for all x .

Theorem 1.20. *Let $f \in \mathcal{C}^2(\mathbb{R}^n)$. Then, the following are equivalent:*

1. f is convex.
2. $f(y) \geq f(x) + \nabla f(x)^\top (y - x)$ for all $x, y \in \mathbb{R}^n$.
3. $\nabla^2 f(x) \succeq 0$ for all $x \in \mathbb{R}^n$.

Proof. We have proved (1) implies (2) in Theorem 1.9.

Suppose (2) holds. Then, for any $x, h \in \mathbb{R}^n$

$$f(x + th) \geq f(x) + t \nabla f(x)^\top h.$$

By Taylor expansion (Lemma 1.19), we have that

$$f(x + th) = f(x) + t \nabla f(x)^\top h + \frac{t^2}{2} h^\top \nabla^2 f(z) h$$

where $z \in [x, x + th]$. By comparing two equations, we have that $h^\top \nabla^2 f(z) h \geq 0$. Taking $t \rightarrow 0$, we have $z \rightarrow x$ and hence $\nabla^2 f(z) \rightarrow \nabla^2 f(x)$. Therefore, we have that

$$h^\top \nabla^2 f(x) h \geq 0$$

for all x and h . Hence, this gives (3).

Suppose (3) holds. Fix $x, y \in \mathbb{R}^n$. Consider the function

$$g(\lambda) = f(\lambda x + (1 - \lambda)y) - \lambda f(x) - (1 - \lambda)f(y).$$

Consider $\lambda^* = \operatorname{argmax}_{\lambda \in [0, 1]} g(\lambda)$. If λ^* is either 0 or 1, then we have $g(\lambda^*) = 0$. Otherwise, by Taylor's theorem, there is a $\zeta \in [\lambda^*, 1]$ such that

$$\begin{aligned} g(1) &= g(\lambda^*) + g'(\lambda^*)(1 - \lambda^*) + \frac{1}{2} g''(\zeta)(1 - \lambda^*)^2 \\ &= g(\lambda^*) + \frac{1}{2} g''(\zeta)(1 - \lambda^*)^2 \end{aligned}$$

where we used that $g'(\lambda^*) = 0$. Note that

$$\begin{aligned} g'(\zeta) &= \nabla f(\zeta x + (1 - \zeta)y)^\top (x - y) - f(x) + f(y), \\ g''(\zeta) &= (x - y)^\top \nabla^2 f(\zeta x + (1 - \zeta)y)(x - y). \end{aligned}$$

By the assumption (3), we have that $g''(\zeta) \geq 0$ and hence $0 = g(1) \geq g(\lambda^*)$. Hence, in both cases, $\max_{\lambda \in [0, 1]} g(\lambda) = g(\lambda^*) \leq 0$. This gives (1). \square

Now, as an example, we prove that the function (1.5) is convex.

Example 1.21. The function (1.5) is convex for $f(z) = \log(1 + \exp(z))$.

Proof. We write $R(\theta) = R_1(\theta) + R_2(\theta)$ where $R_1(\theta) = \frac{1}{n} \sum_{i=1}^n f(y_i \cdot \langle x^i, \theta \rangle)$ and $R_2(\theta) = \lambda \|\theta\|_1$. It is easy to check R_2 is convex. So, it suffices to prove R_1 is convex. Now, we use Theorem 1.20 to prove that R_1 is convex. Note that

$$\begin{aligned} \nabla R_1(\theta) &= \frac{1}{n} \sum_{i=1}^n f'(y^i \langle x^i, \theta \rangle) y^i x^i, \\ \nabla^2 R_1(\theta) &= \frac{1}{n} \sum_{i=1}^n f''(y^i \langle x^i, \theta \rangle) x^i (x^i)^\top \end{aligned}$$

where we used $(y^i)^2 = 1$. Since $x^i (x^i)^\top \succeq 0$, it suffices to prove that $f''(y^i \langle x^i, \theta \rangle) \geq 0$. This follows from the calculation: $f'(z) = \frac{\exp(z)}{1+\exp(z)} = 1 - \frac{1}{1+\exp(z)}$ and $f''(z) = \frac{\exp(z)}{(1+\exp(z))^2} \geq 0$. \square

■ 1.6 Subgradients

The standard definition of a convex function in terms of gradients requires differentiability. However, a more general definition allows us to avoid this requirement. For a convex function $f : \mathbb{R}^n \rightarrow \mathbb{R}$, we say that a function $g : \mathbb{R}^n \rightarrow \mathbb{R}$ is called a *subgradient* if it satisfies the following property: for any $x, y \in \mathbb{R}^n$, $f(y) - f(x) \geq \langle g(x), y - x \rangle$. For the purpose of optimization algorithms, in almost all cases, a subgradient will suffice in place of a gradient.

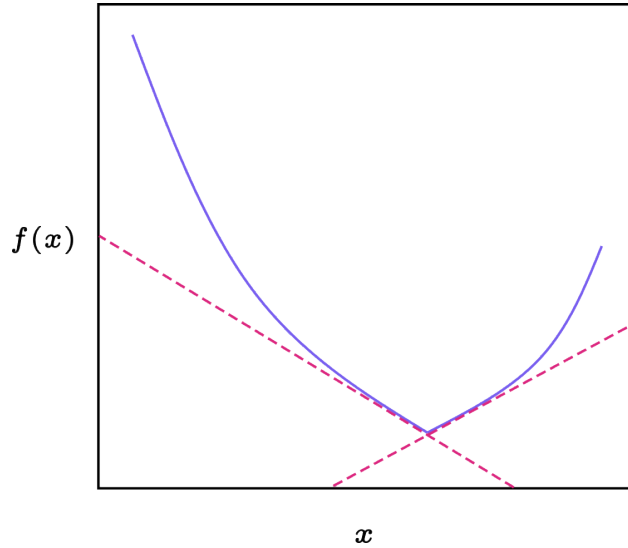


Figure 1.7: Sub-gradient

■ 1.7 Logconcave functions

Definition 1.22. A function $f : \mathbb{R}^n \rightarrow \mathbb{R}_+$ is *logconcave* if $\log f$ is concave, i.e., f is nonnegative and for any $t \in (0, 1)$, we have $f(tx + (1-t)y) \geq f(x)^t f(y)^{1-t}$.

Thus any logconcave function can be viewed as $e^{-f(x)}$ for some convex function f .

Exercise 1.23. Show that for any $t \geq 0$, the level set $L(t) = \{x : f(x) \geq t\}$ of a logconcave function f is convex.

Example 1.24. The indicator function of a convex set $1_K(x) = \begin{cases} 1 & \text{if } x \in K \\ 0 & \text{otherwise} \end{cases}$ is logconcave. The Gaussian density function is logconcave. The Gaussian density restricted to any convex set is logconcave.

To see that the indicator function of a convex set K is logconcave, simply consider two points x, y which (1) both lie in K , (2) both lie outside and (3) one is in K , one is outside. Now check the value of the indicator along any convex combination of x and y .

Lemma 1.25 (Dinghas; Prékopa; Leindler). *The product, minimum and convolution of two logconcave functions is also logconcave; in particular, any linear transformation or any marginal of a logconcave density is logconcave; the distribution function of any logconcave density is logconcave.*

We next describe the basic theorem underlying the above properties. We will see their proofs in a later chapter.

Theorem 1.26 (Prékopa-Leindler). *Fix $\lambda \in [0, 1]$. Let $f, g, h : \mathbb{R}^n \rightarrow \mathbb{R}_+$ be functions satisfying $h(\lambda x + (1 - \lambda)y) \geq f(x)^\lambda g(y)^{1-\lambda}$ for all $x \in \mathbb{R}^n$. Then,*

$$\int_{\mathbb{R}^n} h \geq \left(\int_{\mathbb{R}^n} f \right)^\lambda \left(\int_{\mathbb{R}^n} g \right)^{1-\lambda}.$$

An equivalent version of the lemma for sets in \mathbb{R}^n is often useful. By a *measurable* set below, we mean Lebesgue measurable, which coincides with the definition of volume (for an axis aligned box, it is the product of the axis lengths; for any other set, it is the limit over increasingly finer partitions into boxes, of the sum of volumes of boxes that intersect the set).

Theorem 1.27 (Brunn-Minkowski). *For any $\lambda \in [0, 1]$ and measurable sets $A, B \subset \mathbb{R}^n$, we have*

$$\text{vol}(\lambda A + (1 - \lambda)B)^{1/n} \geq \lambda \text{vol}(A)^{1/n} + (1 - \lambda) \text{vol}(B)^{1/n}.$$

An immediate consequence of the first theorem above is that any one-dimensional marginal distribution of a convex body is logconcave; the second implies that it is in fact $(1/(n-1))$ -concave (a function is s -concave if f^s is concave) if the body is in \mathbb{R}^n .

Exercise 1.28. Prove both corollaries just mentioned.

Example 1.29. We give an example problem related to Bayesian inference. Suppose we have a signal $\theta = (\theta_1, \theta_2, \dots, \theta_n)$ and that we can take a measurement y_i of θ_i . The measurement only incurs unbiased Gaussian noise, i.e., $y_i = \theta_i + \epsilon_i$ where $\epsilon_i \sim N(0, 1)$. The question is to recover the signal θ using y . Without any prior on θ , the only sensible recovery is $\theta = y$. With a prior, one can apply Bayes' theorem:

$$\mathbf{P}(\theta|y) = \frac{\mathbf{P}(y|\theta)\mathbf{P}(\theta)}{\mathbf{P}(y)}.$$

The Bayesian choice is to find θ with maximum likelihood, namely $\theta = \arg\max_{\theta} \log \mathbf{P}(\theta|y) = \arg\min_{\theta} -\log \mathbf{P}(\theta|y)$.

Using the noise assumption, we have that

$$\mathbf{P}(y|\theta) \propto \exp\left(-\frac{1}{2} \sum_i (y_i - \theta_i)^2\right).$$

Now, say we know the signal is smooth and we model the prior as $\mathbf{P}(\theta) \propto \exp(-\lambda \sum_i (\theta_i - \theta_{i+1})^2)$ where λ controls how smooth the signal is. Hence,

$$-\log \mathbf{P}(\theta|y) = c + \sum_i (y_i - \theta_i)^2 + \lambda \sum_i (\theta_i - \theta_{i+1})^2.$$

Since each term in the function above is convex, so is the whole formula. Hence, the recovery question becomes a convex optimization problem

$$\min_{\theta} \sum_i (y_i - \theta_i)^2 + \lambda \sum_i (\theta_i - \theta_{i+1})^2.$$

When we recover a signal, we want to know how confident we are because there are many choices of θ that could explain the same measurement y . One way to do this is to sample multiple $\theta \propto \mathbf{P}(\theta|y)$ and compute the empirical variance or other statistics. Note that

$$\mathbf{P}(\theta|y) \propto e^{-\sum_i (y_i - \theta_i)^2 - \lambda \sum_i (\theta_i - \theta_{i+1})^2}$$

which is a logconcave distribution. Therefore, one can study the signal and quality of signal recovery via logconcave sampling.

Part I

Optimization

■ 2.1 Philosophy

Optimization methods often follow the following framework:

Algorithm 1: OptimizationFramework

```

for  $k = 0, 1, \dots$  do
    Approximate  $f$  by a simpler function  $f_k$  according to the current point  $x^{(k)}$ 
    Do something using  $f_k$  (such as set  $x^{(k+1)} = \arg \min_x f_k(x)$ )
end

```

The runtime depends on the number of iterations and the cost per iteration. Philosophically, the difficulties of a problem can never be created nor destroyed, only converted from one form of difficulty to another. When we decrease the number of iterations, the cost per iteration often increases. The gain of new methods often come from avoiding some wasted computation, utilizing some forgotten information or giving a faster but tailored algorithm for a sub-problem. This is of course just an empirical observation.

One key question to answer in designing an optimization algorithm is what the problem looks like (or how can we approximate f by a simpler function). Here are some approximations we will use in this textbook:

- First-order Approximation: $f(y) \approx f(x) + \langle \nabla f(x), y - x \rangle$ (Section 2.2).
- Second-order Approximation: $f(y) \approx f(x) + \langle \nabla f(x), y - x \rangle + (y - x)^\top \nabla^2 f(x)(y - x)$ (Section 5.4).
- Stochastic/Monte-Carlo Approximation: $\sum_i f_i(x) \approx f_j(x)$ for a random j (Section 6.3).
- Matrix Approximation: Approximate A by a simpler B with $\frac{1}{2}A \preceq B \preceq 2A$ (Section 6.1 and Section 6.2).
- Matrix Approximation: Approximate A by a low-rank matrix.
- Set Approximation: Approximate a convex set by an ellipsoid or a polytope (Section 3.1).
- Barrier Approximation: Approximate a convex set by a smooth function that blows up on the boundary (Section 5.5).
- Polynomial Approximation: Approximate a function by a polynomial (Section 7.1).
- Partial Approximation: Split the problem into two parts and approximate only one part.
- Taylor Approximation: $f(y) \approx \sum_{k=0}^K D^k f(x)[y - x]^k$.
- Mixed ℓ^2 - ℓ^p Approximation: $f(y) \approx f(x) + \langle \nabla f(x), y - x \rangle + \sum_{i=1}^n \alpha_i (y_i - x_i)^2 + \beta_i (y_i - x_i)^p$

Here are other approximation not covered:

- Stochastic Matrix Approximation: Approximate A by a simpler random B with $B \preceq 2A$ and $\mathbf{E}B \succeq \frac{1}{2}A$
- Homotopy Method: Approximate a function by a family of functions
- ... (Please give me more examples here)...

The second question to answer is how to maintain different approximations created in different steps. One simple way would be forget the approximation we got in previous steps, but this is often not optimal. Another way is to keep all previous approximations/information (such as Section 3.1). Often the best way will be combining previous and current approximation carefully to a better approximation (such as Section 7.4).

■ 2.2 Basic Algorithm

Perhaps the most natural algorithm for optimization is gradient descent. In fact, it has many variants with different guarantees. Assume that the function f to be optimized is continuously differentiable. By basic

calculus, either the minimum (or point achieving the minimum) is unbounded or the gradient is zero at a minimum. So we try to find a point with gradient close to zero (which, of course, does not guarantee global optimality). The basic algorithm is the following.

Algorithm 2: GradientDescent (GD)

Input: Initial point $x^{(0)} \in \mathbb{R}^n$, step size $h > 0$.
for $k = 0, 1, \dots$ **do**
 if $\|\nabla f(x^{(k)})\|_2 \leq \epsilon$ **then return** $x^{(k)}$;
 // Alternatively, one can use $x^{(k+1)} \leftarrow \operatorname{argmin}_{x=x^{(k)}+t\nabla f(x^{(k)}), t \in \mathbb{R}} f(x)$.
 $x^{(k+1)} \leftarrow x^{(k)} - h \cdot \nabla f(x^{(k)})$.
end

One can view gradient descent as a greedy method for solving $\min_{x \in \mathbb{R}^n} f(x)$. At a point x , gradient descent goes to the minimizer of

$$\min_{\|\delta\|_2 \leq h/\|\nabla f(x)\|_2} f(x) + \nabla f(x)^\top \delta.$$

The term $f(x) + \nabla f(x)^\top \delta$ is simply the first-order approximation of $f(x + \delta)$. Note that in this problem, the current point x is fixed and we are optimizing the step δ . Certainly, there is no inherent reason for using first-order approximation and the Euclidean norm $\|x\|_2$. For example, if you use second-order approximation, then you would get a method involving Hessian of f .

The step size of the algorithm usually either uses a fixed constant, or follows a predetermined schedule, or determined using a line search.

If the iteration stops, we get a point with $\|\nabla f(x)\|_2 \leq \epsilon$. Why is this good? The hope is that x is a near-minimum in the neighborhood of x . However, this might not be true if the gradient can fluctuate wildly:

Definition 2.1. We say f has L -Lipschitz gradient if ∇f is L -Lipschitz, namely, $\|\nabla f(x) - \nabla f(y)\|_2 \leq L\|x - y\|_2$ for all $x, y \in \mathbb{R}^n$.

Similar to Theorem 1.20, we have the following equivalence.

Theorem 2.2. Let $f \in \mathcal{C}^2(\mathbb{R}^n)$. For any $L \geq 0$, the following are equivalent:

1. $\|\nabla f(x) - \nabla f(y)\|_2 \leq L\|x - y\|_2$ for all $x, y \in \mathbb{R}^n$.
2. $-LI \preceq \nabla^2 f(x) \preceq LI$ for all $x \in \mathbb{R}^n$.
3. $|f(y) - f(x) - \nabla f(x)^\top (y - x)| \leq \frac{L}{2}\|y - x\|_2^2$ for all $x, y \in \mathbb{R}^n$.

Proof. Suppose (1) holds. By the definition of $\nabla^2 f$, we have

$$\nabla^2 f(x)v = \lim_{h \rightarrow 0} \frac{\nabla f(x + hv) - \nabla f(x)}{h}.$$

Since $\|\frac{\nabla f(x + hv) - \nabla f(x)}{h}\|_2 \leq \frac{L}{h}\|hv\|_2 = L\|v\|_2$, we have $\|\nabla^2 f(x)v\|_2 \leq L\|v\|_2$, which means all eigenvalues of $\nabla^2 f$ are at most L in magnitude. This proves (2).

Suppose (2) holds. Since by the fundamental theorem of calculus,

$$\nabla f(x) - \nabla f(y) = \int_0^1 \nabla^2 f(y + t(x - y))(x - y)dt,$$

we have that

$$\|\nabla f(x) - \nabla f(y)\|_2 \leq \int_0^1 \|\nabla^2 f(y + t(x - y))\|_{\text{op}}\|x - y\|_2 dt \leq L\|x - y\|_2.$$

This gives (1).

Suppose (2) holds. By integration along the direction $y - x$ from x to y , we have

$$f(y) = f(x) + \nabla f(x)^\top (y - x) + \int_0^1 (1 - t)(y - x)^\top \nabla^2 f(x + t(y - x))(y - x)dt.$$

Since $-LI \preceq \nabla^2 f(x) \preceq LI$, we have

$$|(y-x)^\top \nabla^2 f(x+t(y-x))(y-x)| \leq L\|y-x\|^2.$$

This gives (3).

Suppose (3) holds, then $g(x) = f(x) + \frac{L}{2}\|x\|^2$ satisfies $g(y) \geq g(x) + \nabla g(x)^\top (y-x)$ for all $x, y \in \mathbb{R}^n$. So Theorem 1.20 shows that g is convex and $\nabla^2 g(x) \succeq 0$. Hence, $\nabla^2 f(x) \succeq -LI$. Similarly, by taking $g(x) = \frac{L}{2}\|x\|^2 - f(x)$, we have $\nabla^2 f(x) \preceq LI$. This gives (2). \square

Exercise 2.3. Prove the implication above (2) \Rightarrow (3) by defining a one-dimensional function.

Exercise 2.4. Prove that if $f \in \mathcal{C}^2(\mathbb{R}^n)$ has an L -Lipschitz gradient then the function $g(x) = \frac{L}{2}\|x\|_2^2 - f(x)$ satisfies $\langle \nabla g(x) - \nabla g(y), x - y \rangle \geq 0$, and so g is convex.

With the equivalent definitions in Thm. 2.2, we can have an alternative view of gradient descent. Each step, we perform

$$x^{(k+1)} = \arg \min_y f(x^{(k)}) + \left\langle \nabla f(x^{(k)}), y - x^{(k)} \right\rangle + \frac{L}{2}\|y - x^{(k)}\|_2^2.$$

To see this is the same step, we let

$$g(y) = f(x^{(k)}) + \left\langle \nabla f(x^{(k)}), y - x^{(k)} \right\rangle + \frac{L}{2}\|y - x^{(k)}\|_2^2.$$

The optimality condition shows that $0 = \nabla g(x^{(k+1)}) = \nabla f(x^{(k)}) + L(x^{(k+1)} - x^{(k)})$. Hence, this gives the step $x^{(k+1)} = x^{(k)} - \frac{1}{L}\nabla f(x^{(k)})$.

By Theorem 2.2, we know that g is an upper bound of f , namely $g(y) \geq f(y)$ for all y . In general, many optimization methods involves minimizing some upper bound function every step. Note that the progress we made for f is at least the progress we made for g . If g is exactly f , we can get all the progress we can make in one step. Hence, we should believe if g is a better approximation of f , then we are making more progress. For gradient descent, it uses the simplest first-order approximation. Although this is not the best approximation one can come up with, it is robust enough to use in all sorts of applications.

Exercise 2.5. Show that any convex function is Lipschitz over any compact subset of its domain.

■ 2.2.1 Analysis for general functions

Gradient descent works for both convex and non-convex functions. For non-convex function, we can only find a point with small gradient (called an approximate saddle point).

Theorem 2.6. Let $f \in \mathcal{C}^2(\mathbb{R}^n)$ with L -Lipschitz gradient and x^* be any minimizer of f . Then **GradientDescent** with step size $h = \frac{1}{L}$ outputs a point x such that $\|\nabla f(x)\|_2 \leq \epsilon$ in at most $\frac{2L}{\epsilon^2} (f(x^{(0)}) - f(x^*))$ iterations.

One practical advantage of line search is that the algorithm does not need to know a bound on the Lipschitz constant of the gradient. The next lemma shows that the function value must decrease along the GD path for a sufficiently small step size, and the magnitude of the decrease depends on the norm of the current gradient.

Lemma 2.7. For any $f \in \mathcal{C}^2(\mathbb{R}^n)$ with L -Lipschitz gradient, we have

$$f(x - \frac{1}{L}\nabla f(x)) \leq f(x) - \frac{1}{2L}\|\nabla f(x)\|_2^2.$$

Proof. Lemma 1.19 shows that

$$f(x - \frac{1}{L}\nabla f(x)) = f(x) - \frac{1}{L}\|\nabla f(x)\|_2^2 + \frac{1}{2L^2}\nabla f(x)^\top \nabla^2 f(z)\nabla f(x)$$

for some $z \in [x, x - \frac{1}{L}\nabla f(x)]$. Since $\|\nabla^2 f(x)\|_{\text{op}} \leq L$, we have that

$$\nabla f(x)^\top \nabla^2 f(z)\nabla f(x) \leq L \cdot \|\nabla f(x)\|_2^2.$$

Putting this back above, we have

$$f(x) - \frac{1}{L} \nabla f(x) \leq f(x) - \frac{1}{L} \|\nabla f(x)\|_2^2 + \frac{L}{2L^2} \|\nabla f(x)\|_2^2 = f(x) - \frac{1}{2L} \|\nabla f(x)\|_2^2.$$

□

We can now prove the theorem.

Proof of Theorem 2.6. We observe that either $\|\nabla f(x)\|_2 \leq \epsilon$, or $\|\nabla f(x)\|_2 \geq \epsilon$ and so by Lemma 2.7, the function value $f(x)$ decreases by at least $\frac{\epsilon^2}{2L}$. Since the function value can decrease by at most $f(x^{(0)}) - f(x^*)$, this bounds the number of iterations — each step of gradient descent decreases f by at least $\frac{\epsilon^2}{2L}$ and since we can decrease f by at most $f(x^{(0)}) - f(x^*)$, we have the result. □

Despite the simplicity of the algorithm and the proof, it is known that this is the best one can do via any algorithm in this general setting [15].

■ 2.3 Analysis for convex functions

Assuming the function is convex, we can prove that gradient descent in fact converges to the global minimum. In particular, when $\|\nabla f(x)\|_2$ is small, convexity shows that $f(x) - f^*$ is small (Theorem 1.9).

Lemma 2.8. *For any convex $f \in \mathcal{C}^1(\mathbb{R}^n)$, we have that $f(x) - f(y) \leq \|\nabla f(x)\|_2 \cdot \|x - y\|_2$ for all x, y .*

Proof. Theorem 1.9 and Cauchy-Schwarz inequality shows that

$$f(x) - f(y) \leq \langle \nabla f(x), x - y \rangle \leq \|\nabla f(x)\|_2 \cdot \|x - y\|_2.$$

□

This in turn give a better bound on the number of iterations because the bound in Theorem 2.6 is affected by $f(x) - f^*$ rather than $\|x - x^*\|_2$

Theorem 2.9. *Let $f \in \mathcal{C}^2(\mathbb{R}^n)$ be convex with L -Lipschitz gradient and x^* be any minimizer of f . With step size $h = \frac{1}{L}$, the sequence $x^{(k)}$ in **GradientDescent** satisfies*

$$f(x^{(k)}) - f(x^*) \leq \frac{2LR^2}{k+4} \text{ where } R = \max_{f(x) \leq f(x^{(0)})} \|x - x^*\|_2.$$

Proof. Let $\epsilon_k = f(x^{(k)}) - f(x^*)$. Lemma 2.7 shows that

$$f(x^{(k+1)}) = f(x^{(k)} - \frac{1}{L} \nabla f(x^{(k)})) \leq f(x^{(k)}) - \frac{1}{2L} \|\nabla f(x^{(k)})\|_2^2.$$

Subtracting $f(x^*)$ from both sides, we have $\epsilon_{k+1} \leq \epsilon_k - \frac{1}{2L} \|\nabla f(x^{(k)})\|_2^2$. Lemma 2.8 shows that

$$\epsilon_k \leq \|\nabla f(x^{(k)})\|_2 \cdot \|x^{(k)} - x^*\|_2 \leq \|\nabla f(x^{(k)})\|_2 \cdot R.$$

Therefore, we have that

$$\epsilon_{k+1} \leq \epsilon_k - \frac{1}{2L} \left(\frac{\epsilon_k}{R} \right)^2.$$

Now, we need to solve the recursion. We note that

$$\frac{1}{\epsilon_{k+1}} - \frac{1}{\epsilon_k} = \frac{\epsilon_k - \epsilon_{k+1}}{\epsilon_k \epsilon_{k+1}} \geq \frac{\epsilon_k - \epsilon_{k+1}}{\epsilon_k^2} \geq \frac{1}{2LR^2}.$$

Also, by Thm. 2.2, we have that

$$\epsilon_0 = f(x^{(0)}) - f(x^*) \leq \nabla f(x^*)^\top (x^{(0)} - x^*) + \frac{L}{2} \|x^{(0)} - x^*\|_2^2 \leq \frac{LR^2}{2}.$$

Therefore, after k iterations, we have

$$\frac{1}{\epsilon_k} \geq \frac{1}{\epsilon_0} + \frac{k}{2LR^2} \geq \frac{2}{LR^2} + \frac{k}{2LR^2} = \frac{k+4}{2LR^2}.$$

□

This style of proof is typical in optimization. It shows that when the gradient is large, then we make large progress and when the gradient is small, we are close to optimal.

This proof above does not make essential use any property of ℓ_2 or inner product space. It can be extended to work for general norms if the gradient descent step is defined using that norm. For the case of ℓ_2 , one can prove that $\|x^{(k)} - x^*\|_2$ is in fact decreasing.

Lemma 2.10. *For $h \leq \frac{2}{L}$, we have that $\|x^{(k+1)} - x^*\|_2 \leq \|x^{(k)} - x^*\|_2$. Therefore, for an L -gradient Lipschitz convex function f , for GD with $h = \frac{1}{L}$, we have*

$$f(x^{(k)}) - f(x^*) \leq \frac{2L\|x^{(0)} - x^*\|_2^2}{k+4}.$$

Proof. We compute the distance to an optimal point as follows, noting that $\nabla f(x^*) = 0$:

$$\begin{aligned} \|x^{(k+1)} - x^*\|_2^2 &= \|x^{(k)} - x^* - h\nabla f(x^{(k)})\|_2^2 \\ &= \|x^{(k)} - x^*\|_2^2 - 2h \langle \nabla f(x^{(k)}), x^{(k)} - x^* \rangle + h^2 \|\nabla f(x^{(k)})\|_2^2 \\ &= \|x^{(k)} - x^*\|_2^2 - 2h \langle \nabla f(x^{(k)}) - \nabla f(x^*), x^{(k)} - x^* \rangle + h^2 \|\nabla f(x^{(k)}) - \nabla f(x^*)\|_2^2. \end{aligned}$$

To handle the term $\nabla f(x) - \nabla f(x^*)$, we note that

$$\nabla f(x^{(k)}) - \nabla f(x^*) = H(x^{(k)} - x^*)$$

with $H = \int_0^1 \nabla^2 f(x^* + t(x^{(k)} - x^*))dt$. Since $0 \preceq H \preceq LI$ and that $H \succeq \frac{1}{L}H^2$, we have

$$\begin{aligned} \langle \nabla f(x^{(k)}) - \nabla f(x^*), x^{(k)} - x^* \rangle &= (x^{(k)} - x^*)^\top H(x^{(k)} - x^*) \\ &\geq \frac{1}{L}(x^{(k)} - x^*)^\top H^2(x^{(k)} - x^*) \\ &= \frac{1}{L}\|\nabla f(x^{(k)}) - \nabla f(x^*)\|_2^2. \end{aligned}$$

Hence, we have

$$\begin{aligned} \|x^{(k+1)} - x^*\|_2^2 &\leq \|x^{(k)} - x^*\|_2^2 - \left(\frac{2h}{L} - h^2\right)\|\nabla f(x^{(k)}) - \nabla f(x^*)\|_2^2 \\ &\leq \|x^{(k)} - x^*\|_2^2. \end{aligned}$$

The error estimate follows from $\|x^{(k)} - x^*\|_2^2 \leq \|x^{(0)} - x^*\|_2^2$ for all k and the proof in Theorem 2.9. □

Rewriting the bound, Theorem 2.9 shows it takes $\frac{2L\|x^{(0)} - x^*\|_2^2}{\epsilon}$ iterations. Compare to the bound $\frac{2L}{\epsilon^2}(f(x^{(0)}) - f^*)$ in Theorem 2.6, it seems the new result has a strictly better dependence on ϵ . However, this is not true because one measures the error in terms of $\|\nabla f(x)\|_2$ while the other is in terms of $f(x) - f^*$. For $f(x) = x^2/2$, we have $f(x) - f^* = \|\nabla f(x)\|_2^2$ and hence both have the same dependence on ϵ for this particular function. So, the real benefit of Theorem 2.9 is its global convergence.

■ 2.4 Strongly Convex Functions

We note that the convergence rate ϵ^{-1} or ϵ^{-2} is not great if we need to solve the problem up to very high accuracy (e.g., up to n bits would mean $\epsilon = 2^{-n}$). Getting to very high accuracy is sometimes important if the optimization problem is used as a subroutine. We note that for the case $f(x) = \frac{1}{2}\|x\|_2^2$, gradient descent with step size $h = 1$ takes exactly 1 step. Therefore, it is natural to ask if one can improve the bound for functions close to quadratics. This motivates the following assumption.

Definition 2.11. We say a function $f \in \mathcal{C}^1(\mathbb{R}^n)$ is μ -strongly convex if for any $x, y \in \mathbb{R}^n$

$$f(y) \geq f(x) + \nabla f(x)^\top (y - x) + \frac{\mu}{2} \|y - x\|_2^2.$$

A “growth” of a strongly convex function around any point is lower bounded by a quadratic function. Clearly a strongly convex function is also convex and the sum of a strongly convex and convex function remains strongly convex. An example of a function that is convex but not strongly convex is $f(x) = |x|$. Similar to the convex case (Theorem 1.20), we have the following.

Theorem 2.12. Let $f \in \mathcal{C}^2(\mathbb{R}^n)$. For any $\mu \geq 0$, the following are equivalent:

- $f(tx + (1-t)y) \leq tf(x) + (1-t)f(y) - \frac{1}{2}\mu t(1-t)\|x - y\|_2^2$ for all $x, y \in \mathbb{R}^n$ and $t \in [0, 1]$.
- $f(y) \geq f(x) + \nabla f(x)^\top (y - x) + \frac{\mu}{2} \|y - x\|_2^2$ for all $x, y \in \mathbb{R}^n$.
- $\nabla^2 f(x) \succeq \mu I$ for all $x \in \mathbb{R}^n$

Proof. It follows from applying Theorem 1.20 on the function $g(x) = f(x) - \frac{\mu}{2}\|x\|^2$. □

Next, we study gradient descent for μ -strongly convex functions.

Lemma 2.13. Let $f \in \mathcal{C}^2(\mathbb{R}^n)$ be μ -strongly convex. Then, for any $x, y \in \mathbb{R}^n$, we have

$$\|\nabla f(x)\|^2 \geq 2\mu(f(x) - f(y)).$$

Proof. By the definition of μ strong convexity, we have

$$f(y) \geq f(x) + \langle \nabla f(x), y - x \rangle + \frac{\mu}{2} \|x - y\|^2.$$

Rearranging, we have

$$f(x) - f(y) \leq \langle \nabla f(x), x - y \rangle - \frac{\mu}{2} \|x - y\|^2 \leq \max_{\Delta} \nabla f(x)^\top \Delta - \frac{\mu}{2} \|\Delta\|^2 = \frac{1}{2\mu} \|\nabla f(x)\|^2.$$

□

This will lead to the following guarantee. Note that the error now decreases geometrically rather than additively.

Theorem 2.14. Let $f \in \mathcal{C}^2(\mathbb{R}^n)$ be μ -strongly convex with L -Lipschitz gradient and x^* be any minimizer of f . With step size $h = \frac{1}{L}$, the sequence $x^{(k)}$ in **GradientDescent** satisfies

$$f(x^{(k)}) - f(x^*) \leq \left(1 - \frac{\mu}{L}\right)^k \left(f(x^{(0)}) - f(x^*)\right).$$

In a later chapter, we will see that an *accelerated* variant of gradient descent improves this further by replacing the $\frac{\mu}{L}$ term with $\sqrt{\frac{\mu}{L}}$.

Proof. Lemma 2.7 shows that

$$f(x^{(k+1)}) - f^* \leq f(x^{(k)}) - f^* - \frac{1}{2L} \|\nabla f(x^{(k)})\|_2^2 \tag{2.1}$$

$$\leq f(x^{(k)}) - f^* - \frac{\mu}{L} \left(f(x^{(k)}) - f^*\right) \tag{2.2}$$

$$= \left(1 - \frac{\mu}{L}\right) \left(f(x^{(k)}) - f^*\right) \tag{2.3}$$

where we used Lemma 2.13. The conclusion follows. □

A similar bound also holds for convergence to the optimal point.

Exercise 2.15. Let $f \in \mathcal{C}^2(\mathbb{R}^n)$ be μ -strongly convex with L -Lipschitz gradient and x^* be the minimizer of f . With step size $h = 1/L$, show that the sequence $x^{(k)}$ in **GradientDescent** satisfies

$$\|x^{(k)} - x^*\|_2^2 \leq \left(1 - \frac{\mu}{L}\right)^k \|x^{(0)} - x^*\|_2^2.$$

It is natural to ask to what extent the assumption of convexity is essential for the bounds we obtained. This is the motivation for the next exercises.

Exercise 2.16. Suppose f satisfies $\langle \nabla f(x), x - x^* \rangle \geq \alpha (f(x) - f(x^*))$. Derive a bound similar to Theorem 2.9 for gradient descent.

Exercise 2.17. Suppose f satisfies $\|\nabla f(x)\|_2^2 \geq \mu (f(x) - f(x^*))$. Derive a bound similar to Theorem 2.14 for gradient descent.

Exercise 2.18. Give examples of nonconvex functions satisfying the above conditions. (Note: convex functions satisfy the first with $\alpha = 1$ and μ -strongly convex functions satisfy the second.)

■ 2.5 Line Search

In practice, we often stop line search early because we can make larger progress in a new direction. A standard stopping condition is called the Wolfe condition.

Definition 2.19. A step size h satisfies the Wolfe condition with respect to direction p if

1. $f(x + hp) \leq f(x) + c_1 h \cdot p^\top \nabla f(x)$,
2. $-p^\top \nabla f(x + hp) \leq -c_2 p^\top \nabla f(x)$.

with $0 < c_1 < c_2 < 1$.

Let the objective for progress be $\phi(h) = f(x) - f(x + hp)$. The first condition requires the algorithm makes sufficient progress ($\phi(h) \geq c_1 h \cdot \phi'(0)$). The second condition requires the slope to reduce significantly ($\phi'(h) \leq c_2 \phi'(0)$). One can think the first condition gives an upper bound on h while the second condition gives a lower bound on h . In general, a step size satisfying the Wolfe conditions will be larger than the step size $h = \frac{1}{L}$. In particular, one can show the following.

Exercise 2.20. Suppose f is μ -strongly convex and has L -Lipschitz gradient. If a step size h satisfies the Wolfe condition with respect to the direction $p = -\nabla f(x)$, then show that

$$\frac{2(1 - c_1)}{\mu} \geq h \geq \frac{1 - c_2}{L}.$$

As a corollary, we have that the function value progress given by such step is $\Omega(\|\nabla f(x)\|^2/L)$. Therefore, this gives the same guarantee Theorem 2.9 and Theorem 2.14. A common way to implement this is via a backtracking line search. The algorithm starts with a large step size and decreases it by a constant factor if the Wolfe conditions are violated. For gradient descent, the next step involves exactly computing $\nabla f(x + hp)$ and hence if our line search accepts the step size immediately, the line search almost costs nothing extra. Therefore, if we maintain a step size throughout the algorithm and decreases it only when it violates the condition, the total cost of the line search will be only an additive logarithmic number of gradient calls throughout the algorithm and is negligible.

Finally, we note that for problems of the form $f(x) = \sum_i f_i(a_i^\top x)$, the bottleneck is often in computing Ax . In this case, exact line search is almost free because we can store the vectors Ax and Ah .

■ 2.6 Generalizing Gradient Descent*

Here we study properties of gradient descent that were actually used for the strongly convex case. There are many ways to generalize this case. One way is to view gradient descent as approximating the function f

by splitting it into two terms, one is the first-order approximation and the second is just a squared ℓ_2 norm. More generally, we can split a function into two terms, one that is easy to optimize and another that we need to approximate with some error. More precisely, we consider the following

Definition 2.21. We say $g + h$ is an α -approximation to f at the point x if

- g is convex, with the same value as f at x , i.e., $g(x) = f(x)$,
- $h(x) = 0$ and $h((1 - \alpha)x + \alpha\hat{x}) \leq \alpha^2 h(\hat{x})$ for all \hat{x} ,
- $g(y) + \alpha h(y) \leq f(y) \leq g(y) + h(y)$ for all y .

To understand this assumption, we note that if f is μ -strongly convex with L -Lipschitz gradient, then for any x , we can use $\alpha = \frac{\mu}{L}$ and

$$g(y) = f(x) + \langle \nabla f(x), y - x \rangle,$$

$$h(y) = \frac{L}{2} \|y - x\|^2.$$

The condition requires h converging to 0 quadratically when $y \rightarrow x$.

Now, we consider the following algorithm:

Algorithm 3: GeneralizedGradientDescent

Input: Initial point $x^{(0)} \in \mathbb{R}^n$, approximation factor $\alpha > 0$.

for $k = 0, 1, \dots$ **do**

 Find an α -approximation of f at $x^{(k)}$ given by $g^{(k)}(x) + h^{(k)}(x)$.
 $x^{(k+1)} \leftarrow \arg \min_y g^{(k)}(y) + h^{(k)}(y)$.

end

Theorem 2.22. Suppose we are given a convex function f such that we can find an α -approximation at any x . Let x^* be any minimizer of f . Then the sequence $x^{(k)}$ in **GeneralizedGradientDescent** satisfies

$$f(x^{(k)}) - f(x^*) \leq (1 - \alpha)^k (f(x^{(0)}) - f(x^*)).$$

Proof. Using the fact that $g^{(k)} + h^{(k)}$ is an upper bound on f , we have that our progress on f is larger than the best possible progress on $g^{(k)} + h^{(k)}$:

$$f(x^{(k+1)}) \leq \min_y g^{(k)}(y) + h^{(k)}(y).$$

To bound the best possible progress, i.e., the RHS above, we consider $\hat{x} = \arg \min_y g^{(k)}(y) + \alpha h^{(k)}(y)$ and $z = (1 - \alpha)x^{(k)} + \alpha\hat{x}$. We have that

$$\begin{aligned} \min_y g^{(k)}(y) + h^{(k)}(y) &\leq g^{(k)}(z) + h^{(k)}(z) \\ &\leq (1 - \alpha)g^{(k)}(x^{(k)}) + \alpha g^{(k)}(\hat{x}) + \alpha^2 h^{(k)}(\hat{x}) \\ &\leq (1 - \alpha)g^{(k)}(x^{(k)}) + \alpha(g^{(k)}(x^*) + \alpha h^{(k)}(x^*)) \end{aligned}$$

where we used $g^{(k)}$ is convex and the assumption on h in the second inequality, we used \hat{x} minimizes $g^{(k)} + \alpha h^{(k)}$.

Combining both and using the fact that $g^{(k)} + \alpha h^{(k)}$ is a lower bound on f , we have

$$f(x^{(k+1)}) \leq (1 - \alpha)f(x^{(k)}) + \alpha f(x^*).$$

This gives the result. □

Although Theorem 2.22 looks weird, it captures many well-known theorems. Here we list some of them.

Exercise 2.23. Show that the second condition in the definition of α -approximation can be replaced by

$$g(y) + \alpha h(y/\alpha) \leq f(y) \leq g(y) + h(y)$$

while maintaining the guarantee for the convergence of generalized GD.

Projected Gradient Descent / Proximal Gradient Descent

Given a convex set K , a μ -strongly convex function f with L -Lipschitz gradient, we consider the problem

$$\min_{x \in K} f(x).$$

To apply Theorem 2.22 to $F(x) \stackrel{\text{def}}{=} f(x) + \delta_K(x)$, for any x , we consider the functions

$$\begin{aligned} g(y) &= f(x) + \langle \nabla f(x), y - x \rangle + \delta_K(y), \\ h(y) &= \frac{L}{2} \|y - x\|_2^2. \end{aligned}$$

Note that $g+h$ is a $\frac{\mu}{L}$ -approximation to F . Theorem 2.22 shows the `GeneralizedGradientDescent` converges in $O(\frac{L}{\mu} \log(1/\epsilon))$ steps where each step involves solving the problem

$$\min_{y \in K} f(x) + \langle \nabla f(x), y - x \rangle + \frac{L}{2} \|y - x\|_2^2.$$

More generally, this works for problems of the form

$$\min_x f(x) + \phi(x)$$

for some convex function $\phi(x)$. Theorem 2.22 requires us to solve a sub-problem of the form

$$\min_y f(x) + \langle \nabla f(x), y - x \rangle + \frac{L}{2} \|y - x\|_2^2 + \phi(y).$$

ℓ^p Regression

One can apply this framework for optimizing ℓ^p regression $\min_x \|Ax - b\|_p^p$. For example, one can approximate the function $f(x) = x^p$ by $g(y) = x^p + px^{p-1}(y - x)$ and $h(y) = p2^{p-1}(x^{p-2}(y - x)^2 + (y - x)^p)$. Using this, one can show that one can solve the problem

$$\min_x \|Ax - b\|_p^p$$

using the problem

$$\min_y v^\top y + \|DA(y - x)\|_2^2 + \|A(y - x)\|_p^p \quad (2.4)$$

for some vector v and some diagonal matrix D . One can show that Theorem 2.22 only need to solve the sub-problem approximately. Therefore, this shows that one can solve ℓ^p regression with $\log(1/\epsilon)$ convergence by solving mixed $\ell_2 + \ell_p$ regression approximately.

Other assumptions

For some special cases, it is possible to analyze this algorithm without convexity. One prominent application is compressive sensing:

$$\min_{\|x\|_0 \leq k} \|Ax - b\|_2^2.$$

For matrices A satisfying restricted isometry property, one can apply `GeneralizedGradientDescent` to solve the problem with the splitting $g(x) = 2A^\top(Ax - b) + \delta_{\|x\|_0 \leq k}$ and $h(x) = \|x\|^2$. In this case, the algorithm is called iterative hard-thresholding [10] and the sub-problem has a closed form expression.

Exercise 2.24. Give the closed form solution for the sub-problem given by the splitting above.

■ 2.7 Gradient Flow

In continuous time, gradient descent follows the Ordinary Differential Equation (ODE)

$$\frac{dx_t}{dt} = -\nabla f(x_t).$$

This can be viewed as the canonical continuous algorithm. Finding the right discretization has led to many fruitful research directions. One benefit of the continuous view is to simplify some calculations. For example, for strongly convex f , Theorem 2.14 now becomes

$$\frac{d}{dt}(f(x_t) - f(x^*)) = \nabla f(x_t)^\top \frac{dx_t}{dt} = -\|\nabla f(x_t)\|_2^2 \leq -2\mu(f(x_t) - f(x^*))$$

where we used Lemma 2.13 at the end. Solving this differential inequality, we have

$$f(x_t) - f(x^*) \leq e^{-2\mu t}(f(x_0) - f(x^*)).$$

Without the strong convexity assumption, gradient flow can behave wildly. For example, the length of the gradient flow can be exponential in d on a unit ball [56].

We emphasize that this continuous view is mainly useful for understanding, indicative of but not necessarily implying an algorithmic result. In some cases, effective algorithmic results can be obtained simply by discretizing time in the gradient flow. The study of such numerical methods and their convergence properties is its own field, and well-known basic methods include the forward Euler method (which results in the basic version of GD), the *backward* Euler method, the Implicit Midpoint method and Runge-Kutta methods. We will see that gradient flow and its discretization also play an important role in the development of sampling algorithms.

■ 2.8 Discussion

Convex optimization by variants of gradient descent is a very active field with an increasing number of applications. Often, methods that are provable for the convex setting are applied as heuristics to nonconvex problems as well, most notably in deep learning. This is one of the principal features of GD, its wide applicability as an algorithmic paradigm.

Researchers are also using GD to get provably faster algorithms for classical problems. For example, [2] and [40] applied the decomposition of Eqn. (2.4) to obtain fast algorithms for ℓ^p regression and the ℓ^p flow problem. [36] showed that the ℓ^p flow problem can be used as a subroutine to solve uncapacitated maximum flow problem in $m^{4/3+o(1)}$ time. Instead of assuming $h(x)$ converges to 0 quadratically, [55] proved Theorem 2.22 assuming h is given by some divergence function and showed its applications in D-optimal design.

■ 3.1 Cutting Plane Methods

The goal of this chapter is to present some polynomial-time algorithms for convex optimization. These algorithms use knowledge of the function in a minimal way, essentially by querying the function value along with weak bounds on its support and range.

Given a continuously differentiable convex function f , Theorem 1.9 shows that

$$f(y) \geq f(x) + \langle \nabla f(x), y - x \rangle \text{ for all } y. \quad (3.1)$$

Let x^* be any minimizer of f . Replacing y with x^* , we have that

$$f(x) \geq f(x^*) \geq f(x) + \langle \nabla f(x), x^* - x \rangle.$$

Therefore, we know that $\langle \nabla f(x), x^* - x \rangle \leq 0$. Namely, x^* lies in a halfspace H with normal vector $-\nabla f(x)$. Roughly speaking, this shows that each gradient computation cuts the set of possible solutions in half. In one dimension, this allows us to do a binary search to minimize convex functions.

It turns out that in \mathbb{R}^n , binary search still works. In this chapter, we will cover several ways to do this binary search. All of them follow the same framework, called the *cutting plane method*. In this method, the convex set or function of interest is given by an oracle, typically a *separation oracle* (for definitions in a broader context, see Defs. 4.2 and 4.8 in the next chapter): for any $x \notin K \subseteq \mathbb{R}^n$, the oracle finds a vector $g(x) \in \mathbb{R}^n$ such that

$$g(x)^\top (y - x) \leq 0 \text{ for all } y \in K.$$

Cutting plane methods address the following class of problems.

Problem 3.1 (Finding a point in a convex set). Given $\epsilon > 0$, $R > 0$, and a convex set $K \subseteq R \cdot B^n$ specified by a separation oracle, find a point $y \in K$ or conclude that $\text{vol}K \leq \epsilon^n$. The complexity of an algorithm is measured by the number of calls to the oracle and the number of arithmetic operations.

Remark. To minimize a convex function, we set $g(x) = \nabla f(x)$ and K to be the set of (approximate) minimizers of f . In Section 3.3, we relate the problem of proving that $\text{vol}(K)$ is small to the problem of finding an approximate minimizer of f .

In this framework, we maintain a convex set $E^{(k)}$ that contains the set K . In each iteration, we choose some $x^{(k)}$ based on $E^{(k)}$ and query the oracle for $g(x^{(k)})$. The guarantee for $g(\cdot)$ implies that K lies in the halfspace

$$H^{(k)} = \{y : g(x^{(k)})^\top (y - x^{(k)}) \leq 0\}$$

and hence $K \subset H^{(k)} \cap E^{(k)}$. The algorithm continues by choosing $E^{(k+1)}$ to be a convex set that contains $H^{(k)} \cap E^{(k)}$.

Algorithm 4: CuttingPlaneFramework**Input:** Initial set $E^{(0)} \subseteq \mathbb{R}^n$ containing K .**for** $k = 0, \dots$ **do** Choose a point $x^{(k)} \in E^{(k)}$. **if** $E^{(k)}$ is “small enough” **then return** $x^{(k)}$; Find $E^{(k+1)} \supset E^{(k)} \cap H^{(k)}$ where

$$H^{(k)} \stackrel{\text{def}}{=} \{x \in \mathbb{R}^n \text{ such that } g(x^{(k)})^\top (x - x^{(k)}) \leq 0\}. \quad (3.2)$$

end

To analyze the algorithm, the main questions we need to answer are:

1. How do we choose $x^{(k)}$ and $E^{(k+1)}$?
2. How do we measure progress?
3. How quickly does the method converge?
4. How expensive is each step?

Progress on the cutting plane method is shown in the next table.

Year	$E^{(k)}$ and $x^{(k)}$	Iter	Cost/Iter
1965 [45, 58]	Center of gravity	n	n^n
1979 [78, 65, 38]	Center of ellipsoid	n^2	n^2
1988 [37]	Center of John ellipsoid	n	$n^{2.878}$
1989 [71]	Volumetric center	n	$n^{2.378}$
1995 [7]	Analytic center	n	$n^{2.378}$
2004 [9]	Center of gravity	n	n^4
2015 [43]	Hybrid center	n	n^2 (amortized)
2020 [30]	Volumetric center	n	n^2 (amortized)

Table 3.1: Different Cutting Plane Methods. Omitted polylogarithmic terms. The number of iterations follows from the rate.

■ 3.2 Ellipsoid Method

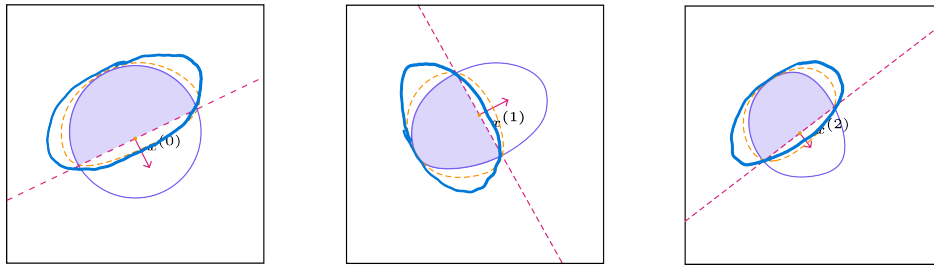


Figure 3.1: Ellipsoid Method

We start by explaining the Ellipsoid method. The algorithm maintains an ellipsoid

$$E^{(k)} \stackrel{\text{def}}{=} \{y \in \mathbb{R}^n : (y - x^{(k)})^\top (A^{(k)})^{-1} (y - x^{(k)}) \leq 1\}$$

that contains K and becomes smaller in volume in each step. Note that for this to be an ellipsoid the matrix $A^{(k)}$ must be symmetric PSD. After we compute $g(x^{(k)})$ and $H^{(k)}$ via (3.2), we define $E^{(k+1)}$ to be the smallest volume ellipsoid containing $E^{(k)} \cap H^{(k)}$. The key observation is that the volume of the ellipsoid $E^{(k)}$ decreases by a factor of $1 - \Theta(\frac{1}{n})$ every iteration. This volume property holds for any halfspace through the

center of the current ellipsoid (not only for the one whose normal is the gradient), a property we will exploit in the next chapter.

Algorithm 5: Ellipsoid

Input: Initial ellipsoid $E^{(0)} = \{y \in \mathbb{R}^n : (y - x^{(0)})^\top (A^{(0)})^{-1} (y - x^{(0)}) \leq 1\}$.
for $k = 0, \dots$ **do**
 if $E^{(k)}$ *is “small enough” or Oracle says YES* **then return** $x^{(k)}$;
 $x^{(k+1)} = x^{(k)} - \frac{1}{n+1} \frac{A^{(k)} g(x^{(k)})}{\sqrt{g(x^{(k)})^\top A^{(k)} g(x^{(k)})}}$.
 $A^{(k+1)} = \frac{n^2}{n^2-1} \left(A^{(k)} - \frac{2}{n+1} \frac{A^{(k)} g(x^{(k)}) g(x^{(k)})^\top A^{(k)}}{g(x^{(k)})^\top A^{(k)} g(x^{(k)})} \right)$.
end

Remark 3.2. We usually obtain $g(x)$ from a *separation oracle*.

Lemma 3.3. *For the Ellipsoid method (Algorithm 5), we have*

$$\text{vol} E^{(k+1)} < e^{-\frac{1}{2n+2}} \text{vol} E^{(k)} \quad \text{and} \quad E^{(k)} \cap H^{(k)} \subset E^{(k+1)}.$$

Remark 3.4. Note that the proof below also shows that $\text{vol} E^{(k+1)} = e^{-\Theta(\frac{1}{n})} \text{vol} E^{(k)}$. Therefore, the ellipsoid method does not run faster even for any function, e.g., a linear function, making it provably “slow” in practice.

Proof. Note that the ratio of $\text{vol} E^{(k+1)} / \text{vol} E^{(k)}$ does not change under any affine transformation, and neither does set containment. Therefore, we can do a transformation so that $A^{(k)} = I$, $x^{(k)} = 0$ and $v(x^{(k)}) = e_1$. Therefore $H^{(k)}$ is simply the halfspace $\{x : x_1 \leq 0\}$. This simplifies our calculation. We need to prove two statements: $\text{vol} E^{(k+1)} < e^{-\frac{1}{2n+2}} \text{vol} E^{(k)}$ and that $E^{(k)} \cap H^{(k)} \subset E^{(k+1)}$.

Claim 1: $\text{vol} E^{(k+1)} < e^{-\frac{1}{2(n+1)}} \text{vol} E^{(k)}$.

Note that since $v(x^{(k)}) = e_1$, we have $A^{(k+1)} = \frac{n^2}{n^2-1} \left(I - \frac{2}{n+1} e_1 e_1^\top \right)$. Therefore, we have that

$$\begin{aligned} \left(\frac{\text{vol} E^{(k+1)}}{\text{vol} E^{(k)}} \right)^2 &= \left| \frac{\det A^{(k+1)}}{\det A^{(k)}} \right| = \left(\frac{n^2}{n^2-1} \right)^n \det \left(I - \frac{2}{n+1} e_1 e_1^\top \right) \\ &= \left(\frac{n^2}{n^2-1} \right)^{n-1} \frac{n^2}{n^2-1} \left(\frac{n-1}{n+1} \right) \\ &= \left(1 + \frac{1}{n^2-1} \right)^{n-1} \left(1 - \frac{1}{n+1} \right)^2 \\ &< \exp\left(\frac{n-1}{n^2-1} - \frac{2}{n+1} \right) = \exp\left(-\frac{1}{n+1} \right) \end{aligned}$$

where we used $1+x \leq e^x$ for all x .

Claim 2. $E^{(k)} \cap H^{(k)} \subset E^{(k+1)}$.

By the definition of $E^{(k)}$ and the assumption $A^{(k)} = I$, we have

$$x^{(k+1)} = -\frac{e_1}{n+1}$$

and, for any $x \in E^{(k)} \cap H^{(k)}$, we have that $\|x\|_2 \leq 1$ and $x_1 \leq 0$. By direct computation, using the fact that

$$\left(I - \frac{2}{n+1} e_1 e_1^\top \right)^{-1} = \left(I + \frac{2}{n-1} e_1 e_1^\top \right)$$

we have

$$\begin{aligned} &\left(x + \frac{e_1}{n+1} \right)^\top \left(1 - \frac{1}{n^2} \right) \left(I + \frac{2}{n-1} e_1 e_1^\top \right) \left(x + \frac{e_1}{n+1} \right) \\ &= \left(1 - \frac{1}{n^2} \right) \left(\|x\|^2 + \frac{2x_1(1+x_1)}{n-1} + \frac{1}{n^2-1} \right) \\ &\leq \left(1 - \frac{1}{n^2} \right) \left(1 + 0 + \frac{1}{n^2-1} \right) = 1 \end{aligned}$$

where we used that $\|x\|_2 \leq 1$ and $x_1(1 + x_1) \leq 0$ (since $-1 \leq x_1 \leq 0$) at the end. This shows that $x \in E^{(k+1)}$. \square

Exercise 3.5. Show that the ellipsoid $E^{(k+1)}$ computed above is the minimum volume ellipsoid containing $E^{(k)} \cap H^{(k)}$.

Exercise 3.6. Suppose that we used a box instead of an ellipsoid. Could we ensure progress in each iteration? What about a simplex?

■ 3.3 From Volume to Function Value

Lemma 3.3 shows that the volume of a set containing all minimizers decreases by a constant factor every n steps. In general, knowing that the optimal x^* lies in a small volume set does not provide enough information to find a point with small function value. For example, if we only knew that x^* lies in the plane $\{x : x_1 = 0\}$, we would still need to search for x^* over an $n - 1$ dimensional space. However, if the set is constructed by the cutting plane framework (Algorithm 4), then we can guarantee that small volume implies that any point in the set has close to optimal function value.

This implies that we can minimize any convex function with ε additive error in $O(n^2 \log(1/\varepsilon))$ iterations. To make the statement more general, we note that the Ellipsoid method can be used for non-differentiable functions. In the next theorem, we allow for a general “progress” function and an arbitrary support Ω . The convergence argument works for any monotonic, scale-and-shift-invariant progress measure. To allow for non-differentiable convex functions, in place of gradient, we use the subgradient (see Sec. 1.6).

Theorem 3.7. Let $x^{(k)}$ be the sequence of points produced by the cutting plane framework (Algorithm 4) for a convex function f . Let \mathcal{V} be a mapping from subsets of \mathbb{R}^n to non-negative real numbers satisfying

1. (Linearity) For any set $S \subseteq \mathbb{R}^n$, any vector y and any scalar $\alpha \geq 0$, we have $\mathcal{V}(\alpha S + y) = \alpha \mathcal{V}(S)$ where $\alpha S + y = \{\alpha x + y : x \in S\}$.
2. (Monotonicity) For any set $T \subset S$, we have that $\mathcal{V}(T) \leq \mathcal{V}(S)$.

Then, for any set $\Omega \subseteq E^{(0)}$, with $\mathcal{V}(\Omega) > 0$, we have

$$\min_{i=1,2,\dots,k} f(x^{(i)}) - \min_{y \in \Omega} f(y) \leq \frac{\mathcal{V}(E^{(k)})}{\mathcal{V}(\Omega)} \cdot \left(\max_{z \in \Omega} f(z) - \min_{x \in \Omega} f(x) \right).$$

Remark 3.8. We can think $\mathcal{V}(E)$ as some way to measure the size of E . It can be radius, mean-width or any other way to measure “size”. For the ellipsoid method, we use $\mathcal{V}(E) = \text{vol}(E)^{\frac{1}{n}}$ for which we have proved volume decrease in Lemma 3.3. We raise the volume to power $1/n$ to satisfy linearity. Also note that we only guarantee that one of the previous query points has a small function value; of course we can simply use the point with minimum function value.

Proof. Let x^* be any minimizer of f over Ω . For any $\alpha > \frac{\mathcal{V}(E^{(k)})}{\mathcal{V}(\Omega)}$ and $S = (1 - \alpha)x^* + \alpha\Omega$, by the linearity of \mathcal{V} , we have that

$$\mathcal{V}(S) = \alpha \mathcal{V}(\Omega) > \mathcal{V}(E^{(k)})$$

Therefore, S is not a subset of $E^{(k)}$ and hence there is a point $y \in S \setminus E^{(k)}$. y is not in $E^{(k)}$. This means it is eliminated by the subgradient halfspace at some step $i \leq k$, namely for some $i \leq k$, we have (denoting the subgradient by ∇f),

$$\nabla f(x^{(i)})^\top (y - x^{(i)}) > 0.$$

By the convexity of f , it follows that $f(x^{(i)}) \leq f(y)$. Since $y \in S$, we have $y = (1 - \alpha)x^* + \alpha z$ for some $z \in \Omega$. Thus, the convexity of f implies that

$$f(x^{(i)}) \leq f(y) \leq (1 - \alpha)f(x^*) + \alpha f(z).$$

Therefore, we have

$$\min_{i=1,2,\dots,k} f(x^{(i)}) - \min_{x \in \Omega} f(x) \leq \alpha \left(\max_{z \in \Omega} f(z) - \min_{x \in \Omega} f(x) \right).$$

Since this holds for any $\alpha > \frac{\mathcal{V}(E^{(k)})}{\mathcal{V}(\Omega)}$, we have the result. \square

Combining Lemma 3.3 and Theorem 3.7, we have the following rate of convergence.

Theorem 3.9. *Let f be a convex function on \mathbb{R}^n , $E^{(0)}$ be any initial ellipsoid and $\Omega \subset E^{(0)}$ be any convex set. Suppose that for any $x \in E^{(0)}$, we can find, in time \mathcal{T} , a nonzero vector $g(x)$ such that*

$$f(y) \geq f(x) \text{ for any } y \text{ such that } g(x)^\top (y - x) \geq 0.$$

Then, we have

$$\min_{i=1,2,\dots,k} f(x^{(i)}) - \min_{y \in \Omega} f(y) \leq \left(\frac{\text{vol}(E^{(0)})}{\text{vol}(\Omega)} \right)^{\frac{1}{n}} \exp \left(-\frac{k}{2n(n+1)} \right) \left(\max_{z \in \Omega} f(z) - \min_{x \in \Omega} f(x) \right).$$

Moreover, each iteration takes $O(n^2 + \mathcal{T})$ time.

Remark 3.10. We note that for this rate of convergence (and hence the entire algorithm) to be polynomial, we need some bound on the range of the function value. This often follows from a bound on the diameter of the support.

Proof. Lemma 3.3 shows that the volume of the ellipsoid maintained decreases by a factor of $\exp(-\frac{1}{2n+2})$ in every iteration. Hence, $\text{vol}^{\frac{1}{n}}$ decreases by $\exp(-\frac{1}{2n(n+1)})$ every iteration. The bound follows by applying Theorem 3.7 with $\mathcal{V}(E) \stackrel{\text{def}}{=} \text{vol}(E)^{\frac{1}{n}}$. Using Theorem 3.7, we have

$$\begin{aligned} \min_{i=1,2,\dots,k} f(x^{(i)}) - \min_{y \in \Omega} f(y) &\leq \left(\frac{\text{vol}(E^{(k)})}{\text{vol}(\Omega)} \right)^{\frac{1}{n}} \left(\max_{z \in \Omega} f(z) - \min_{x \in \Omega} f(x) \right) \\ &\leq \left(\frac{\text{vol}(E^{(0)})}{\text{vol}(\Omega)} \right)^{\frac{1}{n}} \exp \left(-\frac{k}{2n(n+1)} \right) \left(\max_{z \in \Omega} f(z) - \min_{x \in \Omega} f(x) \right). \end{aligned}$$

Next, we note the proof of Theorem 3.7 only used the fact that one side of halfspace defined by the gradient has higher value. Therefore, we can replace the gradient with the vector $g(x)$.

To bound the time per iteration, note that we make one query to the separation oracle per iteration, and then compute the next Ellipsoid using the formulas in Algorithm 5. The most time-consuming operation is multiplying an $n \times n$ matrix by an n -vector, which has complexity $O(n^2)$. \square

This theorem can be used to solve many problems in polynomial time. As an illustration, we show how to solve linear programs to desired approximation in polynomial time here.

Theorem 3.11. *Given a linear program $\min_{x \in \Omega} c^\top x$ where $P = \{x: Ax \geq b\}$. Let the diameter of P be $R \stackrel{\text{def}}{=} \max_{x \in \Omega} \|x\|_2$ and its volume radius be $r = \text{vol}(\Omega)^{\frac{1}{n}}$. Then, we can find $x \in P$ for which*

$$c^\top x - \min_{y \in P} c^\top y \leq \varepsilon \cdot \left(\max_{y \in P} c^\top y - \min_{y \in P} c^\top y \right)$$

in $O(n^2(n^2 + \text{nnz}(A)) \log(\frac{R}{r\varepsilon}))$ time where $\text{nnz}(A)$ is the number of non-zero elements in A .

Remark 3.12. If the dimension n is constant, this algorithm is nearly linear time (linear in the number of constraints)!

Proof. For the linear program $\min_{Ax \geq b} c^\top x$, the function we want to minimize is

$$L(x) = c^\top x + \delta_{Ax \geq b}(x) \quad \text{where} \quad \delta_{Ax \geq b}(x) = \begin{cases} 0 & \text{if } a_i^\top x \geq b_i \text{ for all } i \\ +\infty & \text{otherwise.} \end{cases} \quad (3.3)$$

For this function L , we can use the separation oracle $v(x) = c$ if $Ax \geq b$ and $v(x) = -a_i$ if $a_i^\top x < b_i$. If there are many violated constraints, any one of them will do.

In this case, we can set $\Omega = P$. We can simply pick $E^{(0)}$ be the unit ball centered at 0 with radius R . We apply Theorem 3.9 to find x such that

$$c^\top x - \min_{y \in P} c^\top y \leq \varepsilon \cdot (\max_{y \in P} c^\top y - \min_{y \in P} c^\top y)$$

in time $O(n^2(n^2 + \text{nnz}(A)) \log(\frac{R}{r\varepsilon}))$. Note that the complexity of computer a matrix-vector product Ax is $O(\text{nnz}(A))$. \square

Exercise 3.13. Give a bound on R as a polynomial in $n, \langle A \rangle, \langle b \rangle$, where $\langle A \rangle, \langle b \rangle$ are the numbers of bits needed to represent A, b whose entries are rationals.

To get the solution exactly, i.e., $\varepsilon = 0$, we need to assume the linear program has integral (or rational) coefficients and then the running time will depend on the sizes of the numbers in the matrix A and in the vectors b and c . It is still open how to solve linear programs in time bounded by a polynomial in only the number of variables and constraints (and not the bit sizes of the coefficients). Such a running time is called *strongly polynomial*.

Open Problem. Can we solve linear programs in strongly polynomial time?

■ 3.4 Center of Gravity Method

In the Ellipsoid method, we used an ellipsoid as the current set, and its center as the next query point.

In the center of gravity method, we start with any bounded convex set containing a minimizer, e.g., a large enough cube, and the set maintained is simply the intersection of all halfspaces used so far with the original set. The query point will be the center of gravity (or barycenter) of the current set. Recall that the center of gravity of a bounded set is the average of points in the set, i.e.,

$$z_K = \frac{1}{\text{vol}(K)} \int_K x \, dx.$$

The measure of progress will once again be the volume (or more precisely, volume radius) of the current set.

It is clear that the volume can only decrease in each iteration. But at what rate? The following classical theorem shows that the volume of the convex body decreases by a constant factor (no more than $1 - \frac{1}{e}$) when using the exact center of gravity.

Theorem 3.14. [29] Let K be a convex body in \mathbb{R}^n with center of gravity z . Let H be any halfspace containing z . Then,

$$\text{vol}(K \cap H) \geq \left(\frac{n}{n+1} \right)^n \text{vol}(K).$$

Note that the constant on the RHS is at least $1/e$. We prove the theorem later in this chapter. Unfortunately, computing the center of gravity even of a polytope is #P-hard [62]. For the purpose of efficient approximations, it is important to establish a stable version of the theorem that does not require an exact center of gravity.

Recall that a nonnegative function is logconcave if its logarithm is concave, i.e., for any $x, y \in \mathbb{R}^n$ and any $\lambda \in [0, 1]$,

$$f(\lambda x + (1 - \lambda)y) \geq f(x)^\lambda f(y)^{1-\lambda}.$$

We refer to Section 1.7 for some background on logconcave functions. A distribution p is *isotropic* if the mean of a random variable drawn from the distribution is zero and the covariance is the identity matrix.

The randomized center of gravity method defined as follows:

Algorithm 6: RandomizedCenterOfGravity**Input:** Initial convex set $E^{(0)}$.**for** $k = 0, \dots$ **do** **if** $E^{(k)}$ is “small enough” **then return** $x^{(k)}$; Let $y^{(1)}, \dots, y^{(N)}$ be uniform random points from $E^{(k)}$ and set

$$x^{(k)} = \frac{1}{N} \sum_{i=1}^N y^{(i)}$$

$$E^{(k+1)} = E^{(k)} \cap H^{(k)}$$

 where $H^{(k)} \stackrel{\text{def}}{=} \{x \in \mathbb{R}^n : g(x^{(k)})^\top (x - x^{(k)}) \leq 0\}$ obtained by querying $g(x^{(k)})$.**end**

Remark 3.15. The question of how to sample (nearly) uniform random points is an important one that we will address in detail in this book. Using sampling to approximate the center of gravity leads to the reduction in the time per iteration from n^n to n^4 (Table 3.1).

To prove the convergence of the method, we will use a robust version of Theorem 3.14, which will give a similar result despite using only an approximate center of gravity.

Theorem 3.16 (Robust Grünbaum). *Let p be an isotropic logconcave distribution, namely $\mathbf{E}_{x \sim p} x = 0$ and $\mathbf{E}_{x \sim p} x^2 = 1$. For any unit vector $\theta \in \mathbb{R}^n$, $t \in \mathbb{R}$ we have*

$$\mathbf{P}_{x \sim p}(x^\top \theta \geq t) \geq \frac{1}{e} - |t|.$$

Proof. By taking the marginal with respect to the direction θ , we can assume the distribution is one-dimensional. Let $P(t) = \mathbf{P}_{x \sim p}(x^\top \theta \leq t)$. Note that $P(t)$ is the convolution of p and $1_{(-\infty, 0]}$. Hence, it is logconcave (Lemma 1.25). By some limit arguments, we can assume $P(-M) = 0$ and $P(M) = 1$ for some large enough M (to be rigorous, we do the proof below for finite M and a RHS $\epsilon(M)$ instead of zero, then take the limit $M \rightarrow \infty$). Since $\mathbf{E}_{x \sim p} x = 0$, we have that

$$\int_{-M}^M t \frac{dP(t)}{dt} dt = 0$$

Integration by parts gives that $\int_{-M}^M P(t) dt = M$. Note that $P(t)$ is increasing logconcave, if $P(0)$ is too small, it would make $\int_{-M}^M P(t) dt$ too small. To be precise, since P is logconcave, i.e., $-\log P(t)$ is convex, and so we have,

$$-\log P(t) \geq -\log P(0) - \frac{\frac{d}{dt} P(0)}{P(0)} t.$$

Or we simply write $P(t) \leq P(0)e^{\alpha t}$ for some α . Hence,

$$M = \int_{-M}^M P(t) dt \leq \int_{-\infty}^{\frac{1}{\alpha}} P(0)e^{\alpha t} dt + \int_{1/\alpha}^M 1 dt = \frac{eP(0)}{\alpha} + M - \frac{1}{\alpha}.$$

This shows that $P(0) \geq \frac{1}{e}$.

Next, Lemma 3.17 shows that $\max_x p(x) \leq 1$. Therefore, the cumulative distribution P is 1-Lipschitz and we have

$$\mathbf{P}_{x \sim p}(x^\top \theta \geq t) \geq \mathbf{P}_{x \sim p}(x^\top \theta \geq 0) - t \geq \frac{1}{e} - t.$$

□

Lemma 3.17. *Let p be a one-dimensional isotropic logconcave density. Then $\max p(x) \leq 1$.*

For a proof of this (and for other properties of logconcave functions), we refer the reader to [54].

Exercise 3.18. Give a short proof that $\max_x p(x) = O(1)$ for any one-dimensional isotropic logconcave density.

Using the robust Grünbaum theorem 3.16, we get the following algorithm, which uses uniform random points from the current set. Obtaining such a random sample algorithmically is an interesting problem that we will study in the second part of this book.

Lemma 3.19. Suppose $y^{(1)}, \dots, y^{(N)}$ are i.i.d. uniform random points from a convex body K and $y = \frac{1}{N} \sum_{i=1}^N y^{(i)}$. Then for any halfspace H not containing y ,

$$\mathbf{E}(\text{vol}(K \cap H)) \leq \left(1 - \frac{1}{e} + \sqrt{\frac{n}{N}}\right) \text{vol}(K).$$

Proof. Without loss of generality, we assume that K is in isotropic position, i.e., $\mathbf{E}_K(y^{(i)}) = 0$ and $\mathbf{E}_K(y^{(i)}(y^{(i)})^\top) = I$. Then we have $\mathbf{E}(y) = 0$ and

$$\mathbf{E} \|y\|^2 = \frac{1}{N^2} \mathbf{E} \sum_{i=1}^N \|y^{(i)}\|^2 = \frac{1}{N} \mathbf{E} \|y^{(1)}\|^2 = \frac{n}{N}.$$

Therefore,

$$\mathbf{E} \|y\| \leq \sqrt{\mathbf{E} (\|y\|^2)} = \sqrt{\frac{n}{N}}.$$

Thus, we can apply Theorem 3.16 with $t = \sqrt{\frac{n}{N}}$ to bound $\mathbf{E}(\text{vol}(K \cap H))/\text{vol}(K)$. \square

Theorem 3.7 readily gives the following guarantee for convex optimization, again using volume radius as the measure of progress.

Theorem 3.20. Let f be a convex function on \mathbb{R}^n , $E^{(0)}$ be any initial set and $\Omega \subset E^{(0)}$ be any convex set. Suppose that for any $x \in E^{(0)}$, we can find a nonzero vector $g(x)$ such that

$$f(y) \geq f(x) \text{ for any } y \text{ such that } g(x)^\top (y - x) \geq 0.$$

Then, for the center of gravity method with $N = 10n$, we have

$$\mathbf{E} \left(\min_{i=1,2,\dots,k} f(x^{(i)}) \right) - \min_{y \in \Omega} f(y) \leq \left(\frac{\text{vol}(E^{(0)})}{\text{vol}(\Omega)} \right)^{\frac{1}{n}} (0.95)^{\frac{k}{n}} \left(\max_{z \in \Omega} f(z) - \min_{x \in \Omega} f(x) \right).$$

Now we give a geometric proof of Theorem 3.14. Note that one can modify the proof of Theorem 3.16 to get another proof.

Proof. Since affine transformations do not affect ratios of volumes, without loss of generality, assume that the center of gravity of K is the origin and H is the halfspace $\{x : x_1 \leq 0\}$. For each point $t \in \mathbb{R}$, let $A(t) = K \cap \{x : x_1 = t\}$ be the $(n-1)$ -dimensional slice of K with $x_1 = t$. Define $r(t)$ as the radius of the $(n-1)$ -dimensional ball with the same $(n-1)$ -dimensional volume as $A(t)$.

The goal of the proof is to show that the smallest possible halfspace volume is achieved for a cone by a cut perpendicular to its axis. In the first step, we will symmetrize K as follows: replace each cross-section $A(t)$ by a ball of the same volume, centered at $(t, 0, \dots, 0)^T$. We claim that the resulting rotationally symmetric body is convex. To see this, note that all we have to show is that the radius function $r(t)$ is concave. For any $s, t \in \mathbb{R}$, and any $\lambda \in [0, 1]$, we have by convexity of K that

$$\lambda A(s) + (1 - \lambda) A(t) \subseteq A(\lambda s + (1 - \lambda)t)$$

and by the Brunn-Minkowski theorem (Theorem 1.27) applied to $A(s), A(t)$, the function $\text{vol}_{n-1}(A(s))^{1/(n-1)}$ is a concave function and so we have

$$\text{vol}_{n-1}(A(\lambda s + (1 - \lambda)t))^{1/(n-1)} \geq \lambda \text{vol}_{n-1}(A(s))^{1/(n-1)} + (1 - \lambda) \text{vol}_{n-1}(A(t))^{1/(n-1)}.$$

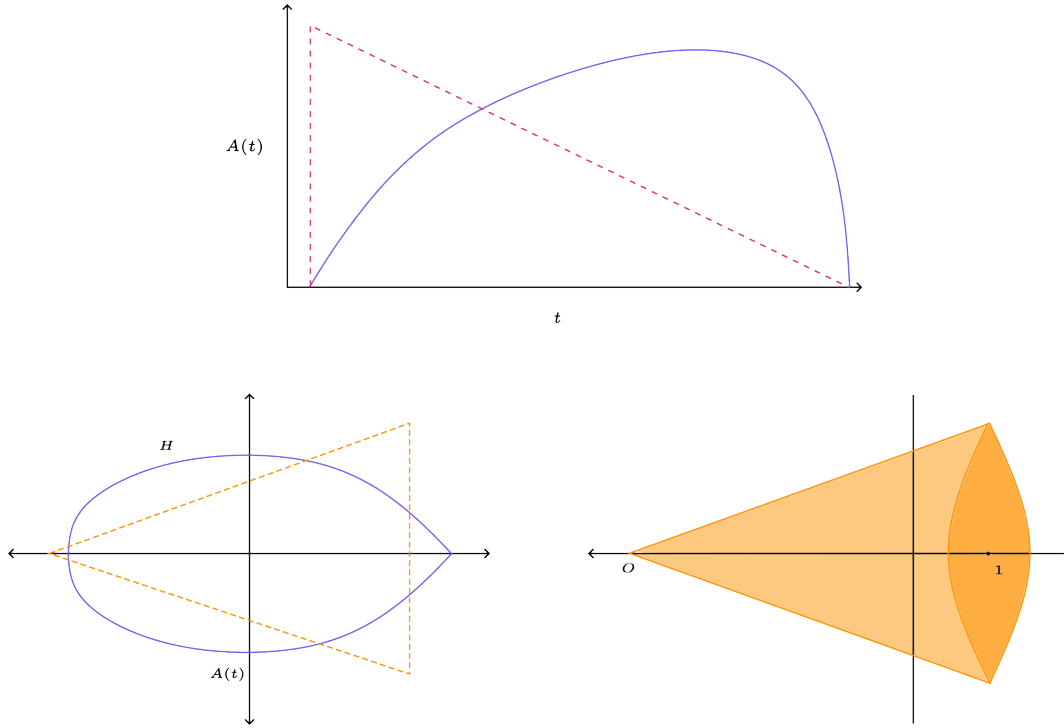


Figure 3.2: Affine transformations for Centre of Gravity method

From this and the definition of $r(t)$, it follows that

$$r(\lambda s + (1 - \lambda)t) \geq \lambda r(s) + (1 - \lambda)r(t)$$

as desired.

Next consider the subset $K_1 = K \cap \{x : x_1 \leq 0\}$. We replace this subset with a cone C having the same base $A(0)$ and apex at some point along the e_1 axis so that the volume of the cone is the same as $\text{vol}(K_1)$. Using the concavity of the radial function, this transformation can only decrease the center of gravity along e_1 . Therefore, proving a lower bound on the transformed body K_1 will give a lower bound for K . So assume we do this and the center of gravity is the origin. Next, extend the cone to the right, so that it remains a rotational cone, and the volume in the positive halfspace along e_1 is the same as $\text{vol}(K \setminus K_1)$. Once again, the center of gravity can only move to the left, and so the volume of K_1 can only decrease by this transformation. At the end we have shown that the lower bound for any convex body follows by proving for a rotational cone with axis along the normal to the halfspace. The intersection of this cone with the halfspace is the original cone scaled down by the ratio of the distance from the apex to the center of gravity, to the height of the cone. So all that remains to be done is to compute the relative distance of the center of gravity from the apex, which is exactly $n/(n+1)$. Now we compute the volume ratio:

$$\frac{\text{vol}(K_1)}{\text{vol}(K)} = \left(\frac{n}{n+1} \right)^n.$$

□

Exercise 3.21. Show that for a cone of height h in \mathbb{R}^n , i.e., the convex hull of a convex body $K \subset \mathbb{R}^{n-1}$ with a single point $a \in \mathbb{R}^n$ at distance h from the hyperplane H containing K , the distance of the center of gravity z of the cone is at distance $h/(n+1)$ from H .

To conclude this section, we note that the number of separation oracle queries made by the center-of-gravity cutting plane method is asymptotically the best possible.

Theorem 3.22. *Any algorithm that solves Problem 3.1 using a separation oracle needs to make $\Omega(n \log(R/\epsilon))$ queries to the oracle.*

Proof. Suppose K is a cube of side length ϵ contained in the cube $[0, R]^n$. Imagine a tiling of the big cube by cubes of side length ϵ . Consider the oracle that always returns an axis parallel halfspace that does not cut any little cube and contains at least half of the volume of the “remaining” region, i.e., the set given by the original cube intersected with all halfspaces given by the oracle so far. This is always possible since for any halfspace either the halfspace or its complement will contain at least half the volume of any set. Thus each query at best halves the remaining volume. To solve the problem, the algorithm needs to cut down to a set of volume ϵ^n starting from a set of volume R^n . Thus it needs at least $n \log_2(R/\epsilon)$ queries. \square

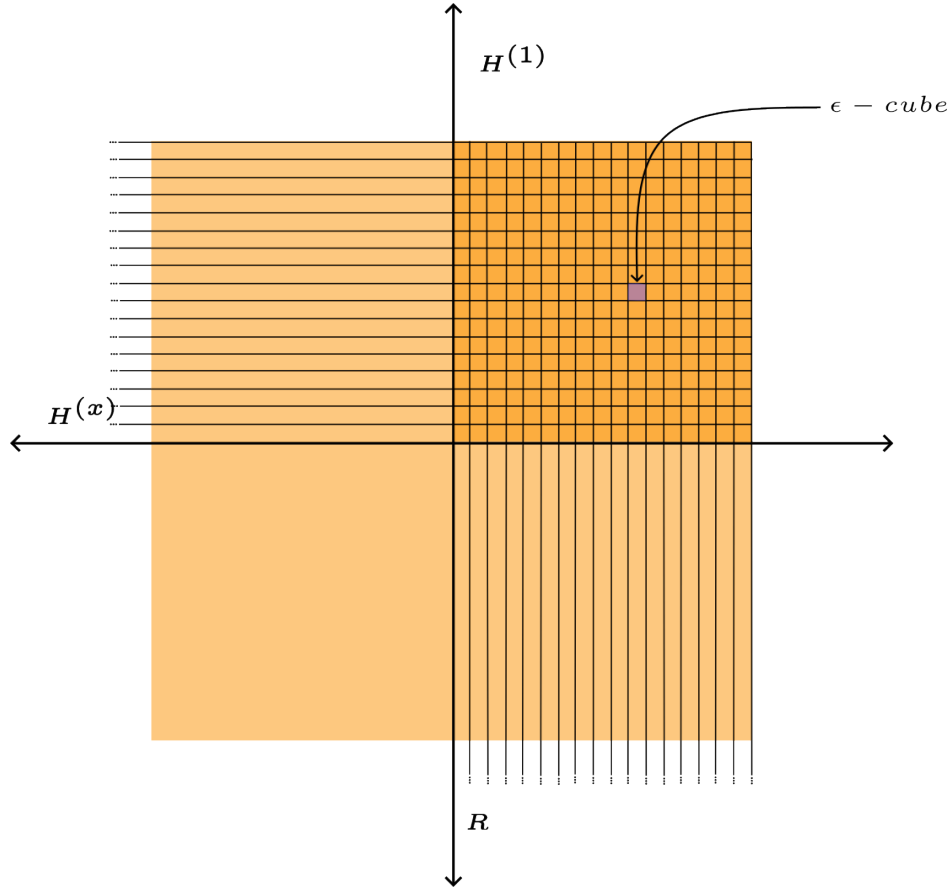


Figure 3.3: Complexity using a separation oracle

Discussion

In later chapters we will see how to implement each iteration of the center of gravity method in polynomial time. Computing the exact center of gravity is #P-hard even for a polytope [62], but we can find an arbitrarily close approximation in randomized polynomial time via sampling. The method generalizes to certain noisy computation models, e.g., when the oracle reports a function value that is within a bounded additive error, i.e., a noisy function oracle.

■ 3.5 Sphere and Parabola Methods

In Section 2.2, we proved that gradient descent converges at the rate $(1 - \frac{\mu}{L})^k$ in function value assuming the function satisfies $\mu \cdot I \preceq \nabla^2 f(x) \preceq L \cdot I$ for all x . Hence, if $\frac{L}{\mu}$ is not too large, this rate of decrease of the function value can be much better than the $(1 - \frac{1}{n^2})^k$ rate of the ellipsoid method or the $(1 - \frac{1}{n})^k$ rate of the center of gravity method (recall that the convergence rate in function value is n times slower than the convergence rate in volume). In this section, we show how to modify the ellipsoid method to get a faster convergence rate when $\frac{L}{\mu}$ is small. One can view this whole section as just an interpretation of accelerated gradient descent (which we haven't seen yet) in the cutting plane framework. In a later section, we will give another interpretation.

■ 3.5.1 Sphere Method

We have been using convexity to find a halfspace containing the optimum with the current point on its boundary. For a strongly convex function, any optimal x^* is contained in a strictly smaller region than a halfspace. In particular, we have

$$f(x^*) \geq f(x) + \nabla f(x)^\top (x^* - x) + \frac{\mu}{2} \|x^* - x\|_2^2.$$

Completing the square, we have that

$$\frac{\mu}{2} \left\| (x^* - x) + \frac{1}{\mu} \nabla f(x) \right\|_2^2 - \frac{\|\nabla f(x)\|_2^2}{2\mu} \leq -(f(x) - f(x^*))$$

Using $x^+ \stackrel{\text{def}}{=} x - \frac{1}{L} \nabla f(x)$ and $x^{++} \stackrel{\text{def}}{=} x - \frac{1}{\mu} \nabla f(x)$, we can write

$$\|x^* - x^{++}\|_2^2 \leq \frac{\|\nabla f(x)\|_2^2}{\mu^2} - \frac{2}{\mu} (f(x) - f(x^*)). \quad (3.4)$$

To use this formula in the cutting plane framework, we need a crude upper bound on $f(x^*)$. One can simply use $f(x^*) \leq f(x)$. Or, we can use Lemma 2.7 and get

$$f(x^*) \leq f(x^+) \leq f(x - \frac{1}{L} \nabla f(x)) \leq f(x) - \frac{1}{2L} \|\nabla f(x)\|_2^2.$$

Putting it into (3.4), we see that

$$\begin{aligned} \|x^* - x^{++}\|_2^2 &\leq \frac{1}{\mu^2} \left(\|\nabla f(x)\|_2^2 - 2\mu \cdot (f(x) - f(x^*)) \right) \\ &\leq \frac{1}{\mu^2} \left(\|\nabla f(x)\|_2^2 - 2\mu \cdot (f(x) - f(x^+)) \right) - \frac{2}{\mu} (f(x^+) - f(x^*)) \\ &\leq \frac{1}{\mu^2} \left(\|\nabla f(x)\|_2^2 - 2\mu \cdot \frac{1}{2L} \|\nabla f(x)\|_2^2 \right) - \frac{2}{\mu} (f(x^+) - f(x^*)) \\ &\leq \frac{(1 - \frac{\mu}{L})}{\mu^2} \|\nabla f(x)\|_2^2 - \frac{2}{\mu} (f(x^+) - f(x^*)). \end{aligned} \quad (3.5)$$

Therefore, using the trivial bound of zero for the second term on the RHS, x^* lies in a ball centered at x^{++} with radius at most

$$\sqrt{1 - \frac{\mu}{L}} \cdot \frac{\|\nabla f(x)\|_2}{\mu}. \quad (3.6)$$

This suggests using balls instead of ellipsoids in a cutting plane algorithm; it would certainly be more efficient to maintain!

We arrive at the following algorithm.

Algorithm 7: SphereMethod

Input: Initial point $x^{(0)} \in \mathbb{R}^n$, strong convexity parameter μ , Lipschitz gradient parameter L .
 $Q^{(0)} \leftarrow \mathbb{R}^n$.
for $k = 0, \dots$ **do**
 Set $Q = \left\{ x \in \mathbb{R}^n : \left\| x - \left(x^{(k)} - \frac{1}{\mu} \nabla f(x^{(k)}) \right) \right\|_2^2 \leq \frac{1 - \frac{\mu}{L}}{\mu^2} \cdot \left\| \nabla f(x^{(k)}) \right\|_2^2 \right\}$.
 $Q^{(k+1)} \leftarrow \text{minSphere}(Q \cap Q^{(k)})$ where $\text{minSphere}(K)$ is the smallest sphere covering K .
 $x^{(k+1)} \leftarrow \text{center of } Q^{(k+1)}$.
end

To analyze **SphereMethod**, we need the following lemma, which is illustrated in Figure 3.4.

Lemma 3.23. *For any $g \in \mathbb{R}^n$ and $\epsilon \in (0, 1)$, we have $B(0, 1) \cap B(g, \|g\|_2 \sqrt{1 - \epsilon}) \subset B(x, \sqrt{1 - \epsilon})$ for some x .*

Proof. By symmetry, it suffices to consider the two-dimensional case, and to assume that $g = ae_1$. If $a \leq 1$, we can simply pick $x = g$. Otherwise, let $(x, 0)$ be the center of the smallest ball containing the required intersection, and y be its radius. (See Figure 3.4). We have $x^2 + y^2 = 1$ and $(x - a)^2 + y^2 = (1 - \epsilon)a^2$. This implies that

$$x = \frac{1 + \epsilon a^2}{2a}$$

and so

$$y^2 = 1 - \frac{\epsilon}{2} - \frac{1}{4a^2} - \frac{\epsilon^2 a^2}{4} \leq 1 - \epsilon$$

as claimed. \square

Lemma 3.24. *Let the measure of progress $\mathcal{V}(Q) = \text{radius}(Q)$. Then, we have that $x^* \in Q^{(k)}$ and $\mathcal{V}(Q^{(k+1)}) \leq \sqrt{1 - \frac{\mu}{L}} \cdot \mathcal{V}(Q^{(k)})$ for all k .*

Remark 3.25. The function value decrease follows from Theorem 3.7.

Proof Sketch. The fact $x^* \in Q^{(k)}$ follows directly from the definition of Q . For the decrease of radius, suppose that

$$Q^{(k)} = \left\{ x \in \mathbb{R}^n : \|x - x^{(k)}\| \leq R^{(k)} \right\}.$$

Then, the new ball is given by

$$Q^{(k+1)} = \text{minSphere} \left(\left\{ \left\| x - \left(x^{(k)} - \frac{1}{\mu} \nabla f(x^{(k)}) \right) \right\|_2^2 \leq \frac{1 - \frac{\mu}{L}}{\mu^2} \cdot \left\| \nabla f(x^{(k)}) \right\|_2^2 \right\} \cap \left\{ \|x - x^{(k)}\| \leq R^{(k)} \right\} \right).$$

To compute $\frac{\text{radius}(Q^{(k+1)})^2}{\text{radius}(Q^{(k)})^2}$, we can assume $x^{(k)} = 0$ and $R^{(k)} = 1$ and let $g = \frac{\nabla f(0)}{\mu}$. Hence, we have

$$Q^{(k+1)} = \text{minSphere} \left(\left\{ \|x - g\|_2^2 \leq \left(1 - \frac{\mu}{L}\right) \cdot \|g\|_2^2 \right\} \cap \left\{ \|x\| \leq 1 \right\} \right).$$

Now Lemma 3.23 (with $\epsilon = \frac{\mu}{L}$) shows that the $\text{radius}(Q^{(k+1)})^2 \leq 1 - \frac{\mu}{L}$. \square

Note that this gives the same convergence rate as gradient descent for strongly convex functions. Each iteration is much faster than the $O(n^2)$ time of the Ellipsoid method.

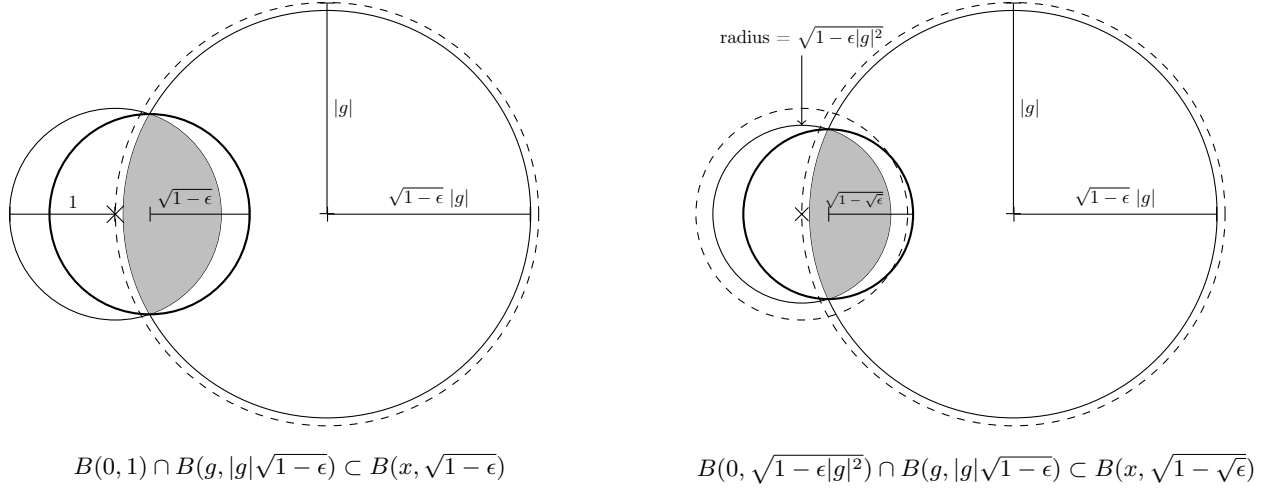


Figure 3.4: The left diagram shows the intersection shrinks at the same rate if only one of the ball shrinks; the right diagram shows the intersection shrinks much faster if two balls shrink at the same absolute amount.

■ 3.5.2 Parabola Method Via Epigraph

In previous sections, we have discussed cutting plane methods that maintain a region that contains the minimizer x^* of f . The proof of such a cutting plane method relies on the following inequality

$$f(x) > f(x^*) \geq f(x) + \langle \nabla f(x), x^* - x \rangle \quad (3.7)$$

Notice that the left-hand side is a strict inequality (unless we already solved the problem). We infer a halfspace containing the optimum using the subgradient at x , namely

$$\langle \nabla f(x), x^* - x \rangle \leq 0.$$

As the algorithm proceeds, we find a new point $x^{(\text{new})}$ such that $f(x^{(\text{new})}) < f(x)$. Therefore, the original inequality can be strengthened to

$$f(x^{(\text{new})}) > f(x) + \langle \nabla f(x), x^* - x \rangle$$

or

$$\langle \nabla f(x), x^* - x \rangle < -(f(x) - f(x^{(\text{new})})).$$

This suggests we should move earlier halfspaces and thereby reduce the measure of the next set. We expect merely updating the halfspaces can improve the convergence rate from $1 - \frac{\mu}{L}$ to $1 - \sqrt{\frac{\mu}{L}}$ because of the right diagram in Figure 3.4. An efficient way to manage all this information is to directly maintain a region that contains $(x^*, f(x^*))$. Now, we can view the inequality $f(y) \geq f(x) + \langle \nabla f(x), y - x \rangle$ as a cutting plane of the epigraph of f and we do not need to update previous cutting planes anymore.

The next algorithm is an epigraph cutting plane method.

Algorithm 8: ParabolaMethod

Input: Initial point $x^{(0)} \in \mathbb{R}^n$ and the strong convexity parameter μ .
 $q^{(0)}(y) \leftarrow -\infty$.
for $k = 0, \dots$ **do**
 Set $q^{(k+\frac{1}{2})}(y) = f(x^{(k)}) + \nabla f(x^{(k)})^\top (y - x^{(k)}) + \frac{\mu}{2} \|y - x^{(k)}\|^2$.
 Let $q^{(k+1)} = \text{maxParabola}(\max(q^{(k+\frac{1}{2})}, q^{(k)}))$ where $\text{maxParabola}(q)$ outputs the parabolic function p such that $p(x) \leq q(x)$ for all x , and p maximizes $\min_x p(x)$.
 // Alternatively, one can use $x^{(k+\frac{1}{2})} \leftarrow x^{(k)} - \frac{1}{L} \nabla f(x^{(k)})$ below.
 Let $x^{(k+\frac{1}{2})} = \text{lineSearch}(x^{(k)}, -\nabla f(x^{(k)}))$ where

$$\text{lineSearch}(x, y) = \operatorname{argmin}_{z=x+ty \text{ with } t \geq 0} f(z).$$

 Let $x^{(k+1)} = \text{lineSearch}(x^{(k+\frac{1}{2})}, c^{(k+1)} - x^{(k+\frac{1}{2})})$ where $c^{(k+1)}$ be the minimizer of $q^{(k+1)}(y)$.
end

As in gradient descent, to avoid using the parameter L , we do a line search from $x^{(k)}$ along the direction $\nabla f(x^{(k)})$. The subroutine `maxParabola` has an explicit formula [21].

Algorithm 9: $q = \text{maxParabola}(\max(q_a, q_b))$

Input: $q_A(x) = v_A + \frac{\mu}{2} \|x - c_A\|_2^2$ and $q_B(x) = v_B + \frac{\mu}{2} \|x - c_B\|_2^2$.
Compute $\lambda = \operatorname{proj}_{[0,1]} \left(\frac{1}{2} + \frac{v_A - v_B}{\mu \|c_A - c_B\|^2} \right)$.
 $c_\lambda = \lambda c_A + (1 - \lambda) c_B$.
 $v_\lambda = \lambda v_A + (1 - \lambda) v_B + \frac{\mu}{2} \lambda(1 - \lambda) \|c_A - c_B\|^2$.
Output: $q(x) = v_\lambda + \frac{\mu}{2} \|x - c_\lambda\|_2^2$.

Exercise 3.26. Show that the formula for `maxParabola` computes the optimal parabola.

The key fact we will be using from the formula is that when $0 < \lambda < 1$, we have

$$v_\lambda = v_A + \frac{\mu}{8} \frac{(\|c_A - c_B\|^2 + \frac{2}{\mu}(v_B - v_A))^2}{\|c_A - c_B\|^2}.$$

This says that the quadratic lower bound improves a lot whenever $\frac{\mu}{2} \|c_A - c_B\|^2 \gg v_B - v_A$ or $\frac{\mu}{2} \|c_A - c_B\|^2 \ll v_B - v_A$. Using this, we can analyze the `ParabolaMethod`.

Theorem 3.27. Assume that f is μ -strongly convex with L -Lipschitz gradient. Let $r_k = f(x^{(k)}) - \min_y q^{(k)}(y)$. Then, we have that

$$r_{k+1}^2 \leq (1 - \sqrt{\frac{\mu}{L}}) \cdot r_k^2.$$

In particular, we have that

$$f(x^{(k+1)}) - f^* \leq \frac{1}{2\mu} (1 - \sqrt{\frac{\mu}{L}})^k \|\nabla f(x^{(0)})\|^2.$$

Remark 3.28. Note that the squared radius of $\{y : q^{(k)}(y) = f(x^{(k)})\}$ is $\frac{2}{\mu}(f(x^{(k)}) - \min_y q^{(k)}(y))$ because $q^{(k)}(y) = \min_y q^{(k)}(y) + \frac{\mu}{2} \|y - \arg \min_x q^{(k)}(x)\|^2$. Hence, r_k is measuring the squared radius of our quadratic lower bound. To relate to the cutting plane framework, we can view the set as $\{y : q^{(k)}(y) \leq f(x^{(k)})\}$ and the measure $\mathcal{V} = f(x^{(k)}) - \min_y q^{(k)}(y)$.

Proof. Fix some k . We write $q^{(k)}(y) = v_A + \frac{\mu}{2} \|y - c_A\|^2$ and $q^{(k+\frac{1}{2})}(y) = v_B + \frac{\mu}{2} \|y - c_B\|^2$ with

$$c_A = c^{(k)}, \quad c_B = x^{(k)} - \frac{\nabla f(x^{(k)})}{\mu} \quad \text{and} \quad v_B = f(x^{(k)}) - \frac{\|\nabla f(x^{(k)})\|^2}{2\mu}.$$

Using the notation in `maxParabola`, we write $q^{(k+1)}(y) = v_\lambda + \frac{\mu}{2} \|y - c_\lambda\|^2$. Note that $r_{k+1}^2 = f(x^{(k+1)}) - v_\lambda$ and $r_k^2 = f(x^{(k)}) - v_A$. Therefore, we have

$$\frac{r_k^2 - r_{k+1}^2}{r_k^2} = \frac{f(x^{(k)}) - f(x^{(k+1)}) + v_\lambda - v_A}{r_k^2}. \quad (3.8)$$

To bound the right hand side, it suffices to bound v_A and v_λ . From the description of the algorithm `maxParabola`, we see that there are three cases $\lambda = 0$, $\lambda = 1$ and $0 < \lambda < 1$. We only focus on proving the nontrivial case $\lambda \in (0, 1)$. In this case, we have that

$$\begin{aligned} v_\lambda &= v_A + \frac{\mu (\|c_A - c_B\|^2 + \frac{2}{\mu} (v_B - v_A))^2}{8 \|c_A - c_B\|^2} \\ &= v_A + \frac{\mu (\|c_A - c_B\|^2 + \frac{2}{\mu} (f(x^{(k)}) - v_A) - \frac{\|\nabla f(x^{(k)})\|^2}{\mu^2})^2}{8 \|c_A - c_B\|^2}. \end{aligned}$$

Since $f \geq q^{(k)}$, we have $f(x^{(k)}) \geq q^{(k)}(x^{(k)}) \geq \min_x q^{(k)}(x) = v_A$. Next, we claim that $\|c_A - c_B\|^2 \geq \frac{\|\nabla f(x^{(k)})\|^2}{\mu^2}$. Using these two facts, we can prove that

$$v_\lambda \geq v_A + \frac{\mu (\frac{2}{\mu} (f(x^{(k)}) - v_A))^2}{8 \frac{\|\nabla f(x^{(k)})\|^2}{\mu^2}} = v_A + \frac{\mu \cdot r_k^4}{2 \|\nabla f(x^{(k)})\|^2}.$$

Putting this into (3.8), we have

$$\begin{aligned} \frac{r_k^2 - r_{k+1}^2}{r_k^2} &\geq \frac{f(x^{(k)}) - f(x^{(k+1)})}{r_k^2} + \frac{\mu \cdot r_k^2}{2 \|\nabla f(x^{(k)})\|^2} \\ &\geq \frac{f(x^{(k+\frac{1}{2})}) - f(x^{(k+1)})}{r_k^2} + \frac{\mu \cdot r_k^2}{2 \|\nabla f(x^{(k)})\|^2} \\ &\geq \frac{\|\nabla f(x^{(k)})\|^2}{2Lr_k^2} + \frac{\mu \cdot r_k^2}{2 \|\nabla f(x^{(k)})\|^2} \\ &\geq \sqrt{\frac{\mu}{L}} \end{aligned} \quad (3.9)$$

where the second inequality is due to the fact $x^{(k+\frac{1}{2})}$ is a line search from $x^{(k)}$, the third inequality is due to the assumption on L (Lemma 2.7), the last inequality follows from the Cauchy-Schwarz inequality.

For the final conclusion, we note that

$$\begin{aligned} q^{(1)}(y) &= f(x^{(0)}) + \nabla f(x^{(0)})^\top (y - x^{(0)}) + \frac{\mu}{2} \|y - x^{(0)}\|^2 \\ &= f(x^{(0)}) - \frac{1}{2\mu} \|\nabla f(x^{(0)})\|^2 + \frac{\mu}{2} \left\| y - \left(x^{(0)} - \frac{1}{\mu} \nabla f(x^{(0)}) \right) \right\|^2. \end{aligned}$$

Hence, we have $v^{(1)} = f(x^{(0)}) - \frac{1}{2\mu} \|\nabla f(x^{(0)})\|^2$ and hence $r_1 \leq f(x^{(1)}) - v^{(1)} \leq \frac{1}{2\mu} \|\nabla f(x^{(0)})\|^2$.

To prove the claim, we note that $x^{(k)}$ is the result of a line search of f between $c^{(k)}$ and some point. Therefore, we have that $\nabla f(x^{(k)}) \perp (x^{(k)} - c^{(k)})$ and hence

$$\|c_A - c_B\|^2 = \|c^{(k)} - x^{(k)} + \frac{\nabla f(x^{(k)})}{\mu}\|^2 \geq \frac{\|\nabla f(x^{(k)})\|^2}{\mu^2}.$$

□

Remark 3.29. We can view (3.9) as the key equation of the proof above. It shows that the progress is roughly $\frac{\|\nabla f\|^2}{L} + \frac{\mu}{\|\nabla f\|^2}$ where the first term comes from the progress on the function value and the second term comes from “the curvature” of the cutting sphere.

Exercise 3.30. Prove the following extension of Lemma 3.23: There exists x s.t. $B(0, \sqrt{1 - \epsilon|g|^2}) \cap B(g, |g|\sqrt{1 - \epsilon}) \subset B(x, \sqrt{1 - \sqrt{\epsilon}})$.

■ 3.5.3 Discussion

This section was about the idea of managing cutting planes, and as a byproduct we get an accelerated rate of convergence. As we will see later, standard accelerated gradient descent does not use line search and achieves the rate $1 - \sqrt{\frac{\mu}{L}}$. However, it seems that the use of line search helps in practice and that with a careful implementation, line search can be as cheap as gradient computation. For more difficult problems, one may want to store multiple quadratic lower bounds (see [21]).

■ 3.6 Lower Bounds

In this chapter, we have discussed a few cutting plane methods. In particular, we showed that $O(\min(n, \sqrt{\frac{L}{\mu}}) \log(\frac{1}{\epsilon}))$ gradient computations suffice. We conclude this section by showing that $\min(n, \sqrt{\frac{L}{\mu}})$ is in fact optimal among “gradient-based” methods. For convenience the reader may consider $\mu = 1$ and $L = \kappa$.

Theorem 3.31. *Fix any $L \geq \mu > 0$. Consider the function*

$$f(x) = -\frac{L-\mu}{4}x_1 + \frac{L-\mu}{8} \sum_{i=1}^{n-1} (x_i - x_{i+1})^2 + \frac{L-\mu}{8}x_1^2 + \frac{\mu}{2} \sum_{i=1}^n x_i^2 + \frac{\sqrt{L\mu} - \mu}{4}x_n^2 \quad (3.10)$$

which satisfies $\mu \cdot I \preceq \nabla^2 f(x) \preceq L \cdot I$. Assume that our algorithm satisfies $x^{(k)} \in \text{span}(x^{(0)}, \nabla f(x^{(0)}), \dots, \nabla f(x^{(k-1)}))$ with the initial point $x^{(0)} = 0$. Then, for $k < n$,

$$f(x^{(k)}) - \min_x f(x) \geq \left(\frac{\mu}{L}\right)^{3/2} \left(\frac{\sqrt{L/\mu} - 1}{\sqrt{L/\mu} + 1}\right)^{2k} (f(x^{(0)}) - \min_x f(x)).$$

Proof. First, we check the strong convexity and smoothness. Note that $f(x) = -x_1 + \frac{1}{2}x^\top A x$ for some matrix A . Hence, $\nabla^2 f(x) = A$. Hence, we have

$$\theta^\top \nabla^2 f(x) \theta = \frac{L-\mu}{4} \sum_{i=1}^{n-1} (\theta_i - \theta_{i+1})^2 + \frac{L-\mu}{4} \theta_1^2 + \mu \sum_{i=1}^n \theta_i^2 + \frac{\sqrt{L\mu} - \mu}{2} \theta_n^2$$

For the upper bound $\nabla^2 f(x) \preceq L \cdot I$, we note that

$$\begin{aligned} \theta^\top \nabla^2 f(x) \theta &\leq \frac{L-\mu}{4} \sum_{i=1}^{n-1} (2\theta_i^2 + 2\theta_{i+1}^2) + \frac{L-\mu}{4} \theta_1^2 + \mu \sum_{i=1}^n \theta_i^2 + \left(\frac{\sqrt{L\mu} - \mu}{2}\right) \theta_n^2 \\ &\leq (L-\mu) \sum_{i=1}^n \theta_i^2 + \mu \sum_{i=1}^n \theta_i^2 \\ &= L \sum_{i=1}^n \theta_i^2. \end{aligned}$$

For the lower bound $\nabla^2 f(x) \succeq \mu \cdot I$, we note that

$$\theta^\top \nabla^2 f(x) \theta \geq \mu \sum_{i=1}^n \theta_i^2.$$

To lower bound the error, we note that the gradient at $x^{(0)}$ is of the form $(?, 0, 0, 0, \dots)$ and hence by the assumption $x^{(1)} = (?, 0, 0, 0, \dots)$ and $\nabla f(x^{(1)}) = (?, ?, 0, 0, \dots)$. By induction, only the first k coordinates of $x^{(k)}$ are non-zero.

Now, we compute the minimizer of $f(x)$. Let x^* be the minimizer of $f(x)$. By the optimality condition, we have that

$$\begin{aligned} -\frac{L-\mu}{4} + \frac{L-\mu}{4}(x_1^* - x_2^*) + \frac{L-\mu}{4}x_1^* + \mu x_1^* &= 0, \\ \frac{L-\mu}{4}(x_i^* - x_{i-1}^*) + \frac{L-\mu}{4}(x_i^* - x_{i+1}^*) + \mu x_i^* &= 0, \text{ for } i \in \{2, 3, \dots, n-1\} \\ \frac{L-\mu}{4}(x_n^* - x_{n-1}^*) + \frac{\sqrt{L\mu} + \mu}{2}x_n^* &= 0. \end{aligned}$$

By a direct substitution, we have that $x_i^* = (\frac{\sqrt{L/\mu}-1}{\sqrt{L/\mu}+1})^i$ is a solution of the above equation. Now, we note that

$$\|x^{(k)} - x^*\|_2^2 \geq \sum_{i=k+1}^n \left(\frac{\sqrt{L/\mu}-1}{\sqrt{L/\mu}+1}\right)^{2i} \geq \left(\frac{\sqrt{L/\mu}-1}{\sqrt{L/\mu}+1}\right)^{2(k+1)}$$

and that

$$\|x^{(0)} - x^*\|_2^2 \leq \sum_{i=1}^{\infty} \left(\frac{\sqrt{L/\mu}-1}{\sqrt{L/\mu}+1}\right)^{2i} = \left(\frac{\sqrt{L/\mu}-1}{\sqrt{L/\mu}+1}\right)^2 \frac{\sqrt{L/\mu}+1}{2}.$$

Now, by smoothness and by the strong convexity of f , we have

$$\frac{f(x^{(k)}) - f(x^*)}{f(x^{(0)}) - f(x^*)} \geq \frac{\mu}{L} \cdot \frac{\|x^{(k)} - x^*\|_2^2}{\|x^{(0)} - x^*\|_2^2} \geq \left(\frac{\mu}{L}\right)^{3/2} \left(\frac{\sqrt{L/\mu}-1}{\sqrt{L/\mu}+1}\right)^{2k}.$$

□

Note that this “worst” function naturally appears in many problems. So, it is a problem we need to address. In some sense, the proof points out a common issue of any algorithm which only uses gradient information. Given any convex function, we construct the dependence graph G on the set of variables x_i by connecting x_i to x_j if $\nabla f(x)_i$ depends on x_j or $\nabla f(x)_j$ depends on x_i (given all other variables). Note that the dependence graph G of the worst function is simply a n vertex path, whose diameter is $n-1$. Also, note that gradient descent can only transmit information from one vertex to another in each iteration. Therefore, it takes at least $\Omega(\text{diameter})$ time to solve the problem unless we know the solution is sparse (when L/μ is small). However, we note that this is not a lower bound for all algorithms.

The problem (3.10) belongs to a general class of functions called Laplacian systems and it can be solved in nearly linear time using spectral graph theory.

■ 4.1 Equivalences between Oracles

■ 4.1.1 Oracles for Convex Sets

Grötschel, Lovász and Schrijver [28] defined five different oracles to access convex sets, showed they are equivalent and used them to get polynomial-time algorithms for a variety of combinatorial problems (including the first ones in many cases).

Here are four basic oracles¹ for a convex set $K \subseteq \mathbb{R}^n$. Later we will allow for error parameters in each oracle, i.e., approximate versions of all the oracles below. We begin with exact oracles for simplicity.

Definition 4.1 (Membership Oracle (MEM)). Queried with a vector $y \in \mathbb{R}^n$, the oracle either

- asserts that $y \in K$, or
- asserts that $y \notin K$.

Definition 4.2 (Separation Oracle (SEP)). Queried with a vector $y \in \mathbb{R}^n$, the oracle either

- asserts that $y \in K$, or
- finds a unit vector $c \in \mathbb{R}^n$ such that $c^T x \leq c^T y$ for all $x \in K$.

Definition 4.3 (Validity Oracle (VAL)). Queried with a unit vector $c \in \mathbb{R}^n$, the oracle either²

- outputs $\max_{x \in K} c^T x$, or
- asserts that K is empty.

Definition 4.4 (Optimization Oracle (OPT)). Queried with a unit vector $c \in \mathbb{R}^n$, the oracle either

- finds a vector $y \in K$ and $c^T x \leq c^T y$ for all $x \in K$, or
- asserts that K is empty.

According to the definitions, the separation oracle gives more information than the membership oracle and the optimization oracle gives more information than the validity oracle. Depending on the problem, usually one of the oracles will be the preferred or more natural way to access the convex set. For example, for the polytope given by $\{Ax \geq b\}$, the separation oracle is the preferred way because the membership oracle takes as much time as the separation oracle, and both validity and optimization involve solving a linear program. On the contrary, the preferred oracle for the convex set $\text{conv}(\{a_i\})$ is the optimization oracle because $\max_{x \in \text{conv}(\{a_i\})} \theta^T x$ can be solved by only checking $x = a_i$ for each i . In combinatorial optimization, many polytopes have exponentially many vertices and constraints but one can use combinatorial structure to solve the optimization problem efficiently.

Example 4.5. The spanning tree polytope of an undirected graph $G = (V, E)$ is given by

$$P = \{x \in \mathbb{R}_+^{|E|} \mid \sum_{e \in E} x_e = |V| - 1, \quad \sum_{(u,v) \in E \cap (S \times S)} x_{(u,v)} \leq |S| - 1 \quad \forall S \subseteq V, |S| \geq 1\}.$$

The extreme points of this polytope can be shown to exactly correspond to the indicator vectors of spanning trees of G . Thus, the optimization oracle in this case is to simply find a maximum cost spanning tree.

Exercise 4.6. Design a membership oracle for the spanning tree polytope.

¹We also omit the fifth oracle VIOL defined by [28], which checks whether the convex set satisfies a given inequality or gives a violating point in the convex set, since this is equivalent to the OPT oracle below up to a logarithmic factor.

²We use a slightly different definition than [28] for clarity.

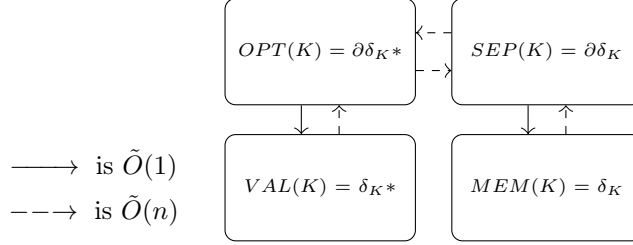


Figure 4.1: The relationships among the four oracles for convex sets. The arrows are implications.

■ 4.1.2 Oracles for Convex Functions

Now, we generalize the oracles for convex sets to convex functions. The membership oracle and separation oracle can be generalized as follows

Definition 4.7 (Evaluation Oracle (EVAL)). Queried with a vector y , the oracle outputs $f(y)$.

The next oracle generalizes gradients to subgradients so that they can be computed for general convex functions. Any vector output by the oracle is a subgradient of the function at the query point.

Definition 4.8 (Subgradient Oracle (GRAD)). Queried with a vector y , the oracle outputs $f(y)$ and a vector $g \in \mathbb{R}^n$ such that

$$f(x) \geq f(y) + g^\top(x - y) \text{ for all } x \in \mathbb{R}^n \quad (4.1)$$

or outputs “ $f(y)$ undefined.”

To generalize the validity oracle, we define the convex (Fenchel) conjugate of f :

Definition 4.9 (Convex Conjugate). For any function f , we define the convex conjugate

$$f^*(\theta) \stackrel{\text{def}}{=} \sup_{x \in \mathbb{R}^n} \theta^\top x - f(x).$$

Note that f^* is convex because it is the supremum of linear functions. Also, we have $f^*(0) = -\inf_{x \in \mathbb{R}^n} f(x)$. Note that³ $\delta_K^*(c) = \sup_{x \in K} c^\top x$. Therefore, the validity oracle for δ_K is simply the evaluation oracle for δ_K^* . The following lemma shows that the optimization oracle is simply the (sub)gradient oracle for δ_K^* . We use ∇f to represent subgradient.

Lemma 4.10. For any continuous function f with differentiable f^* , we have that $\nabla f^*(\theta) = \arg \max_x \theta^\top x - f(x)$.

Proof. First we observe that the supremum is achieved. Fix θ . Let $g_\theta(x) = \theta^\top x - f(x)$. We assume $\sup_x g_\theta(x) = f^*(\theta)$ is finite. Let $\epsilon > 0$. Then, $g_\theta(x)$ is a continuous function, so $S = g_\theta^{-1}([f^*(\theta) - \epsilon, \infty))$ is a closed set. The set S is not empty because there is some x for which $g_\theta(x) \geq \sup_z g_\theta(z) - \epsilon$. Now suppose for a contradiction that S is not bounded. Then, there exists a sequence $x_i \in \mathbb{R}^n$ such that $\|x_i\| \geq i$ and $g_\theta(x_i) \geq f^*(\theta) - \epsilon$ for all i . By the compactness of the unit sphere, we may assume by taking a subsequence that $x_i/\|x_i\| \rightarrow u$ for some unit vector $u \in \mathbb{R}^n$. Then, $u^\top x_i/\|x_i\| \rightarrow u^\top u = 1$, and since $\|x_i\| \rightarrow \infty$, we have $u^\top x_i \rightarrow \infty$. Since $g_{\theta+u}(x_i) = g_\theta(x_i) + u^\top x_i \geq f^*(\theta) - \epsilon + u^\top x_i$, this means that $g_{\theta+u}(x_i) \rightarrow \infty$, contradicting $f^*(\theta + u)$ being finite. Hence, S is bounded and thus compact, so $g_\theta(x)$ attains its maximum in S , and thus in \mathbb{R}^n .

Let $x_\theta \in \arg \sup_x \theta^\top x - f(x)$. By definition, we have that $f^*(\theta) = \theta^\top x_\theta - f(x_\theta)$ and that $f^*(\eta) \geq \eta^\top x_\theta - f(x_\theta)$ for all η . Therefore,

$$f^*(\eta) \geq f^*(\theta) + x_\theta^\top(\eta - \theta) \text{ for all } \eta.$$

Therefore, $x_\theta \in \nabla f^*(\theta)$. □

³Recall that $\delta_C(x) = 0$ if $x \in C$ and $+\infty$ otherwise.

Note that this lemma shows that $\nabla \delta_K^*(\theta) = \arg \max_{x \in K} \theta^\top x$. So, the gradient oracle for δ_K^* is exactly the optimization oracle for K .

Figure 4.2 shows the current best reduction between these four function oracles. Note that according to our definition of the GRAD oracle, it also outputs the function value (EVAL). It is not hard to show that you can use $n + 1$ calls to evaluation oracle to compute one gradient approximately (using finite difference) and that you can use $\tilde{O}(n)$ calls to gradient oracle of f to compute one gradient of f^* (using the cutting plane method). In the next section (Sec. 4.2), we will see the remaining reductions. However, it is still an open question if all of these reductions are the best possible.

Open Problem. Prove that it takes $\Omega(n^2)$ calls to the evaluation oracle of f to compute the gradient of f^* .

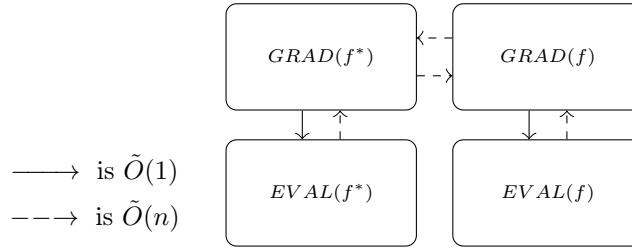


Figure 4.2: This illustrates the relationships of oracles for a convex function f and its convex conjugate f^* .

■ 4.1.3 Convex Conjugate and Equivalences

Here are some examples of conjugates.

Exercise 4.11. Show that

- The conjugate of $f(x) = \frac{1}{p} \|x\|_p^p$ is $f^*(\theta) = \frac{1}{q} \|\theta\|_q^q$ where $\frac{1}{p} + \frac{1}{q} = 1$ (with $p, q \geq 1$).
- The conjugate of $f(x) = \langle a, x \rangle - b$ is $f^*(\theta) = \begin{cases} b, & \theta = a \\ +\infty & \text{otherwise} \end{cases}$.
- The conjugate of $f(x) = \sum_i e^{x_i}$ is $f^*(\theta) = \begin{cases} \sum_i \theta_i \log \theta_i - \theta_i & \text{if } \theta_i \geq 0 \text{ for all } i \\ +\infty & \text{otherwise} \end{cases}$.

Exercise 4.12. For any x, θ , we have $\theta^\top x \leq f(x) + f^*(\theta)$.

Exercise 4.13. Prove that the gradient of f is L -Lipschitz if and only if f^* is $\frac{1}{L}$ strongly convex.

The following lemma shows that one can recover f from f^* .

Lemma 4.14 (Involution property). *For any convex function f with a closed epigraph, we have that $f^{**} = f$.*

Proof. Since $\text{epi} f$ is a closed, convex set, Corollary 1.7 shows that it must be an intersection of halfspaces, i.e., a set \mathcal{H} s.t.

$$f(x) = \sup_{(\theta, b) \in \mathcal{H}} \theta^\top x - b$$

where \mathcal{H} is the set of supporting planes of $\text{epi} f$ and contains all affine lower bounds on f , namely, $f(x) \geq \theta^\top x - b$ for all x . Alternatively, we can write

$$\text{epi}(f) = \bigcap_{\mathcal{H} = \{(\theta, b) : \forall x, f(x) \geq \theta^\top x - b\}} \{(x, t) : t \geq \theta^\top x - b\}.$$

For a fixed θ , any feasible b satisfies $b \geq \theta^\top x - f(x)$ for all x . So, the smallest feasible value satisfies

$$b^* = \sup_x \theta^\top x - f(x) = f^*(\theta).$$

Hence,

$$f(x) = \sup_{(\theta, b) \in \mathcal{H}} \theta^\top x - b^* = \sup_{\theta} \theta^\top x - f^*(\theta) = f^{**}(x).$$

□

Exercise 4.15. Let f be a convex function with closed epigraph. Show that $f = f^*$ iff $f(x) = \frac{\|x\|^2}{2}$.

Since we can use the gradient, ∇f , to compute the gradient of the dual, ∇f^* (via cutting plane method), the involution property shows that we can do the reverse – use ∇f^* to compute ∇f . Going back to the example about $\text{conv}(\{a_i\})$, since we know how to compute $\max_{x \in \text{conv}(\{a_i\})} \theta^\top x = \delta_{\text{conv}(\{a_i\})}^*(\theta)$, this reduction gives us a way to separate $\text{conv}(\{a_i\})$, or equivalently, to compute the (sub)gradient of $\delta_{\text{conv}(\{a_i\})}^*$. This is formalized in the next exercise.

Exercise 4.16. Show how to implement the separation oracle SEP for a convex set K given access to an optimization oracle OPT for K .

Recall that for any linear space X , X^* denotes the dual space, i.e., the set of all linear functions on X and that under mild assumptions⁴, we have $X^{**} = X$. Therefore, there are two natural “coordinate systems” to record a convex function, the primal space X and the dual space X^* . Under these “coordinate systems”, we have the dual functions f and f^* .

Exercise 4.17 (Order reversal). Show that $f \geq g \iff f^* \leq g^*$ (both for all $x \in \mathbb{R}^n$).

Interestingly, the convex conjugate is the *unique* transformation on convex functions that satisfies both involution and order reversal.

Theorem 4.18 ([6]). *Given a transformation \mathcal{T} that maps the set of lower semi-continuous⁵ convex functions onto itself such that $\mathcal{T}\mathcal{T}\phi = \phi$ and $\phi \leq \psi \implies \mathcal{T}\phi \geq \mathcal{T}\psi$ for all lower-semi-continuous convex functions ϕ and ψ . Then, \mathcal{T} is essentially the convex conjugate, namely, there is an invertible symmetric linear transformation B , a vector v_0 and a constant C_0 such that*

$$(\mathcal{T}\phi)(x) = \phi^*(Bx + v_0) + v_0^\top x + C_0.$$

In combinatorial optimization, many convex sets are given by the convex hull for some discrete objects. In many cases, the only known way to do the separation is via such reductions. In this chapter, we will study the following general theorem showing that optimization can be reduced to membership/evaluation with a quadratic overhead in dimension for the number of oracle queries.

Theorem 4.19. *Let K be a convex set specified by a membership oracle, a point $x_0 \in \mathbb{R}^n$, and numbers $0 < r < R$ such that $B(x_0, r) \subseteq K \subseteq B(x_0, R)$. For any convex function f given by an evaluation oracle and any $\epsilon > 0$, there is a randomized algorithm that computes a point $z \in B(K, \epsilon)$ such that*

$$f(z) \leq \min_{x \in K} f(x) + \epsilon \left(\max_{x \in K} f(x) - \min_{x \in K} f(x) \right)$$

with constant probability using $O(n^2 \log^2(\frac{nR}{\epsilon r}))$ calls to the membership oracle and evaluation oracle and $O(n^3 \log^{O(1)}(\frac{nR}{\epsilon r}))$ total arithmetic operations.

■ 4.2 Gradient from Evaluation via Finite Difference

When the function f is in \mathcal{C}^1 , we can approximate the gradient of a function by calculating a finite difference for sufficiently small h :

$$\frac{\partial f}{\partial x_i} = \frac{f(x + he_i) - f(x)}{h} + O(h)$$

⁴The dual of the dual of a vector space X is isomorphic to X if and only if X is a finite-dimensional vector space.

⁵See Def. 0.3.

which only takes $n + 1$ calls to the evaluation oracle (for computing $f(x), f(x + he_1), \dots, f(x + he_n)$). The only issue is that the convex function may not be differentiable. However, any convex Lipschitz function is twice differentiable almost everywhere (see the proof below). Therefore, we can simply perturb x with random noise, then apply a finite difference. To see the idea more precisely, we first observe that the norm of the Hessian can be bounded in expectation for a Lipschitz function. Note that this is Lipschitzness of the function, not its gradient. The proof below uses the basic fact that the gradient is defined almost everywhere for Lipschitz functions.

Lemma 4.20. *For any L -Lipschitz convex function f defined in a unit ball, we have $\nabla^2 f(x)$ exists almost everywhere and that $\mathbf{E}_{x \in B(0,1)} \|\nabla^2 f(x)\|_F \leq nL$.*

Proof. The existence almost everywhere is classical (Alexandrov Theorem, see e.g., [59]; see also Rademacher's theorem about the existence of the derivative almost everywhere for Lipschitz functions). We will only prove the part $\mathbf{E}_{x \in B(0,1)} \|\nabla^2 f(x)\|_F \leq nL$. Since $\nabla^2 f \succeq 0$ (where defined), we have $\|\nabla^2 f(x)\|_F \leq \text{tr} \nabla^2 f(x)$. Therefore,

$$\int_{B(0,1)} \|\nabla^2 f(x)\|_F dx \leq \int_{B(0,1)} \text{tr} \nabla^2 f(x) dx = \int_{B(0,1)} \Delta f(x) dx.$$

Using Stokes' Theorem, and letting $\nu(x)$ be the normal vector at x , we have

$$\int_{B(0,1)} \Delta f(x) dx = \int_{\partial B(0,1)} \langle \nabla f(x), \nu(x) \rangle dx \leq |\partial B(0,1)| \cdot L.$$

Hence, we have

$$\mathbf{E}_{x \in B(0,1)} \|\nabla^2 f(x)\|_F \leq \frac{|\partial B(0,1)|}{|B(0,1)|} L = nL.$$

□

To turn this into an algorithm, we need to develop it a bit further.

Lemma 4.21 ([42]). *Let $B_\infty(x, r) = \{y : \|x - y\|_\infty \leq r\}$. For any $0 < r_2 \leq r_1$ and any convex function f defined on $B_\infty(x, r_1 + r_2)$ with $\|\nabla f(z)\|_\infty \leq L$ for any $z \in B_\infty(x, r_1 + r_2)$ we have*

$$\mathbf{E}_{y \in B_\infty(x, r_1)} \mathbf{E}_{z \in B_\infty(y, r_2)} \|\nabla f(z) - g(y)\|_1 \leq n^{3/2} \frac{r_2}{r_1} L$$

where $g(y)$ is the average of ∇f over $B_\infty(y, r_2)$.

Proof. Let $\omega_i(z) = \langle \nabla f(z) - g(y), e_i \rangle$ for all $i \in [n]$. Then, we have that

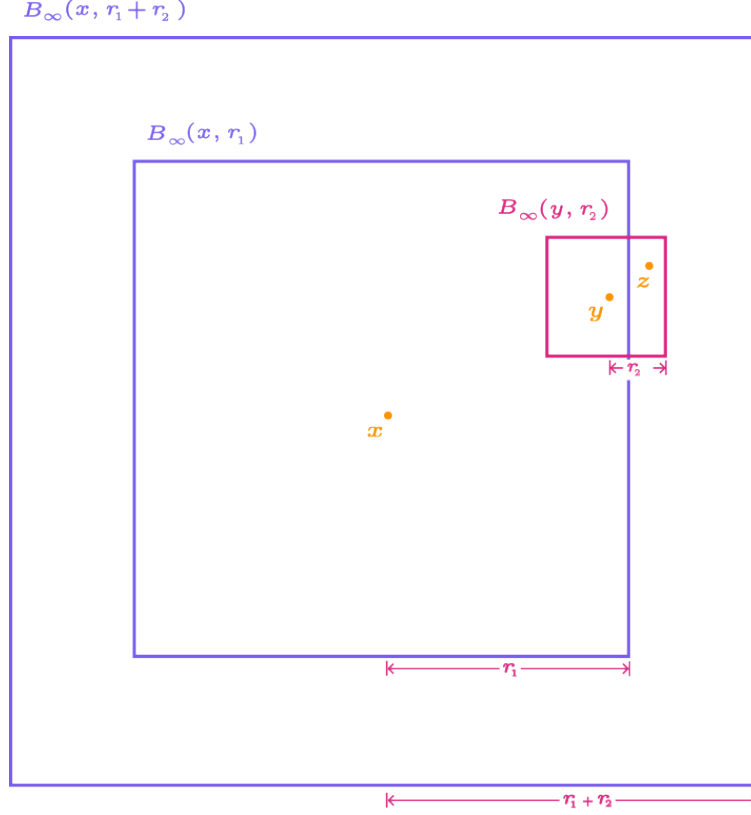
$$\int_{B_\infty(y, r_2)} \|\nabla f(z) - g(y)\|_1 dz = \sum_i \int_{B_\infty(y, r_2)} |\omega_i(z)| dz.$$

Since $\int_{B_\infty(y, r_2)} \omega_i(z) dz = 0$, the Poincaré inequality for a box (Theorem 4.25 below) shows that

$$\begin{aligned} \int_{B_\infty(y, r_2)} |\omega_i(z)| dz &\leq r_2 \int_{B_\infty(y, r_2)} \|\nabla \omega_i(z)\|_2 dz \\ &= r_2 \int_{B_\infty(y, r_2)} \|\nabla^2 f(z) e_i\|_2 dz \\ \sum_i \int_{B_\infty(y, r_2)} |\omega_i(z)| dz &\leq \sqrt{n} r_2 \int_{B_\infty(y, r_2)} \|\nabla^2 f(z)\|_F dz \end{aligned}$$

Since f is convex, eigenvalues of the Hessian are nonnegative and so we have

$$\|\nabla^2 f(z)\|_F = \sqrt{\sum_i \lambda_i^2} \leq \sum_i \lambda_i = \text{tr} \nabla^2 f(z) = \Delta f(z).$$



Therefore, we have

$$\begin{aligned} \mathbf{E}_{z \in B_\infty(y, r_2)} \|\nabla f(z) - g(y)\|_1 &\leq \sqrt{n} r_2 \mathbf{E}_{z \in B_\infty(y, r_2)} \Delta f(z) \\ &= \sqrt{n} r_2 \Delta h(y) \end{aligned}$$

where $h = \frac{1}{(2r_2)^n} f * \chi_{B_\infty(0, r_2)}$ where $\chi_{B_\infty(0, r_2)}$ is 1 on the set $B_\infty(0, r_2)$ and 0 on outside.

Integrating by parts, we have that

$$\int_{B_\infty(x, r_1)} \Delta h(y) dy = \int_{\partial B_\infty(x, r_1)} \langle \nabla h(y), n(y) \rangle dy$$

where $\Delta h(y) = \sum_i \frac{d^2 h}{dx_i^2}(y)$ and $n(y)$ is the normal vector on $\partial B_\infty(x, r_1)$ the boundary of the box $B_\infty(x, r_1)$, i.e. standard basis vectors. Since f is L -Lipschitz with respect to $\|\cdot\|_\infty$ so is h , i.e. $\|\nabla h(z)\|_\infty \leq L$. Hence, we have that

$$\mathbf{E}_{y \in B_\infty(x, r_1)} \Delta h(y) \leq \frac{1}{(2r_1)^n} \int_{\partial B_\infty(x, r_1)} \|\nabla h(y)\|_\infty \|n(y)\|_1 dy \leq \frac{1}{(2r_1)^n} \cdot 2n(2r_1)^{n-1} \cdot L = \frac{nL}{r_1}.$$

Therefore, we have that

$$\mathbf{E}_{y \in B_\infty(x, r_1)} \mathbf{E}_{z \in B_\infty(y, r_2)} \|\nabla f(z) - g(y)\|_1 \leq n^{3/2} \frac{r_2}{r_1} L.$$

□

Exercise 4.22. For an L -gradient-Lipschitz function $f : \mathbb{R}^n \rightarrow \mathbb{R}$, and $h = f * \chi_{B_\infty(0, 1/2)}$, prove that h is also L -gradient-Lipschitz and $\Delta h(y) = \mathbf{E}_{z \sim B_\infty(y, 1/2)} (\Delta f(z))$.

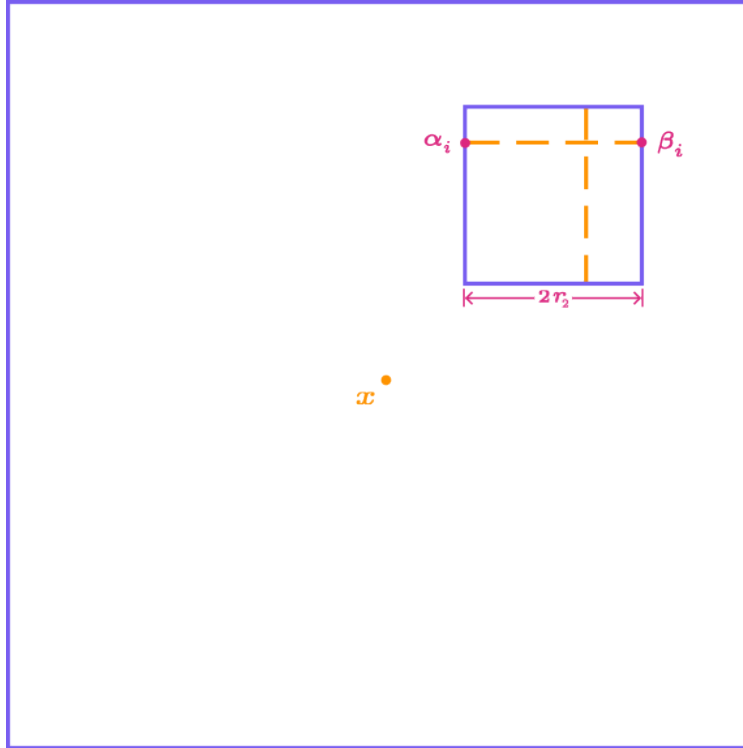
Algorithm 10: SubgradConvexFunc(f, x, r_1, ε)**Require:** $r_1 > 0$, $\|\partial f(z)\|_\infty \leq L$ for any $z \in B_\infty(x, 2r_1)$.Set $r_2 = \sqrt{\frac{\varepsilon r_1}{\sqrt{n}L}}$.Sample $y \in B_\infty(x, r_1)$ and $z \in B_\infty(y, r_2)$ independently and uniformly at random.**for** $i = 1, 2, \dots, n$ **do** Let α_i and β_i denote the end points of the interval $B_\infty(y, r_2) \cap \{z + se_i : s \in \mathbb{R}\}$. Set $\tilde{g}_i = \frac{f(\beta_i) - f(\alpha_i)}{2r_2}$ where we compute f to within ε additive error.**end****Output** \tilde{g} as the approximate subgradient of f at x .

This lemma shows that we can implement an approximate gradient oracle (GRAD) using an evaluation oracle (EVAL) even for non-differentiable functions. By the involution property again, this completes all the reductions in Figure 4.2. With the above fact asserting that, on average, the gradient is approximated by its average in a small ball, we now proceed to construct an approximate subgradient, using only an approximate evaluation oracle. The parameter r_2 in the algorithm is chosen to optimize the final error of the output. By making the ratio r_2/r_1 sufficiently small, we can get a desired error for the subgradient.

Lemma 4.23. *Let $r_1 > 0$ and f be a convex function. Suppose that $\|\nabla f(z)\|_\infty \leq L$ for any $z \in B_\infty(x, 2r_1)$ and suppose that we can evaluate f to within ε additive error for $\varepsilon \leq r_1\sqrt{n}L$. Let $\tilde{g} = \text{SubgradConvexFunc}(f, x, r_1, \varepsilon)$. Then, there is random variable $\zeta \geq 0$ with $\mathbf{E}\zeta \leq 2\sqrt{\frac{L\varepsilon}{r_1}}n^{5/4}$ such that for any y*

$$f(y) \geq f(x) + \langle \tilde{g}, y - x \rangle - \zeta \|y - x\|_\infty - 4nr_1L.$$

Proof. We assume that f is twice differentiable. For general f , we can reduce to this case by viewing it as a limit of twice-differentiable functions.



First, we assume that we can compute f exactly, namely $\varepsilon = 0$. Fix $i \in [n]$. Let $g(y)$ be the average of

∇f over $B_\infty(y, r_2)$. Then, for the function \tilde{g} computed by the algorithm, we have that

$$\begin{aligned} \mathbf{E}_z |\tilde{g}_i - g(y)_i| &= \mathbf{E}_z \left| \frac{f(\beta_i) - f(\alpha_i)}{2r_2} - g(y)_i \right| \\ &\leq \mathbf{E}_z \frac{1}{2r_2} \int \left| \frac{df}{dx_i}(z + se_i) - g(y)_i \right| ds \\ &= \mathbf{E}_z \left| \frac{df}{dx_i}(z) - g(y)_i \right| \end{aligned}$$

where we used that both $z + se_i$ and z are uniform distribution on $B_\infty(y, r_2)$ in the last line. Hence, we have

$$\mathbf{E}_z \|\tilde{g} - \nabla f(z)\|_1 \leq \mathbf{E}_z \|\nabla f(z) - g(y)\|_1 + \mathbf{E}_z \|\tilde{g} - g(y)\|_1 \leq 2\mathbf{E}_z \|\nabla f(z) - g(y)\|_1.$$

Now, applying the convexity of f yields that

$$\begin{aligned} f(q) &\geq f(z) + \langle \nabla f(z), q - z \rangle \\ &= f(z) + \langle \tilde{g}, q - x \rangle + \langle \nabla f(z) - \tilde{g}, q - x \rangle + \langle \nabla f(z), x - z \rangle \\ &\geq f(z) + \langle \tilde{g}, q - x \rangle - \|\nabla f(z) - \tilde{g}\|_1 \|q - x\|_\infty - \|\nabla f(z)\|_\infty \|x - z\|_1. \end{aligned}$$

Now, using f is L -Lipschitz between x and z , we have that $f(z) \geq f(x) - L \cdot \|x - z\|_1$. Hence, we have

$$f(q) \geq f(x) + \langle \tilde{g}, q - x \rangle - \|\nabla f(z) - \tilde{g}\|_1 \|q - x\|_\infty - 2L \|x - z\|_1.$$

Note that $\|x - z\|_1 \leq n \cdot \|x - z\|_\infty \leq n(r_1 + r_2)$ by assumption. Moreover, we can apply Lemma 4.21 to bound $\|\nabla f(z) - \tilde{g}\|_1$ and use $r_2 = \sqrt{\frac{\varepsilon r_1}{\sqrt{n}L}} \leq r_1$ to get

$$f(q) \geq f(x) + \langle \tilde{g}, q - x \rangle - \zeta \|q - x\|_\infty - 4nr_1L$$

with $\mathbf{E}\zeta \leq 2n^{3/2} \frac{r_2}{r_1} L$.

Since we only compute f up to ε additive error, it introduces $\frac{\varepsilon}{r_2}$ additive error in \tilde{g}_i . Hence, we instead have that

$$\mathbf{E}\zeta \leq 2n^{3/2} \frac{r_2}{r_1} L + \frac{\varepsilon n}{2r_2}.$$

Setting $r_2 = \frac{1}{2} \sqrt{\frac{\varepsilon r_1}{\sqrt{n}L}}$ completes the proof. \square

Note that if we happened to have an exact oracle for f , then we can make r_2 arbitrarily small.

Exercise 4.24. What is the best possible bound in Lemma 4.21, in particular is the dependence on the dimension tight?

In the proof of Lemma 4.21, we used the following fact applied to the case when Ω is a cube. In this case, the coefficient on the RHS is given by the Cheeger or KLS constant of the cube and is 1. This is an example of an isoperimetric inequality. Such inequalities will play an important role later in this book.

Theorem 4.25 (L^1 -Poincaré inequality). *Let Ω be connected, bounded and open. Then the following (best-possible) inequality holds for any smooth function $f : \Omega \rightarrow \mathbb{R}$:*

$$\left\| f - \frac{1}{|\Omega|} \int_\Omega f(x) dx \right\|_{L^1(\Omega)} \leq \left(\sup_{S \subset \Omega} \frac{2|S||\Omega \setminus S|}{|\partial S||\Omega|} \right) \|\nabla f\|_{L^1(\Omega)}$$

where the supremum is over all subsets S s.t. S and $\Omega \setminus S$ are both connected.

Exercise 4.26. Prove the inequality in Theorem 4.25 using the classical co-area formula.

■ 4.3 Separation via Membership

In this section, we show that how to implement a separation oracle for a convex set using a nearly linear number of queries to a membership oracle. We divide this into two steps. In the first step (Algorithm ??), we compute an approximate subgradient of a given Lipschitz convex function. Using this, in the second step (Algorithm ??), we compute an approximate separating hyperplane.

Theorem 4.27. *Let K be a convex body s.t. $B(0, 1) \subseteq K \subseteq B(0, R)$. Then, for any $0 < \eta \leq 1/2$, we can compute an η -approximate separation oracle for K using $O(n \log(nR/\eta))$ queries to a membership oracle for K .*

Throughout this section, let $K \subseteq \mathbb{R}^n$ be a convex set that contains $B_2(0, r)$ and is contained in $B_2(0, R)$. Recall that $B_p(x, r)$ is the p -norm ball of radius r centered at x . By an approximate separation oracle we mean that either the queried point x lies within distance η of K , or the oracle provides a halfspace $c^T y \leq c^T x + \eta$ for all points $y \in K$ at distance at least η from the boundary of K . We also define

$$B_p(K, -\delta) \stackrel{\text{def}}{=} \{x \in \mathbb{R}^n : B_p(x, \delta) \subseteq K\}.$$

Given some point $x \notin K$, we wish to separate x from K using a halfspace. To do this, we reduce this problem to computing an approximate subgradient of a Lipschitz convex function $h_x(d)$ defined for points in K . Roughly speaking, it is the “height” (or distance from the boundary) of a point d in the direction of x . Let

$$\alpha_x(d) = \max_{d + \alpha x \in K} \alpha \quad \text{and} \quad h_x(d) = -\alpha_x(d) \|x\|_2.$$

Note that $d + \alpha_x(d)x$ is the last point in K on the line through $d \in K$ in the direction of x , and $-h_x(d)$ is the ℓ_2 distance from this boundary point to d (see Fig.4.3).

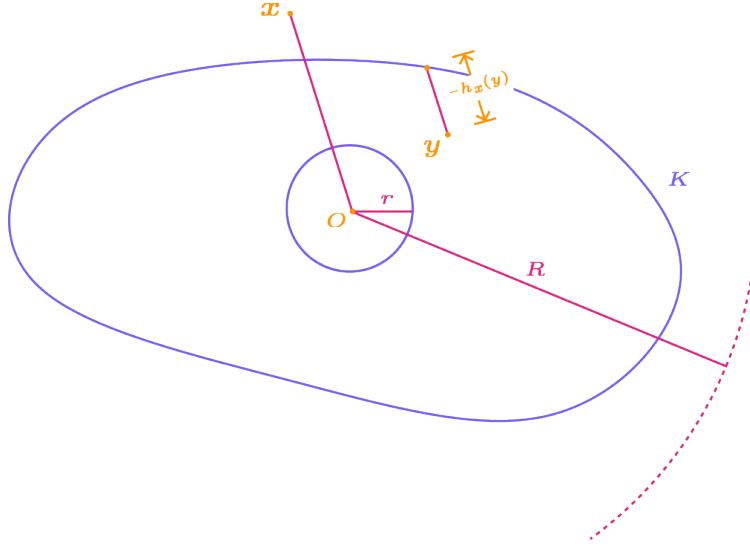


Figure 4.3: The convex height function h_x

The output of the algorithm for separation is a halfspace that approximately contains K , and the input point x is close to its bounding hyperplane. It uses a call to the subgradient function above.

We now proceed to analyze the height function.

Lemma 4.28. *$h_x(d)$ is convex on K .*

Proof. Let $d_1, d_2 \in K$ and $\lambda \in [0, 1]$. Now $d_1 + \alpha_x(d_1)x \in K$ and $d_2 + \alpha_x(d_2)x \in K$. Consequently,

$$[\lambda d_1 + (1 - \lambda)d_2] + [\lambda \cdot \alpha_x(d_1) + (1 - \lambda) \cdot \alpha_x(d_2)]x \in K.$$

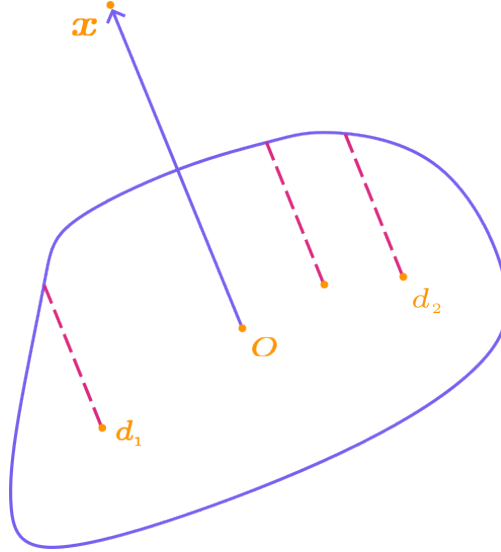
Therefore, if we let $d \stackrel{\text{def}}{=} \lambda d_1 + (1 - \lambda)d_2$ we see that $\alpha_x(d) \geq \lambda \cdot \alpha_x(d_1) + (1 - \lambda) \cdot \alpha_x(d_2)$ and $h_x(\lambda d_1 + (1 - \lambda)d_2) \leq \lambda h_x(d_1) + (1 - \lambda) h_x(d_2)$ as claimed. \square

Algorithm 11: $\text{Separate}_{\varepsilon, \rho}(K, x)$

Require: $B_2(0, r) \subset K \subset B_2(0, R)$.
if $\text{MEM}_{\varepsilon}(K)$ asserts that $x \in B(K, \varepsilon)$ **then**
 | **Output:** “ $x \in B(K, \varepsilon)$ ”.
else if $x \notin B_2(0, R)$ **then**
 | **Output:** the halfspace $\{y : 0 \geq \langle y - x, x \rangle\}$.
end
Let $\kappa = R/r$, $\alpha_x(d) = \max_{d+\alpha x \in K} \alpha$ and $h_x(d) = -\alpha_x(d) \|x\|_2$.
The evaluation oracle of $\alpha_x(d)$ can be implemented via binary search and $\text{MEM}_{\varepsilon}(K)$.
Compute $\tilde{g} = \text{SubgradConvexFunc}(h_x, 0, r_1, 4\varepsilon)$ with $r_1 = n^{1/6} \varepsilon^{1/3} R^{2/3} \kappa^{-1}$ and the evaluation oracle of $\alpha_x(d)$.
Output: the halfspace

$$\left\{ y : \frac{31}{\rho} n^{7/6} R^{2/3} \kappa \varepsilon^{1/3} \geq \langle \tilde{g}, y - x \rangle \right\}$$

Lemma 4.29. h_x is $\left(\frac{R+\delta}{r-\delta}\right)$ -Lipschitz over points in $B_2(0, \delta)$ for any $\delta < r$.



Proof. Let d_1, d_2 be arbitrary points in $B(0, \delta)$. We wish to upper bound $|h_x(d_1) - h_x(d_2)|$ in terms of $\|d_1 - d_2\|_2$. We assume without loss of generality that $\alpha_x(d_1) \geq \alpha_x(d_2)$ and therefore

$$|h_x(d_1) - h_x(d_2)| = |\alpha_x(d_1) \|x\|_2 - \alpha_x(d_2) \|x\|_2| = (\alpha_x(d_1) - \alpha_x(d_2)) \|x\|_2.$$

Consequently, it suffices to lower bound $\alpha_x(d_2)$. We split the analysis into two cases.

Case 1: $\|d_2 - d_1\|_2 \geq r - \delta$. Since $0 \geq h_x(d_1), h_x(d_2) \geq -R - \delta$, we have that

$$|h_x(d_1) - h_x(d_2)| \leq R + \delta \leq \frac{R + \delta}{r - \delta} \|d_2 - d_1\|_2.$$

Case 2: $\|d_2 - d_1\|_2 \leq r - \delta$. We consider the point $d_3 = d_1 + \frac{d_2 - d_1}{\lambda}$ with $\lambda = \|d_2 - d_1\|_2 / (r - \delta)$. Note that

$$\|d_3\|_2 \leq \|d_1\|_2 + \frac{1}{\lambda} \|d_2 - d_1\|_2 \leq \delta + \frac{1}{\lambda} \|d_2 - d_1\|_2 \leq r.$$

Hence, $d_3 \in K$. Since $\lambda \in [0, 1]$ and K is convex, we have that $\lambda \cdot d_3 + (1 - \lambda) \cdot [d_1 + \alpha_x(d_1)x] \in K$. Now, we note that

$$\lambda \cdot d_3 + (1 - \lambda) \cdot [d_1 + \alpha_x(d_1)x] = d_2 + (1 - \lambda) \cdot \alpha_x(d_1)x$$

and this shows that

$$\alpha_x(d_2) \geq (1 - \lambda) \cdot \alpha_x(d_1) = \left(1 - \frac{\|d_2 - d_1\|_2}{r - \delta}\right) \cdot \alpha_x(d_1).$$

Since $d_1 + \alpha_x(d_1)x \in K \subset B_2(0, R)$, we have that $\alpha_x(d_1) \cdot \|x\|_2 \leq R + \delta$ and hence

$$|h_x(d_1) - h_x(d_2)| = (\alpha_x(d_1) - \alpha_x(d_2)) \cdot \|x\|_2 \leq \alpha_x(d_1) \cdot \|x\|_2 \frac{\|d_2 - d_1\|_2}{r - \delta} \leq \frac{R + \delta}{r - \delta} \|d_2 - d_1\|_2.$$

In either case, as claimed we have

$$|h_x(d_1) - h_x(d_2)| \leq \frac{R + \delta}{r - \delta} \|d_2 - d_1\|_2.$$

□

The next lemma shows that h_x gives us a way to implement an approximation separation oracle and only needs access to an approximation evaluation oracle for h_x which in turn only needs an approximate membership oracle for K . To be precise, we define approximate oracles.

Definition 4.30 (Separation Oracle (SEP)). Queried with a vector $y \in \mathbb{R}^n$ and real numbers $\delta, \delta' > 0$, with probability at least $1 - \delta'$, the oracle either

- assert that $y \in B(K, \delta)$, or
- find a unit vector $c \in \mathbb{R}^n$ such that $c^T x \leq c^T y + \delta$ for all $x \in B(K, -\delta)$.

We let $\text{SEP}_{\delta, \delta'}(K)$ be the time complexity of this oracle.

Definition 4.31 (Membership Oracle (MEM)). Queried with a vector $y \in \mathbb{R}^n$ and real numbers $\delta, \delta' > 0$, with probability at least $1 - \delta'$, either

- assert that $y \in B(K, \delta)$, or
- assert that $y \notin B(K, -\delta)$.

We let $\text{MEM}_{\delta, \delta'}(K)$ be the time complexity of this oracle.

We can now state the main lemma for the separation oracle. Since the algorithm is randomized, we have a parameter $\rho \in (0, 1)$ to denote the probability of failure.

Lemma 4.32. *Let K be a convex set satisfying $B_2(0, r) \subset K \subset B_2(0, R)$. Given any $0 < \rho < 1$ and $0 \leq \varepsilon \leq r$. With probability $1 - \rho$, $\text{Separate}_{\varepsilon, \rho}(K, x)$ outputs a halfspace that contains K .*

Proof. When $x \notin B_2(0, R)$, the algorithm outputs a valid separation for $B_2(0, R)$. For the rest of the proof, we assume $x \notin B(K, -\varepsilon)$ (due to the membership oracle) and $x \in B_2(0, R)$.

By Lemma 4.28 and Lemma 4.29, h_x is convex with Lipschitz constant 3κ on $B_2(0, \frac{r}{2})$. By our assumption on ε and our choice of r_1 , we have that $B_\infty(0, 2r_1) \subset B_2(0, \frac{r}{2})$. Hence, we can apply Lemma 4.23 to get that

$$h_x(y) \geq h_x(0) + \langle \tilde{g}, y \rangle - \zeta \|y\|_\infty - 12nr_1\kappa \quad (4.2)$$

for any $y \in K$. Note that $-\frac{x}{\kappa} \in K$ and $h_x(-\frac{x}{\kappa}) = h_x(0) - \frac{1}{\kappa} \|x\|_2$. Hence, we have

$$h_x(0) - \frac{1}{\kappa} \|x\|_2 = h_x(-\frac{1}{\kappa}x) \geq h_x(0) + \left\langle \tilde{g}, -\frac{1}{\kappa}x \right\rangle - \frac{1}{\kappa} \zeta \|x\|_\infty - 12nr_1\kappa.$$

Therefore, we have

$$\langle \tilde{g}, x \rangle \geq \|x\|_2 - \zeta \|x\|_\infty - 12nr_1\kappa^2. \quad (4.3)$$

Now, we note that $x \notin B(K, -\varepsilon)$. Using that $B(0, r) \subset K$, we have $(1 - \frac{\varepsilon}{r})K \subset B(K, -\varepsilon)$. Hence,

$$h_x(0) \geq -\left(1 - \frac{\varepsilon}{r}\right) \|x\|_2 \geq -\|x\|_2.$$

Therefore, we have

$$h_x(0) + \langle \tilde{g}, x \rangle \geq -\zeta \|x\|_\infty - 12nr_1\kappa^2$$

Combining this with (4.2), we have that

$$\begin{aligned} h_x(y) &\geq \langle \tilde{g}, y - x \rangle - \zeta \|y\|_\infty - \zeta \|x\|_\infty - 12nr_1\kappa - 12nr_1\kappa^2 \\ &\geq \langle \tilde{g}, y - x \rangle - 2\zeta R - 24nr_1\kappa^2 \end{aligned}$$

for any $y \in K$. Recall from Lemma 4.23 that ζ is a positive random scalar independent of y satisfying $\mathbf{E}\zeta \leq 2\sqrt{\frac{3\kappa\varepsilon}{r_1}}n^{5/4}$. For any $y \in K$, we have that $h_x(y) \leq 0$ and hence $\tilde{\zeta} \geq \langle \tilde{g}, y - x \rangle$ where $\tilde{\zeta}$ is a random scalar independent of y satisfying

$$\begin{aligned} \mathbf{E}\tilde{\zeta} &\leq 4\sqrt{\frac{3\kappa\varepsilon}{r_1}}n^{5/4}R + 24nr_1\kappa^2 \\ &\leq 31n^{7/6}R^{2/3}\varepsilon^{1/3}\kappa. \end{aligned}$$

where we used $r_1 = n^{1/6}\varepsilon^{1/3}R^{2/3}/\kappa$ and $0 \leq \varepsilon \leq r$. The result then follows using Markov's inequality. \square

Exercise 4.33. Suppose we can evaluate the subgradient of h_x exactly for a convex set K containing the origin. Give a short proof that for any $x \notin K$, we have $\langle \nabla h_x(0), y - x \rangle \leq 0$ for all $y \in K$.

Theorem 4.34. Let K be a convex set satisfying $B_2(0, 1/\kappa) \subset K \subset B_2(0, 1)$. For any $0 \leq \eta < \frac{1}{2}$, we have that

$$\text{SEP}_\eta(K) \leq O\left(n \log\left(\frac{n\kappa}{\eta}\right)\right) \text{MEM}_{(\eta/n\kappa)^{O(1)}}(K).$$

Proof. First, we bound the running time. Note that the bottleneck is to compute h_x with δ additive error. Since $-O(1) \leq h_x(y) \leq 0$ for all $y \in B_2(0, O(1))$, one can compute $h_x(y)$ by binary search with $O(\log(1/\delta))$ calls to the membership oracle.

Next, we check that $\text{Separate}_{\delta, \rho}(K, x)$ is indeed a separation oracle. Note that \tilde{g} may not be a unit vector and we need to re-normalize the \tilde{g} by $1/\|\tilde{g}\|_2$. So, we need a lower bound $\|\tilde{g}\|_2$.

From (4.3) and our choice of r_1 , if $\delta \leq \frac{\rho^3}{10^6 n^6 \kappa^6}$, then we have that

$$\langle \tilde{g}, x \rangle \geq \|x\|_2 - \zeta \|x\|_\infty - 12nr_1\kappa^2 \geq \frac{r}{4}.$$

Hence, we have that $\|\tilde{g}\|_2 \geq \frac{1}{4\kappa}$. Therefore, this algorithm is a separation oracle with error $\frac{400}{\rho}n^{7/6}\kappa^2\delta^{1/3}$ and failure probability $O(\rho + \log(1/\delta)\delta)$.

$$\text{SEP}_{\Omega(\max(n^{7/6}\kappa^2\delta^{1/3}/\rho + \rho + \log(1/\delta)\delta))}(K) \leq O(\log(1/\delta))\text{MEM}_\delta(K).$$

Setting $\rho = \sqrt{n^{7/6}\kappa^2\delta^{1/3}}$ and $\delta = \Theta\left(\frac{\eta^6}{n^{7/2}\kappa^6}\right)$, we have that

$$\text{SEP}_\eta(K) \leq O(\log(\frac{n\kappa}{\eta}))\text{MEM}_{\eta^6/(n^{7/2}\kappa^6)}(K).$$

\square

■ 4.3.1 Gradient from Evaluation via Auto Differentiation

In this section, we give yet another way to compute gradients using evaluations.

Theorem 4.35. Given a function $f : \mathbb{R}^n \rightarrow \mathbb{R}$ represented by an circuit whose gates compute differentiable functions of a finite number of variables. Suppose that $f(x)$ can be computed in time \mathcal{T} (namely, the circuit has \mathcal{T} edges). Then we can compute $\nabla f(x)$ in $O(\mathcal{T})$ time.

Remark. In practice, the runtime is roughly $2\mathcal{T}$ assuming we have enough memory. Check out google/jax for a modern implementation.

Before proving it formally, we first go through an example. Consider the function $f(x_1, x_2) = \sin(x_1/x_2) + x_1x_2$. We use x_i to denote both the input and all intermediate variables. Then, we can write the program in $\mathcal{T} = 6$ steps:

• $x_1 = x_1, x_2 = x_2, x_3 = x_1/x_2, x_4 = \sin(x_3), x_5 = x_1x_2$, Output $x_6 = x_4 + x_5$.
 Note that each step involves computing

$$x_i = f_i(\overbrace{(x_1, \dots, x_{i-1})}^{\text{only few } x_j})$$

with simple functions f_i whose derivatives we know how to compute. The key idea is compute $\frac{\partial f}{\partial x_1}$ not just for the inputs x_1 and x_2 , but also for all intermediate variables. Here, we use $\frac{\partial f}{\partial x_i}$ to denote the derivative of f with respect to x_i while fixing x_1, x_2, \dots, x_{i-1} (and other inputs if x_i is an input). For the example above, suppose we want to compute $\nabla f(\pi, 2)$, we can simply compute first compute all x_i from $i = 1, 2, \dots, 6$, then $\frac{\partial f}{\partial x_i}$ in the reverse order from $i = 6, 5, \dots, 1$:

- $x_1 = \pi, x_2 = 2, x_3 = \pi/2, x_4 = \sin(x_3) = 1, x_5 = x_1x_2 = 2\pi, x_6 = x_4 + x_5 = 2\pi + 1$.
- $\frac{\partial f}{\partial x_6} = 1, \frac{\partial f}{\partial x_5} = \frac{\partial(x_4+x_5)}{\partial x_5} = 1, \frac{\partial f}{\partial x_4} = \frac{\partial(x_4+x_5)}{\partial x_4} = 1$,
- $\frac{\partial f}{\partial x_3} = \frac{\partial f}{\partial x_4} \frac{\partial x_4}{\partial x_3} = 1 \cdot \cos(x_3) = 0$,
- $\frac{\partial f}{\partial x_2} = \frac{\partial f}{\partial x_3} \frac{\partial x_3}{\partial x_2} + \frac{\partial f}{\partial x_5} \frac{\partial x_5}{\partial x_2} = 0 \cdot (-\frac{x_1}{x_2^2}) + 1 \cdot x_1 = \pi$,
- $\frac{\partial f}{\partial x_1} = \frac{\partial f}{\partial x_3} \frac{\partial x_3}{\partial x_1} + \frac{\partial f}{\partial x_5} \frac{\partial x_5}{\partial x_1} = 0 \cdot (\frac{1}{x_2}) + 1 \cdot x_2 = 2$.

The general case is similar. See `AutoDifferentiation` for the algorithm.

Algorithm 12: AutoDifferentiation

Input: a function $f(x_1, x_2, \dots, x_n)$ given by $f(x_1, x_2, \dots, x_n) = x_m$ and

$$x_i = f_i(x_1, \dots, x_{i-1}) \text{ for } i = n+1, n+2, \dots, m$$

for $i = n+1, n+2, \dots, m$ **do**

 | Compute $x_i = f_i(x_1, \dots, x_{i-1})$.

end

Let $\frac{\partial f}{\partial x_m} = 1$.

for $i = m-1, \dots, 1$ **do**

 | Let L_i be the set of j such that f_j depends on x_i (i.e. x_j directly depends on x_i).

 | Compute $\frac{\partial f}{\partial x_i} = \sum_{j \in L_i} \frac{\partial f}{\partial x_j} \frac{\partial x_j}{\partial x_i}$.

end

Proof of Theorem 4.35. We prove by induction that the formula $\frac{\partial f}{\partial x_i} = \sum_{j \in L_i} \frac{\partial f}{\partial x_j} \frac{\partial x_j}{\partial x_i}$ is correct. For the base case $i = m$, we have $f = x_m$ and hence $\frac{\partial f}{\partial x_m} = 1$. For the induction, we let $L_i = \{x_{j_1}, x_{j_2}, \dots, x_{j_k}\}$. If we fix variables x_1, x_2, \dots, x_{i-1} , then f is a function of x_i (and of other inputs if x_i is an input). Since only $x_{j_1}, x_{j_2}, \dots, x_{j_k}$ depend on x_i , we can also view f as a function of $x_{j_1}, x_{j_2}, \dots, x_{j_k}$. More precisely, we have

$$f(x_i) = f(x_{j_1}(x_i, x_{j_{-1}}), x_{j_2}(x_i, x_{j_{-2}}), \dots, x_{j_k}(x_i, x_{j_{-k}}))$$

where we use $x_{j_{-1}}$ to denote the variables $x_{j_2}, x_{j_3}, \dots, x_{j_k}$. By chain rule, we have

$$\frac{\partial f}{\partial x_i} = \sum_{j \in L_i} \frac{\partial f}{\partial x_j} \frac{\partial x_j}{\partial x_i}.$$

To bound the runtime, we define the computation graph G be a graph on x_1, x_2, \dots, x_m such that $i \rightarrow j$ if f_j depends on x_i . Note that each edge is examined $O(1)$ times whether evaluating f or its gradient. Hence, the cost of computing f and the cost of our algorithm are both $\Theta(m)$ where m is the number of edges in G . This completes the proof. \square

We note that an efficient implementation of the chain rule is the heart of the backpropagation algorithm for neural networks. To conclude this section, we see that Theorem 4.35 can be surprisingly useful even for some simple explicit functions.

Corollary 4.36. *If we can compute $f(A) = \det A$ exactly in time \mathcal{T} , then we can compute A^{-1} exactly in $O(\mathcal{T})$.*

Proof. Note that $\frac{\partial}{\partial A_{ij}} \det A = \text{adj}(A)_{ji} = \det A \cdot (A^{-1})_{ji}$. Hence, $\nabla \log \det A = A^{-\top}$. Theorem 4.35 shows that computing $A^{-\top}$ can be done as fast as $\det A$. \square

■ 4.3.2 Gradient from Evaluation via Complex Step Differentiation

Auto differentiation is great if the function can be computed exactly. However, it does not work well if f can be only approximated or the computation of f involves too many variables. For example, if f is the energy usage of some aircraft design, then f can only be computed approximately via simulation and such computation is memory expensive (if we need to store all intermediate variables) and not exact, so the method in the previous subsection is not practical.

To introduce complex step differentiation, we recall the formula of finite difference:

- Forward/Backward difference: $\frac{f(x \pm h) - f(x)}{\pm h} = f'(x) + hf''(\zeta)$.
- Central difference: $\frac{f(x+h) - f(x-h)}{2h} = f'(x) + O(h^2)f'''(\zeta)$.

Note that the error analysis above assumes no numerical error involved. The formula involves subtracting two close numbers and dividing by a small number and this step creates lots of error. If we are computing f as floating point, we have

$$\begin{aligned} \frac{(1 \pm \epsilon)f(x \pm h) - (1 \pm \epsilon)f(x)}{\pm h} &= f'(x) + O\left(\frac{\epsilon}{h}\right)f(\zeta_1) + O(h)f''(\zeta_2) \\ \frac{(1 \pm \epsilon)f(x+h) - (1 \pm \epsilon)f(x-h)}{2h} &= f'(x) + O\left(\frac{\epsilon}{h}\right)f(\zeta_1) + O(h^2)f'''(\zeta_2) \end{aligned}$$

where ϵ is the floating point precision. Suppose that f, f', f'', f''' are all bounded by constants and suppose $\epsilon = (10)^{-8}$ (single precision floating point), then we should pick $h = \sqrt{\epsilon}$ for the first case and $h = \epsilon^{1/3}$ in the second case. Hence, forward/backward difference gives only accuracy $\epsilon^{1/2} \approx (10)^{-4}$ and the central difference gives only accuracy $\epsilon^{2/3} \approx (10)^{-5}$. In reality, the error will be larger because f'' and f''' usually are large.

The complex step differentiation uses the step

$$\frac{\text{Im}f(x + ih)}{h} \approx f'(x) + O(h^2)f''(\zeta).$$

This formula works only for complex analytic functions, but it avoids subtracting numbers. In practice, this really allows us to compute $f'(x)$ close to machine accuracy. In general, ensuring algorithms give close to machine accuracy is important because algorithms often stack on top of each other.

■ 4.4 Composite Problem via Duality

■ 4.4.1 Motivation

In this section, we will discuss a few algorithmic applications of duality. In general, two reasons to consider a dual problem are that (1) the dual problem might have smaller dimension and (2) (sub)gradients are easier to compute. We will see such examples.

Suppose we have a “difficult” convex problem $\min_x f(x)$, i.e., one that does not satisfy some smoothness condition which directly suggests a faster than worst-case optimization method. Often, we can decompose the difficult problem as $f(x) = g(x) + h(Ax)$ such that the (sub)gradients $\nabla g^*(x)$ and $\nabla h^*(x)$ are easy to compute. Then, it is useful to compute its dual as follows:

$$\begin{aligned} \min_x g(x) + h(Ax) &= \min_x \max_{\theta} g(x) + \theta^\top Ax - h^*(\theta) \\ &= \max_{\theta} \min_x g(x) + (A^\top \theta)^\top x - h^*(\theta) \\ &= \max_{\theta} -g^*(-A^\top \theta) - h^*(\theta) \\ &= -\min_{\theta} g^*(-A^\top \theta) + h^*(\theta) \end{aligned}$$

where we used $h = h^{**}$ in the first line, the following minimax theorem on the second line, and the definition of g^* on the third line.

Theorem 4.37 (Sion's minimax theorem). *Let $X \subset \mathbb{R}^n$ be a compact convex set and $Y \subset \mathbb{R}^m$ be a convex set. If $f : X \times Y \rightarrow \mathbb{R} \cup \{+\infty\}$ such that $f(x, \cdot)$ is upper semi-continuous and quasi-concave on Y for all $x \in X$ and $f(\cdot, y)$ is lower semi-continuous and quasi-convex on X for all $y \in Y$. Then, we have*

$$\min_{x \in X} \sup_{y \in Y} f(x, y) = \sup_{y \in Y} \min_{x \in X} f(x, y).$$

Remark. Compactness is necessary. Consider $f(x, y) = x + y$. This theorem generalizes Von Neumann's minimax theorem.

We call “ $g(x) + h(Ax)$ ” the primal problem and “ $g^*(-A^\top \theta) + h^*(\theta)$ ” the dual problem. Often, the dual problem gives us some insight on the primal problem. However, we note that there are many ways to split a problem into two and hence many candidate dual problems.

Example 4.38. Consider the unit capacity flow problem on a graph $G = (V, E)$:

$$\max_{Af=d, -1 \leq f \leq 1} c^\top f$$

where $f \in \mathbb{R}^E$ is the flow vector, $A \in \mathbb{R}^{V \times E}$ encodes the vertex-edge adjacency matrix with two nonzeros per column, d is the demand vector so that $Af = d$ is flow conservation, and c is the cost vector. We can write the dual as follows:

$$\begin{aligned} \max_{Af=d, -1 \leq f \leq 1} c^\top f &= \max_{-1 \leq f \leq 1} \min_{\phi} c^\top f - \phi^\top (Af - d) \\ &= \min_{\phi} \max_{-1 \leq f \leq 1} \phi^\top d + (c - A^\top \phi)^\top f \\ &= \min_{\phi} \phi^\top d + \sum_{e \in E} |c - A^\top \phi|_e. \end{aligned}$$

When $c = 0$ and $d = F \cdot 1_{st}$ this is the maximum flow problem with flow value F , and the dual problem is the minimum $s - t$ cut problem with the cut given by $\{v \in V \text{ such that } \phi(v) \geq t\}$. We can view ϕ as assigning a “potential” to every vertex of the graph. Note that there are $|E|$ variables in primal and $|V|$ variables in dual. So, in this sense, the dual problem is easier for dense graphs. Although we do not have a way to turn a minimum $s - t$ cut to a maximum $s - t$ flow in general, we will see various tricks to reconstruct the primal solution from the dual solution by modifying the problem.

■ 4.4.2 Example: Semidefinite Programming

When you can solve the dual problem, the proof of the optimality of the dual problem often directly gives you the solution of the primal problem, or gives you some way to solve the primal problem efficiently. Here, we use the semidefinite programming as an concrete example. Define \bullet as the inner product of matrices, i.e.,

$$A \bullet B = \sum_{i,j} A_{ij} B_{ij}.$$

Consider the semidefinite programming (SDP) problem:

$$\max_{X \succeq 0} C \bullet X \text{ s.t. } A_i \bullet X = b_i \text{ for } i = 1, 2, \dots, m \quad (4.4)$$

and its dual

$$\min_y b^\top y \text{ s.t. } \sum_{i=1}^m y_i A_i \succeq C \quad (4.5)$$

where X, C, A_i are $n \times n$ symmetric matrices and $b, y \in \mathbb{R}^m$. SDP is a generalization of linear programming and is useful for various problems involving matrices. If we apply the current-best cutting plane method

naively on the primal problem, we would get $\tilde{O}(n^2(Z + n^4))$ time algorithm for the primal (because there are n^2 variables) and $\tilde{O}(m(Z + n^\omega + m^2))$ for the dual where Z is the total number of non-zeros in A_i . (The term $Z + n^\omega$ is the cost of computing $\sum y_i A_i$ and finding its minimum eigenvalue.) Generally, $n^2 \gg m$ and hence it takes much less time to solve the dual.

We note that

$$\min_{\sum_{i=1}^m y_i A_i \succeq C} b^\top y = \min_{v^\top (\sum_{i=1}^m y_i A_i - C) v \geq 0 \ \forall \|v\|_2=1} b^\top y.$$

In each step of the cutting plane method, the (sub)gradient oracle either outputs b or outputs one of the cutting planes

$$v^\top (\sum_{i=1}^m y_i A_i - C) v \geq 0.$$

Let S be the set of all cutting planes used in the algorithm. Then, the proof of the cutting plane method shows that

$$\min_{\sum_{i=1}^m y_i A_i \succeq C} b^\top y = \min_{v^\top (\sum_{i=1}^m y_i A_i - C) v \geq 0 \ \forall v \in S} b^\top y \pm \varepsilon. \quad (4.6)$$

The key idea to obtaining the primal solution is to take the dual of the right hand side (which is an approximate dual of the original problem). Now, we have

$$\begin{aligned} \min_{v^\top (\sum_{i=1}^m y_i A_i - C) v \geq 0 \ \forall v \in S} b^\top y &= \min_y \max_{\lambda_v \geq 0} b^\top y - \sum_{v \in S} \lambda_v v^\top (\sum_{i=1}^m y_i A_i - C) v \\ &= \max_{\lambda_v \geq 0} \min_y C \bullet \sum_{v \in S} \lambda_v v v^\top + b^\top y - \sum_{i=1}^m y_i \sum_{v \in S} \lambda_v v v^\top \bullet A_i \\ &= \max_{X = \sum_{v \in S} \lambda_v v v^\top, \lambda_v \geq 0} \min_y C \bullet X + \sum_{i=1}^m y_i (b_i - X \bullet A_i) \\ &= \max_{X = \sum_{v \in S} \lambda_v v v^\top, \lambda_v \geq 0, X \bullet A_i = b_i} C \bullet X. \end{aligned}$$

Note that this is exactly the primal SDP problem, except that we restrict the set of solutions to the form $\sum_{v \in S} \lambda_v v v^\top$ with $\lambda_v \geq 0$. Also, we can write this problem as a linear program:

$$\max_{\sum_v \lambda_v v v^\top A_i v = b_i \text{ for all } i, \lambda_v \geq 0} \sum_v \lambda_v v^\top C v. \quad (4.7)$$

Therefore, we can simply solve this linear program and recover an approximate solution for the SDP. By (4.6), we know that this is an approximate solution with the same guarantee as the dual SDP.

Now, we analyze the runtime of this algorithm. This algorithm contains two phases: solve the dual SDP via cutting plane method, and solve the primal linear program. Note that each step of the cutting plane method involves finding a separating hyperplane of $\sum_{i=1}^m y_i A_i \succeq C$.

Exercise 4.39. Let $\Omega = \{y \in \mathbb{R}^m : \sum_{i=1}^m y_i A_i \succeq C\}$. Show that one can implement the separation oracle in time $O^*(Z + n^\omega)$ via eigenvalue computation.

Therefore, the first phase takes $O^*(m(Z + n^\omega + m^2))$ time in total. Since the cutting plane method takes $O^*(m)$ steps, we have $|\mathcal{S}| = O^*(m)$. In the second phase, we need to solve a linear program (4.7) with $O^*(m)$ variables with $O(m)$ constraints. It is known how to solve such linear programs in time $O^*(m^{2.38})$ [18]. Hence, the total cost is dominated by the first phase

$$O^*(mZ + mn^\omega + m^3).$$

Problem 4.40. In the first phase, each step involves computing an eigenvector of similar matrices. So, can we use matrix update formulas to decrease the cost per step in the cutting plane to $O^*(Z + n^2)$? Namely, can we solve SDP in time $O^*(mZ + m^3)$?

■ 4.4.3 Duality and Convex Hull

The problem $\min_x g(x) + h(Ax)$ in general can be solved by a similar trick. To make this geometric picture clearer, we consider its linear optimization version: $\min_{(x,t_1) \in \text{epi } g, (Ax,t_2) \in \text{epi } h} t_1 + t_2$. To simplify the notation, we consider the problem

$$\min_{x \in K_1, Mx \in K_2} c^\top x$$

where $M \in \mathbb{R}^{m \times n}$, and we have convex sets $K_1 \subset \mathbb{R}^n$ and $K_2 \subset \mathbb{R}^m$.

To be concrete, let us consider the following example. Let V_1 be a set of students, V_2 be a set of schools. Each edge $e \in E$ represents a possible choice of a student. Let w_e be the happiness of a school/student if the student is assigned to that school. Suppose that every student can only be assigned to one school and school b can accept c_b students. Then, the problem can be formulated as

$$\max_{x_e \geq 0} \sum_{e \in E} w_e x_e \text{ subject to } \sum_{(a,b) \in E} x_{(a,b)} \leq 1 \quad \forall a \in V_1, \quad \sum_{(a,b) \in E} x_{(a,b)} \leq c_b \quad \forall b \in V_2.$$

This is the weighted b-matching problem. Typically, the number of students is much more than the number of schools. Therefore, an algorithm with running time linear in the number of students is preferable. To apply our framework, we let

$$K_1 = \{x \in \mathbb{R}^E, x_e \geq 0, \sum_{(a,b) \in E} x_{(a,b)} \leq 1 \quad \forall a \in V_1\},$$

$$K_2 = \{y \in \mathbb{R}^{V_2}, y_b \leq c_b\},$$

and $M \in \mathbb{R}^E \rightarrow \mathbb{R}^{V_2}$ is the map $(Tx)_b = \sum_{a:(a,b) \in E} x_{(a,b)}$.

To further emphasize its importance, consider some general examples here:

- Linear programming: $\min_{Ax=b, x \geq 0} c^\top x$: $K_1 = \{x \geq 0\}$, $K_2 = \{b\}$ and $M = A$.
- Semidefinite programming: $\min_{A_i \bullet X = b_i, X \succeq 0} C \bullet X$: $K_1 = \{X \succeq 0\}$, $K_2 = \{b\}$ and $M : \mathbb{R}^{n \times n} \rightarrow \mathbb{R}^m$ defined by $(MX)_i = A_i \bullet X$.
- Matroid intersection: $\min_{x \in M_1 \cap M_2} 1^\top x$: $K_1 = M_1$ and $K_2 = M_2$, $M = I$.
- Submodular minimization: $K_1 = \{y \in \mathbb{R}^n : \sum_{i \in S} y_i \leq f(S) \text{ for all } S \subset [n]\}$, $K_2 = \{y \leq 0\}$, $M = I$.
- Submodular flow: $K_1 = \{\varphi \in \mathbb{R}^E, \ell_e \leq \varphi_e \leq u_e \text{ for all } e \in E\}$, $K_2 = \{y \in \mathbb{R}^V : \sum_{i \in S} y_i \leq f(S) \text{ for all } S \subset [n]\}$, M is the incidence matrix.

In all of these examples, it is easy to compute the gradient of $\delta_{K_1}^*$ and $\delta_{K_2}^*$. For the last three examples, it is not clear how to compute gradient of δ_{K_1} and/or δ_{K_2} directly. Furthermore, in all examples, M maps from a larger space to the same or smaller space. Therefore, it is good to take advantage of the smaller space.

Before [43], the standard way was to use the equivalence of $\nabla \delta_{K_1}^*$ and $\nabla \delta_{K_1}$, and apply cutting plane methods. With the running time of cutting plane methods, such an algorithm usually had theoretical running time at least n^5 and was of little practical value.

Now we rewrite the problem as we did in the beginning:

$$\begin{aligned} \min_{x \in K_1, Mx \in K_2} c^\top x &= \min_{x \in \mathbb{R}^n} c^\top x + \delta_{K_1}(x) + \delta_{K_2}(Mx) \\ &= \min_{x \in \mathbb{R}^n} \max_{\theta \in \mathbb{R}^m} c^\top x + \delta_{K_1}(x) + \theta^\top Mx - \delta_{K_2}^*(\theta) \\ &= \max_{\theta \in \mathbb{R}^m} \min_{x \in \mathbb{R}^n} c^\top x + \delta_{K_1}(x) + \theta^\top Mx - \delta_{K_2}^*(\theta) \\ &= \max_{\theta \in \mathbb{R}^m} -\delta_{K_1}^*(-c - M^\top \theta) - \delta_{K_2}^*(\theta). \end{aligned}$$

Taking the dual has two benefits. First, the number of variables is smaller. Second, the gradient oracle is something we can compute efficiently. Hence, cutting plane methods can be used to solve it in $O^*(m\mathcal{T} + m^3)$ where \mathcal{T} is the time to evaluate $\nabla \delta_{K_1}^*$ and $\nabla \delta_{K_2}^*$. The only problem left is to recover the primal x .

The key observation is the following lemma:

Lemma 4.41. *Let $x_i \in K_1$ be the set of points output by the oracle $\nabla \delta_{K_1}^*$ during the cutting plane method. Define $y_i \in K_2$ similarly. Suppose that the cutting plane method ends with the guarantee that the additive*

error is less than ε . Then, we have that

$$\min_{x \in K_1, Tx \in K_2} c^\top x \leq \min_{x \in \widetilde{K}_1, Tx \in \widetilde{K}_2} c^\top x \leq \min_{x \in K_1, Tx \in K_2} c^\top x + \varepsilon$$

where $\widetilde{K}_1 = \text{conv}(x_i)$ and $\widetilde{K}_2 = \text{conv}(y_i)$.

Proof. Let θ_i be the set of directions queried by the oracle for $\nabla \delta_{K_1}^*$ and φ_i be the directions queried by the oracle for $\nabla \delta_{K_2}^*$. We claim that $x_i \in \nabla \delta_{\widetilde{K}_1}^*(\theta_i)$ and $y_i \in \nabla \delta_{\widetilde{K}_2}^*(\varphi_i)$. Having this, the algorithm cannot distinguish between \widetilde{K}_1 and K_1 , and between \widetilde{K}_2 and K_2 . Hence, the algorithm runs exactly the same, i.e., uses the same sequence of points. Therefore, we get the same value $c^\top x$. However, by the guarantee of cutting plane method, we have that

$$\min_{x \in \widetilde{K}_1, Tx \in \widetilde{K}_2} c^\top x \leq c^\top x \leq \min_{x \in K_1, Tx \in K_2} c^\top x + \varepsilon.$$

To prove the claim, we note that $x_i \in \nabla \delta_{\widetilde{K}_1}^*(\theta_i)$. Note that $\widetilde{K}_1 \subset K_1$ and hence $\min_{x \in \widetilde{K}_1} \theta_i^\top x \geq \min_{x \in K_1} \theta_i^\top x$. Also, note that

$$x_i = \arg \min_{x \in K_1} \theta_i^\top x \in \widetilde{K}_1$$

and hence $\min_{x \in \widetilde{K}_1} \theta_i^\top x \leq \min_{x \in K_1} \theta_i^\top x$. Therefore, we have that $\min_{x \in \widetilde{K}_1} \theta_i^\top x = \min_{x \in K_1} \theta_i^\top x$. Therefore, $x_i \in \arg \min_{x \in K_1} \theta_i^\top x$. This proves the claim for \widetilde{K}_1 . The proof for \widetilde{K}_2 is the same. \square

This reduces the problem into the form $\min_{x \in \widetilde{K}_1, Tx \in \widetilde{K}_2} c^\top x$. For the second phase, we let $z_i = Mx_i \in \mathbb{R}^m$. Then, we have

$$\begin{aligned} \min_{x \in \widetilde{K}_1, Mx \in \widetilde{K}_2} c^\top x &= \min_{t_i \geq 0, s_i \geq 0, M \sum_i t_i x_i = \sum_i s_i y_i} c^\top \left(\sum_i t_i x_i \right) \\ &= \min_{t_i \geq 0, s_i \geq 0, \sum_i t_i z_i = \sum_i s_i y_i} \sum_i t_i \cdot c^\top x_i. \end{aligned}$$

Note that it takes $O^*(mZ)$ time to write down this linear program where Z is the number of non-zeros in M . Next, we note that this linear program has $O^*(m)$ variables and m constraints. Therefore, we can solve it in $O^*(m^{2.38})$ time.

Therefore, the total running time is

$$O^*(m(\mathcal{T} + m^2) + (mZ + m^{2.38})).$$

To conclude, we have the following theorem.

Theorem 4.42. *Given convex sets $K_1 \subset \mathbb{R}^n$ and $K_2 \subset \mathbb{R}^m$ with $m \leq n$ and a matrix $M : \mathbb{R}^n \rightarrow \mathbb{R}^m$ with Z non-zeros, let \mathcal{T} be the cost to compute $\nabla \delta_{K_1}^*$ and $\nabla \delta_{K_2}^*$. Then, we can solve the problem*

$$\min_{x \in K_1, Mx \in K_2} c^\top x$$

in time $O^(m\mathcal{T} + mZ + m^3)$.*

Remark. We hid all sorts of terms in the log term hidden in O^* such as the diameter of the set. Also this is the number of arithmetic operations, not the bit complexity.

Going back to the school/student problem, this algorithm gives a running time of

$$O^*(|V_2||E| + |V_2|^3)$$

which is linear in the number of students!

In general, this statement says that if we can split a convex problem into two parts, with both being easy to solve and one part having fewer variables, then we can solve the entire problem in time depending on the smaller dimension.

Exercise 4.43. How fast can we solve $\min_{x \in \cap_{i=1}^k K_i} c^\top x$ given the oracles $\nabla \delta_{K_i}^*$?

In this chapter, we study techniques that further exploit the geometry of convex functions and associated norms. Many of these techniques are effective in practice for large scale problems. We recall the following relevant definitions.

■ 5.1 Norms and Local Metrics

Any 0-symmetric convex body K induces the following norm:

$$\|x\|_K = \inf \{t : x \in tK\}.$$

For the usual Euclidean norm, the convex body is the Euclidean ball, B_2^n . Similarly, for an ℓ_p norm, the convex body is the unit ℓ_p ball.

It is often useful to consider affine transformations, and the norms they induce, e.g., for a PSD matrix A , we can define the associated norm as follows:

$$\|x\|_A = \sqrt{x^\top A x}.$$

The convex body (unit ball) of this norm is an ellipsoid centered at zero and defined by the matrix A .

As we have encountered previously in this book, convex sets and functions have duals. For a convex body K , the dual (or polar) is defined as follows:

$$K^* = \{y : \forall x \in K, \langle x, y \rangle \leq 1\}.$$

The dual norm for $\|\cdot\|_K$ is $\|\cdot\|_{K^*}$. We can state a generalized Cauchy-Schwarz inequality.

Fact 5.1. *For $x, y \in \mathbb{R}^n$ and any centrally symmetric convex body K , we have $\langle x, y \rangle \leq \|x\|_K \|y\|_{K^*}$.*

In this chapter, an important idea will be *local* norms, i.e., at each point x in the domain, there could be a different norm. Indeed, in a Riemannian metric \mathcal{M} , for every $x \in \mathcal{M}$, there is a matrix $A(x)$ s.t. the norm at x is defined as $\|v\|_x = \sqrt{v^\top A(x)v}$. A special class of Riemannian metrics of particular interest for us will be *Hessian* metrics (corresponding to Hessian manifolds). Here the matrix defining the local norm is the Hessian of a convex, twice-differentiable function, i.e.,

$$A(x) = \nabla^2 \phi(x)$$

for some convex function ϕ .

■ 5.2 Mirror Descent

The cutting plane method is well-suited for minimizing non-smooth convex functions with high accuracy. However, its relatively large polynomial time complexity and quadratic space requirement are not favorable for large scale problems. Here we discuss a different approach to minimize a non-smooth function with low accuracy.

■ 5.2.1 Subgradient method

In this section, we consider the constrained non-smooth minimization problem $\min_{x \in \mathcal{D}} f(x)$. Recall how to define gradient for non-smooth functions:

Definition 5.2. For any convex function f , we define $\partial f(x)$ be the set of vectors g such that

$$f(y) \geq f(x) + g^\top (y - x) \text{ for all } y \in \mathbb{R}^n.$$

Such a vector g is called a *subgradient* of f at x .

Algorithm 13: SubgradientMethod

Input: Initial point $x^{(0)} \in \mathbb{R}^n$, step size $h > 0$.
for $k = 0, 1, \dots, T - 2$ **do**
 Pick any $g^{(k)} \in \partial f(x^{(k)})$.
 $y^{(k+1)} \leftarrow x^{(k)} - h \cdot g^{(k)}$.
 $x^{(k+1)} \leftarrow \pi_{\mathcal{D}}(y^{(k+1)})$ where $\pi_{\mathcal{D}}(y) = \arg \min_{x \in \mathcal{D}} \|x - y\|_2$
end
return $\frac{1}{T} \sum_{k=0}^{T-1} x^{(k)}$.

Note that we return the average of all iterates, rather than the last iterate, as the average is better behaved in the worst case. To analyze the algorithm, we first need the following Pythagorean theorem. This shows that when we project a point to a convex set, we get closer to each point in the convex set, and how much closer depends on how much we move.

Lemma 5.3 (Pythagorean Theorem). *Given a convex set \mathcal{D} and a point y , let $\pi(y) = \arg \min_{x \in \mathcal{D}} \|x - y\|_2$. For any $z \in \mathcal{D}$, we have that*

$$\|z - \pi(y)\|_2^2 + \|\pi(y) - y\|_2^2 \leq \|z - y\|_2^2.$$

Proof. Let $h(t) = \|(\pi(y) + t(z - \pi(y))) - y\|^2$. Since $\pi(y)$ is the closest point to y , $h(t)$ must be minimized at $t = 0$. So, we have that $h'(0) \geq 0$. i.e.,

$$h'(0) = (\pi(y) - y)^\top (z - \pi(y)) \geq 0.$$

(If y is in the set, then the statement is trivial since $\pi(y) = y$. Otherwise, since $\pi(y)$ is the closest point in \mathcal{D} to y , the hyperplane normal to $\pi(y) - y$ through $\pi(y)$ separates y from z .) Hence,

$$\begin{aligned} \|z - y\|_2^2 &= \|z - \pi(y) + \pi(y) - y\|_2^2 \\ &= \|z - \pi(y)\|_2^2 + 2(z - \pi(y))^\top (\pi(y) - y) + \|\pi(y) - y\|_2^2 \\ &\geq \|z - \pi(y)\|_2^2 + \|\pi(y) - y\|_2^2. \end{aligned}$$

□

Now, we are ready to analyze the subgradient method. It basically involves tracking the squared distance to the optimum, $\|x^{(k+1)} - x^*\|_2^2$.

Theorem 5.4. *Let f be a convex function that is G -Lipschitz in ℓ_2 norm. After T steps, the subgradient method outputs a point x such that*

$$f(x) \leq f(x^*) + \frac{\|x^{(0)} - x^*\|_2^2}{2hT} + \frac{h}{2}G^2$$

where x^* is any point that minimizes f over \mathcal{D} .

Remark. If the distance $\|x^{(0)} - x^*\|$ and the Lipschitz constant G are known, we can pick $h = \frac{\|x^{(0)} - x^*\|_2}{G\sqrt{T}}$ and get

$$f(x) \leq f(x^*) + \frac{G \cdot \|x^{(0)} - x^*\|_2}{\sqrt{T}}.$$

Proof. Let x^* be any point that minimizes f . Then, we have

$$\begin{aligned}\|x^{(k+1)} - x^*\|_2^2 &= \|\pi_{\mathcal{D}}(y^{(k+1)}) - x^*\|_2^2 \\ &\leq \|y^{(k+1)} - x^*\|_2^2 \\ &= \|x^{(k)} - hg^{(k)} - x^*\|_2^2 \\ &= \|x^{(k)} - x^*\|_2^2 - 2h \langle g^{(k)}, x^{(k)} - x^* \rangle + h^2 \|g^{(k)}\|_2^2.\end{aligned}$$

where we used Lemma 5.3 in the inequality. Since x^* lies on the $-g^{(k)}$ direction, we expect $x^{(k+1)}$ is closer to x^* than $x^{(k)}$ if the step size is small enough (or if we ignore the second order term $\|g^{(k)}\|_2^2$). To bound the distance improvement, we apply the definition of subgradient and get

$$f(x^*) \geq f(x^{(k)}) + \langle g^{(k)}, x^* - x^{(k)} \rangle.$$

Therefore, we have that

$$\begin{aligned}\|x^{(k+1)} - x^*\|_2^2 &\leq \|x^{(k)} - x^*\|_2^2 - 2h \cdot (f(x^{(k)}) - f(x^*)) + h^2 \|g^{(k)}\|_2^2 \\ &\leq \|x^{(k)} - x^*\|_2^2 - 2h \cdot (f(x^{(k)}) - f(x^*)) + h^2 G^2.\end{aligned}$$

Note that this equation shows that if the error $f(x^{(k)}) - f(x^*)$ is larger, then we move faster towards the optimum. Rearranging the terms, we have

$$f(x^{(k)}) - f(x^*) \leq \frac{1}{2h} \left(\|x^{(k)} - x^*\|_2^2 - \|x^{(k+1)} - x^*\|_2^2 \right) + \frac{h}{2} G^2.$$

We sum over all iterations, to get

$$\begin{aligned}\frac{1}{T} \sum_{k=0}^{T-1} (f(x^{(k)}) - f(x^*)) &\leq \frac{1}{T} \cdot \frac{1}{2h} (\|x^{(0)} - x^*\|_2^2 - \|x^{(T)} - x^*\|_2^2) + \frac{h}{2} G^2 \\ &\leq \frac{\|x^{(0)} - x^*\|_2^2}{2hT} + \frac{h}{2} G^2.\end{aligned}$$

The result follows from observing that for a convex function,

$$f\left(\frac{1}{T} \sum_{k=0}^{T-1} x^{(k)}\right) - f(x^*) \leq \frac{1}{T} \sum_{k=0}^{T-1} (f(x^{(k)}) - f(x^*)).$$

□

■ 5.2.2 Intuition of Mirror Descent

Consider using the subgradient method above to minimize $f(x) = \sum_i |x_i|$ over the unit ball $B(0, 1)$. The subgradient of f is given by $\text{sign}(x)$ (assuming $x_i \neq 0$ for all i). Therefore, we have that the Lipschitz constant is bounded by the Euclidean norm of a vector with ± 1 entries, i.e., $G = \sqrt{n}$ and the set is contained in a ball of radius $R = 1$. Hence, by the main theorem of the previous section, the error is bounded by $\sqrt{\frac{n}{T}}$ after T steps, which grows with the dimension. Intuitively, the dimension dependence comes from the fact that we must take a tiny step size to avoid changing the variables too much. For example, if we take a constant step size h and start at the point $x = (1, \frac{1}{n}, \frac{1}{n}, \dots, \frac{1}{n})$, then we will get a point with x_i constant in all directions $i \neq 1$, and this increases the function f dramatically from $\Theta(1)$ to $\Theta(nh)$. Therefore, to get constant error, we need to take step size $h \leq \frac{1}{n}$ and hence we need $\Omega(n)$ iterations.

Conceptually, the step $x = x - \eta g$ does not make sense either. Imagine the problem is infinitely dimensional. Note that $f(x) < +\infty$ for any

$$x \in \ell_1 = \{x \in \mathbb{R}^{\mathbb{N}} : \sum_i |x_i| < \infty\}.$$

On the other hand, its gradient g lives in ℓ_∞ space; the dual space of ℓ_1 is ℓ_∞ (in general, ℓ_p is dual to ℓ_q where $(1/p) + (1/q) = 1$). Since x and g are not in the same space, the term $x - \eta g$ does not make sense. More precisely, we have the following tautology (directly follows from the definition of dual space, namely the set of all linear maps in the original space).

Definition 5.5. A *Banach space* over the reals is a vector space over the reals together with a norm that defines a complete metric space, i.e., for any Cauchy sequence, $X = (x_i)_{i=1}^\infty$, there is a vector x s.t. $\lim_{n \rightarrow \infty} \|x_n - x\| = 0$.

Fact 5.6. Given any Banach space \mathcal{D} over the reals and a continuously differentiable function f from \mathcal{D} to \mathbb{R} , its gradient $\nabla f(x) \in \mathcal{D}^*$ for any x .

In general, if the function f is on the primal space \mathcal{D} , then the gradient g lives in the dual space \mathcal{D}^* . Therefore, we need to map x from the primal space \mathcal{D} to the dual space \mathcal{D}^* , update its position, then map the point back to the original space \mathcal{D} .

In fact, Lemma 5.6 gives us one such map, ∇f . Consider the following algorithm: Starting at x . We use $\nabla f(x)$ to map x to the dual space $y = \nabla f(x)$. Then, we apply the gradient step on the dual $y^{(\text{new})} = y - \nabla f(x)$ and map it back to the primal space, namely finding $x^{(\text{new})}$ such that $\nabla f(x^{(\text{new})}) = y^{(\text{new})}$. Note that $y^{(\text{new})} = 0$ and hence $x^{(\text{new})}$ is exactly a minimizer of f . So, if we can map it back, this algorithm solves the problem in one step. Unfortunately, the task of mapping it back is exactly our original problem.

Instead of using the same f , mirror descent uses some other convex function Φ , called the *mirror map*. For constrained problems, the mirror map may not bring the point back to a point in \mathcal{D} . Naively, one may consider the algorithm

$$\begin{aligned}\nabla \Phi(y^{(t+1)}) &= \nabla \Phi(x^{(t)}) - h \cdot \nabla f(x^{(t)}), \\ x^{(t+1)} &= \arg \min_{x \in \mathcal{D}} \|x - y^{(t+1)}\|_2.\end{aligned}$$

Note that the first step of finding $y^{(t+1)}$ involves solving an optimization problem. We will show how to do this optimization later (see 5.1) but with a proper formulation of the algorithm which takes into account the distance as measured by the mirror map Φ .

Definition 5.7. For any strictly convex function Φ , we define the Bregman divergence as

$$D_\Phi(y, x) = \Phi(y) - \Phi(x) - \langle \nabla \Phi(x), y - x \rangle.$$

Note that $D_\Phi(y, x)$ is the error of the first order Taylor expansion of Φ at x . Due to the convexity of Φ , we have that $D_\Phi(y, x) \geq 0$. Also, we note that $D_\Phi(y, x)$ is convex in y , but not necessarily in x .

Example 5.8. $D_\Phi(y, x) = \|y - x\|^2$ for $\Phi(x) = \|x\|^2$. $D_\Phi(y, x) = \sum_i y_i \log \frac{y_i}{x_i} - \sum y_i + \sum x_i$ for $\Phi(x) = \sum x_i \log x_i$.

Algorithm 14: MirrorDescent

Input: Initial point $x^{(0)} = \arg \min_{x \in \mathcal{D}} \Phi(x)$, step size $h > 0$.
for $k = 0, 1, \dots, T - 2$ **do**
 Pick any $g^{(k)} \in \partial f(x^{(k)})$.
 // As shown in (5.1), the next 2 steps can be implemented by an optimization over D_Φ .
 Find $y^{(k+1)}$ such that $\nabla \Phi(y^{(k+1)}) = \nabla \Phi(x^{(k)}) - h \cdot g^{(k)}$.
 $x^{(k+1)} \in \pi_{\mathcal{D}}^\Phi(y^{(k+1)})$ where $\pi_{\mathcal{D}}^\Phi(y) = \arg \min_{x \in \mathcal{D}} D_\Phi(x, y)$.
end
return $\frac{1}{T} \sum_{k=0}^{T-1} x^{(k)}$.

The Mirror Descent step can be written as follows. In the second step below, we use the fact that the

optimization is only over x (and hence all terms in y can be ignored):

$$\begin{aligned}
x^{(k+1)} &= \arg \min_{x \in \mathcal{D}} D_{\Phi}(x, y^{(k+1)}) \\
&= \arg \min_{x \in \mathcal{D}} \Phi(x) - \Phi(y^{(k+1)}) - \nabla \Phi(y^{(k+1)})^{\top} (x - y^{(k+1)}) \\
&= \arg \min_{x \in \mathcal{D}} \Phi(x) - \nabla \Phi(y^{(k+1)})^{\top} x \\
&= \arg \min_{x \in \mathcal{D}} \Phi(x) - \nabla \Phi(x^{(k)})^{\top} x + hg^{(k)\top} x \\
&= \arg \min_{x \in \mathcal{D}} hg^{(k)\top} x + D_{\Phi}(x, x^{(k)}).
\end{aligned} \tag{5.1}$$

Note that this is a natural generalization of $x^{(k+1)} = \arg \min_{x \in \mathcal{D}} hg^{(k)\top} x + \|x - x^{(k)}\|^2$.

■ 5.2.3 Analysis of Mirror Descent

Lemma 5.9 (Pythagorean Theorem). *Given a convex set \mathcal{D} and a point y , let $\pi(y) = \arg \min_{x \in \mathcal{D}} D_{\Phi}(x, y)$. For any $z \in \mathcal{D}$, we have that*

$$D_{\Phi}(z, \pi(y)) + D_{\Phi}(\pi(y), y) \leq D_{\Phi}(z, y).$$

Proof. Let $h(t) = D_{\Phi}(\pi(y) + t(z - \pi(y)), y)$. Since $h(t)$ is minimized at $t = 0$, we have that $h'(0) \geq 0$. Hence, we have

$$h'(0) = (\nabla \Phi(\pi(y)) - \nabla \Phi(y))^{\top} (z - \pi(y)) \geq 0.$$

Hence,

$$\begin{aligned}
D_{\Phi}(z, y) &= D_{\Phi}(z, \pi(y)) + 2(z - \pi(y))^{\top} (\nabla \Phi(\pi(y)) - \nabla \Phi(y)) + D_{\Phi}(\pi(y), y) \\
&\geq D_{\Phi}(z, \pi(y)) + D_{\Phi}(\pi(y), y).
\end{aligned}$$

□

Theorem 5.10. *Let f be a G -Lipschitz convex function on \mathcal{D} with respect to some norm $\|\cdot\|$. Let Φ be a ρ -strongly convex function on \mathcal{D} with respect to $\|\cdot\|$ with squared diameter $R^2 = \sup_{x \in \mathcal{D}} \Phi(x) - \Phi(x^{(0)})$. Then, mirror descent outputs x such that*

$$f(x) - \min_x f(x) \leq \frac{R^2}{hT} + \frac{h}{2\rho} G^2.$$

Remark 5.11. We say a function f is ρ strongly convex with respect to the norm $\|\cdot\|$ if for any x, y , we have

$$f(y) \geq f(x) + \langle \nabla f(x), y - x \rangle + \frac{\rho}{2} \|y - x\|^2.$$

The usual strong convexity is with respect to the Euclidean norm.

Remark 5.12. Picking $h = \frac{R}{G} \sqrt{\frac{2\rho}{T}}$, we get the rate $f(x) \leq \min_x f(x) + GR \sqrt{\frac{2}{\rho T}}$.

Proof. This proof is a complete “mirror” of the proof in Theorem 5.4.

$$\begin{aligned}
D_{\Phi}(x^*, x^{(k+1)}) &\leq D_{\Phi}(x^*, y^{(k+1)}) - D_{\Phi}(x^{(k+1)}, y^{(k+1)}) \\
&= D_{\Phi}(x^*, x^{(k)}) + (x^* - x^{(k)})^{\top} (\nabla \Phi(x^{(k)}) - \nabla \Phi(y^{(k+1)})) + D_{\Phi}(x^{(k)}, y^{(k+1)}) - D_{\Phi}(x^{(k+1)}, y^{(k+1)}) \\
&= D_{\Phi}(x^*, x^{(k)}) - h \cdot \left\langle g^{(k)}, x^{(k)} - x^* \right\rangle + D_{\Phi}(x^{(k)}, y^{(k+1)}) - D_{\Phi}(x^{(k+1)}, y^{(k+1)})
\end{aligned}$$

where we used Lemma 5.9 in the inequality. Using the definition of subgradient, we have that

$$f(x^*) \geq f(x^{(k)}) + \left\langle g^{(k)}, x^* - x^{(k)} \right\rangle.$$

Therefore, we have that

$$D_{\Phi}(x^*, x^{(k+1)}) \leq D_{\Phi}(x^*, x^{(k)}) - h \cdot (f(x^{(k)}) - f(x^*)) + D_{\Phi}(x^{(k)}, y^{(k+1)}) - D_{\Phi}(x^{(k+1)}, y^{(k+1)}).$$

Next we note that

$$\begin{aligned} & D_{\Phi}(x^{(k)}, y^{(k+1)}) - D_{\Phi}(x^{(k+1)}, y^{(k+1)}) \\ &= \Phi(x^{(k)}) - \Phi(x^{(k+1)}) - \nabla \Phi(y^{(k+1)})^{\top} (x^{(k)} - x^{(k+1)}) \\ &\leq \left\langle \nabla \Phi(x^{(k)}) - \nabla \Phi(y^{(k+1)}), x^{(k)} - x^{(k+1)} \right\rangle - \frac{\rho}{2} \|x^{(k)} - x^{(k+1)}\|^2 \\ &= h \cdot \left\langle g^{(k)}, x^{(k)} - x^{(k+1)} \right\rangle - \frac{\rho}{2} \|x^{(k)} - x^{(k+1)}\|^2 \\ &\leq hG \|x^{(k)} - x^{(k+1)}\| - \frac{\rho}{2} \|x^{(k)} - x^{(k+1)}\|^2 \\ &\leq \frac{(hG)^2}{2\rho}. \end{aligned}$$

Hence, we have

$$D_{\Phi}(x^*, x^{(k+1)}) \leq D_{\Phi}(x^*, x^{(k)}) - h \cdot (f(x^{(k)}) - f(x^*)) + \frac{(hG)^2}{2\rho}.$$

Rearranging the terms, we have

$$f(x^{(k)}) - f(x^*) \leq \frac{1}{h} \left(D_{\Phi}(x^*, x^{(k)}) - D_{\Phi}(x^*, x^{(k+1)}) \right) + \frac{hG^2}{2\rho}.$$

Summing over all iterations, we have

$$\begin{aligned} \frac{1}{T} \sum_{k=0}^{T-1} (f(x^{(k)}) - f(x^*)) &\leq \frac{1}{T} \cdot \frac{1}{h} (D_{\Phi}(x^*, x^{(0)}) - D_{\Phi}(x^*, x^{(T)})) + \frac{h}{2\rho} G^2 \\ &\leq \frac{1}{hT} D_{\Phi}(x^*, x^{(0)}) + \frac{h}{2\rho} G^2 \\ &\leq \frac{R^2}{hT} + \frac{h}{2\rho} G^2. \end{aligned}$$

Using the fact that $x^{(0)}$ was chosen as a minimum of $\Phi(x)$,

$$\begin{aligned} D_{\Phi}(x^*, x^{(0)}) &= (\Phi(x^*) - \Phi(x^{(0)})) - \left\langle \nabla \Phi(x^{(0)}), x^* - x^{(0)} \right\rangle \\ &= \Phi(x^*) - \Phi(x^{(0)}) \\ &\leq R^2 \end{aligned}$$

The result follows from the convexity of f . □

■ 5.2.4 Multiplicative Weight Update

In this section, we discuss mirror descent under the map $\Phi(x) = \sum x_i \log x_i$ with the convex set being the simplex $\mathcal{D} = \{x_i \geq 0, \sum x_i = 1\}$.

Step Formula As we showed in (5.1), we have that

$$x^{(k+1)} = \arg \min_{x \in \mathcal{D}} hg^{(k)\top} x + D_{\Phi}(x, x^{(k)}).$$

Note that

$$\begin{aligned} D_\Phi(x, x^{(k)}) &= \sum_i x_i \log x_i - \sum_i x_i^{(k)} \log x_i^{(k)} - \sum_i (1 + \log x_i^{(k)})(x_i - x_i^{(k)}) \\ &= \sum_i x_i \log \frac{x_i}{x_i^{(k)}} \end{aligned}$$

where we used that $\sum_i x_i = \sum_i x_i^{(k)}$. Hence, the step is simply

$$x^{(k+1)} = \arg \min_{\sum x_i = 1, x_i \geq 0} hg^{(k)\top} x + \sum_i x_i \log \frac{x_i}{x_i^{(k)}}.$$

Note that the optimality condition is given by

$$hg_i^{(k)} + \log \frac{x_i^{(k+1)}}{x_i^{(k)}} + 1 - \lambda = 0$$

for some Lagrangian multiplier λ . Rewriting, we have

$$x_i^{(k+1)} = e^{-hg_i^{(k)}} x_i^{(k)} / Z$$

for some normalization constant Z . Note that this algorithm multiplies the current x with a multiplicative factor and hence it is also called multiplicative weight update.

Strong Convexity To bound the strong convexity parameter, we note that

$$\Phi(y) - \Phi(x) - \langle \nabla \Phi(x), y - x \rangle = \frac{1}{2} (y - x)^\top \nabla^2 \Phi(\zeta) (y - x)$$

for some ζ between x and y . Since $\nabla^2 \Phi(\zeta) = \frac{1}{\zeta}$, we have

$$(y - x)^\top \nabla^2 \Phi(\zeta) (y - x) = \sum_i \frac{(y_i - x_i)^2}{\zeta_i} \geq \frac{(\sum_i |y_i - x_i|)^2}{\sum_i \zeta_i} = (\sum_i |y_i - x_i|)^2$$

where we used that $\sum_i x_i = \sum_i y_i = 1$ and so $\sum_i \zeta_i = 1$. Hence,

$$\Phi(y) - \Phi(x) - \langle \nabla \Phi(x), y - x \rangle \geq \frac{1}{2} \|y - x\|_1^2.$$

Therefore, Φ is 1-strongly convex in $\|\cdot\|_1$. Hence, $\rho = 1$.

Diameter Direct calculation shows that $-\log n \leq \Phi(x) \leq 0$. We start at $x^{(0)} = \frac{1}{n}(1, \dots, 1)^T$. Hence, $R^2 = \log n$.

Result

Theorem 5.13. *Let f be a 1-Lipschitz function on $\|\cdot\|_1$. Then, mirror descent with the mirror map $\Phi(x) = \sum_i x_i \log x_i$.*

$$f(x^T) - \min_x f(x) \leq \sqrt{\frac{2 \log n}{T}}.$$

In comparison, projected gradient descent had the bound of $\sqrt{\frac{n}{T}}$.

■ 5.3 Frank–Wolfe

Mirror descent is not suitable for all spaces. The guarantee of mirror descent crucially depends on the fact that there is a 1-strongly convex mirror map Φ such that $\max_x \Phi(x) - \min_x \Phi(x)$ is small on the domain. For some domains such as $\{x : \|x\|_\infty \leq 1\}$, the range $\max_x \Phi(x) - \min_x \Phi(x)$ can be large.

Lemma 5.14. *Let Φ be a 1-strongly convex function on \mathbb{R}^n over $\|\cdot\|_\infty \leq 1$. Then,*

$$\max_{\|x\|_\infty \leq 1} \Phi(x) \geq \min_{\|x\|_\infty \leq 1} \Phi(x) + \frac{n}{2}.$$

Proof. By the strong convexity of Φ , we have that

$$\begin{aligned} \mathbf{E}_{s_k \in \{\pm 1\} \ \forall k \in [n]} \Phi(s_1, \dots, s_n) &\geq \mathbf{E}_{s_k \in \{\pm 1\} \ \forall k \in [n-1]} \Phi(s_1, \dots, s_{n-1}, 0) + \mathbf{E}_{s_n} \langle \nabla \Phi(s_1, \dots, s_{n-1}, 0), s_n \rangle + \frac{1}{2} \\ &= \mathbf{E}_{s_k \in \{\pm 1\} \ \forall k \in [n-1]} \Phi(s_1, \dots, s_{n-1}, 0) + \frac{1}{2} \\ &\vdots \\ &\geq \Phi(0) + \frac{n}{2}. \end{aligned}$$

□

Remark. This inequality is tight because $\frac{1}{2}\|x\|^2$ is 1-strongly convex in $\|\cdot\|_\infty$ and its value is between 0 and $\frac{n}{2}$.

■ 5.3.1 Algorithm

Now we give another geometry dependent algorithm that relies on a different set of assumptions. The problem we study in this section is of the form

$$\min_{x \in \mathcal{D}} f(x)$$

for f such that ∇f is “Lipschitz” in a certain sense. The algorithm reduces the problem to a sequence of linear optimization problems.

Algorithm 15: FrankWolfe

Input: Initial point $x^{(0)} \in \mathbb{R}^n$, step size $h > 0$.
for $k = 0, 1, \dots, T-1$ **do**
 Compute $y^{(k)} = \arg \min_{y \in \mathcal{D}} \langle y, \nabla f(x^{(k)}) \rangle$.
 $x^{(k+1)} \leftarrow (1 - h_k)x^{(k)} + h_k y^{(k)}$ with $h_k = \frac{2}{k+2}$.
end
return $x^{(T)}$.

Analysis

Theorem 5.15. *Let f be a convex function on a convex set \mathcal{D} with a constant C_f such that*

$$f((1-h)x + hy) \leq f(x) + h \langle \nabla f(x), y - x \rangle + \frac{1}{2} C_f h^2.$$

Then, for any $x, y \in \mathcal{D}$ and $h \in [0, 1]$, we have

$$f(x^{(k)}) - f(x^*) \leq \frac{2C_f}{k+2}.$$

Remark. If ∇f is L -Lipschitz with respect to the norm $\|\cdot\|$ over the domain \mathcal{D} , then $C_f \leq L \cdot \text{diam}_{\|\cdot\|}(\mathcal{D})^2$.

Proof. By the definition of C_f , we have that

$$f(x^{(k+1)}) \leq f(x^{(k)}) + h_k \langle \nabla f(x^{(k)}), y^{(k)} - x^{(k)} \rangle + \frac{1}{2} C_f h_k^2.$$

Note that

$$f(x^*) \geq f(x^{(k)}) + \langle \nabla f(x^{(k)}), x^* - x^{(k)} \rangle \geq f(x^{(k)}) + \langle \nabla f(x^{(k)}), y^{(k)} - x^{(k)} \rangle$$

where we used the fact that $y^{(k)} = \arg \min_{y \in \mathcal{D}} \langle y, \nabla f(x^{(k)}) \rangle$ and that $x^* \in \mathcal{D}$. Hence, we have that

$$f(x^{(k+1)}) \leq f(x^{(k)}) - h_k (f(x^{(k)}) - f(x^*)) + \frac{1}{2} C_f h_k^2.$$

Let $e_k = f(x^{(k)}) - f(x^*)$. Then,

$$e_{k+1} \leq (1 - h_k) e_k + \frac{1}{2} C_f h_k^2.$$

Note that $e_0 = f(x^{(0)}) - f^* \leq \frac{1}{2} C_f$. By induction, we have that $e_k \leq \frac{2C_f}{k+2}$. \square

Remark. Note that this proof is in fact the same as Theorem 2.9.

■ 5.4 The Newton Method

We begin with the Newton-Raphson method for finding the zeros of a function g , i.e. finding x such that $g(x) = 0$. In optimization, the goal is to find a root of the gradient, $\nabla f(x) = 0$. The Newton-Raphson iteration approximates a function by its gradient/Jacobian, then guesses where the gradient intersects the zero line as a likely zero, repeating this process until a sufficient approximation has been found. In one dimension, we approximate the function g by its gradient

$$g(x) \sim g(x^{(k)}) + g'(x^{(k)})(x - x^{(k)}).$$

Finding the zeros of the right hand side, we have the Newton step

$$x^{(k+1)} = x^{(k)} - \frac{g(x^{(k)})}{g'(x^{(k)})}.$$

In high dimension, we can approximate the function by its Jacobian $g(x) \sim g(x^{(k)}) + Dg(x^{(k)})(x - x^{(k)})$ and this gives the step

$$x^{(k+1)} = x^{(k)} - \left(Dg(x^{(k)}) \right)^{-1} g(x^{(k)}).$$

When the function $g(x) = \nabla f(x)$, then the Newton step becomes

$$x^{(k+1)} = x^{(k)} - \left(\nabla^2 f(x^{(k)}) \right)^{-1} \nabla f(x^{(k)}).$$

Alternatively, we can derive the Newton step as

$$x^{(k+1)} \leftarrow \min_x f(x^{(k)}) + \langle \nabla f(x^{(k)}), x - x^{(k)} \rangle + \frac{1}{2} (y - x^{(k)})^\top (\nabla^2 f(x^{(k)})) (y - x^{(k)}).$$

In words, the Newton step finds the minimum of the second order approximation of the function. We note that the Newton iteration is a natural idea, since

1. It is affine invariant (changing coordinate systems does not affect convergence).
2. It is the fastest descent direction taking the Hessian into account.

To see why affine-invariance is important for optimization, we consider the following function

$$f(x_1, x_2) = \frac{100}{2}x_1^2 + \frac{1}{2}x_2^2.$$

The gradient descent for this function is

$$(x_1, x_2) \leftarrow (x_1, x_2) - h\nabla f(x_1, x_2) = ((1 - 100h)x_1, (1 - h)x_2).$$

We need $h < \frac{1}{100}$ in order the first coordinate to converge, but this will make the second coordinate converges too slowly. In general, we may want to take different step sizes for different directions and Newton method gives the best step if the function is quadratic.

For many classes of functions, gradient methods converge to the solution linearly (namely, it takes $c \cdot \log \frac{1}{\epsilon}$ iterations for some c depending on the problem) while the Newton method converges to the solution quadratically (namely, it takes $c' \cdot \log \log \frac{1}{\epsilon}$ for some c') if the starting point is sufficiently close to a root. However, each step of Newton method involves solving a linear system, which can be much more expensive. Furthermore, Newton method may not converges if the starting point is far away.

Algorithm 16: NewtonMethod

Input: Initial point $x^{(0)} \in \mathbb{R}^n$
for $k = 0, 1, \dots, T - 1$ **do**
 $x^{(k+1)} = x^{(k)} - (Dg(x^{(k)}))^{-1} g(x^{(k)}).$
end
return $x^{(T)}.$

Theorem 5.16 (Quadratic convergence). *Assume that $g : \mathbb{R}^n \rightarrow \mathbb{R}^n$ is twice continuously differentiable. Let $x^{(k)}$ be the sequence given by the Newton method. Suppose that $x^{(k)}$ converges to some x^* such that $g(x^*) = 0$ and $Dg(x^*)$ is invertible. Then, for k large enough, we have*

$$\|x^{(k+1)} - x^*\| \leq \|(Dg(x^*))^{-1} D^2 g(x^*)\|_{\text{op}} \cdot \|x^{(k)} - x^*\|^2.$$

Proof. Let $e^{(k)} = x^* - x^{(k)}$. Then, we have that

$$g(x^*) = g(x^{(k)}) + Dg(x^{(k)})[e^{(k)}] + \int_0^1 (1-s) D^2 g(x^{(k)} + se^{(k)})[e^{(k)}, e^{(k)}] ds.$$

Hence, we have

$$0 = Dg(x^{(k)})^{-1} g(x^{(k)}) + x^* - x^{(k)} + \int_0^1 (1-s) Dg(x^{(k)})^{-1} D^2 g(x^{(k)} + se^{(k)})[e^{(k)}, e^{(k)}] ds.$$

Since $x^{(k+1)} = x^{(k)} - Dg(x^{(k)})^{-1} g(x^{(k)})$, we have

$$x^{(k+1)} - x^* = \int_0^1 (1-s) Dg(x^{(k)})^{-1} D^2 g(x^{(k)} + se^{(k)})[e^{(k)}, e^{(k)}] ds.$$

So, we have

$$\begin{aligned} \|x^{(k+1)} - x^*\| &\leq \int_0^1 (1-s) \|Dg(x^{(k)})^{-1} D^2 g(x^{(k)} + se^{(k)})[e^{(k)}, e^{(k)}]\| ds \\ &\leq \int_0^1 (1-s) \|Dg(x^{(k)})^{-1} D^2 g(x^{(k)} + se^{(k)})\|_{\text{op}} ds \cdot \|x^{(k)} - x^*\|^2. \end{aligned}$$

Since $x^{(k)} \rightarrow x^*$, we have that

$$Dg(x^{(k)})^{-1} D^2 g(x^{(k)} + se^{(k)}) \rightarrow Dg(x^*)^{-1} D^2 g(x^*)$$

and for large enough k , we can assume

$$\|Dg(x^{(k)})^{-1} D^2 g(x^{(k)} + se^{(k)})\|_{\text{op}} \leq 2 \|Dg(x^*)^{-1} D^2 g(x^*)\|_{\text{op}}.$$

The result follows. □

This argument above uses only that $g \in \mathcal{C}^2$ and does not require convexity. Without further global assumptions on g , the Newton method does not always converge to a root. The argument above only shows that if the algorithm converges, then it converges quadratically eventually. We call this “local” convergence since it only gives a bound when $x^{(k)}$ is close enough to x^* . In comparison, all earlier analyses in this book are about global convergence, bounding the total number of iterations. In practice, both analyses are important; global convergence makes sure the algorithm is robust and local quadratic convergence makes sure the algorithm converges to machine accuracy quickly enough. The local quadratic convergence is particularly important for simple problems such as computing \sqrt{x} .

Finding the largest root of a real-rooted polynomial

In general, the Newton method does not converge globally. Here, we give an application that does converge “globally”.

Theorem 5.17. *Given a polynomial $g(x) = \sum_{i=1}^n a_i x^i$ with only real roots. Let λ_1 be its largest root. Suppose that $\lambda_1 \leq x^{(0)}$. Then, after $O(n \log(\frac{1}{\epsilon}))$ iterations, the Newton method finds $x^{(k)}$ such that*

$$\lambda_1 \leq x^{(k)} \leq \lambda_1 + \epsilon \cdot (x^{(0)} - \lambda_1).$$

Proof. Since the roots of g are real, we can write

$$g(x) = a_n \cdot \prod_{i=1}^n (x - \lambda_i)$$

with $\lambda_n \leq \lambda_{n-1} \leq \dots \leq \lambda_1$. Then, we have that $g'(x) = a_n \cdot \sum_i \prod_{j \neq i} (x - \lambda_j)$ and hence

$$\frac{g(x)}{g'(x)} = \frac{1}{\sum_i \frac{1}{x - \lambda_i}}.$$

For any $x \geq \lambda_1$, we have

$$\begin{aligned} \frac{g(x)}{g'(x)} &\leq \frac{1}{\frac{1}{x - \lambda_1}} = x - \lambda_1, \\ \frac{g(x)}{g'(x)} &\geq \frac{1}{\sum_i \frac{1}{x - \lambda_1}} = \frac{x - \lambda_1}{n}. \end{aligned}$$

Hence, by induction, we have that $x^{(k)} \geq \lambda_1$ every step and that

$$x^{(k+1)} - \lambda_1 \leq \left(1 - \frac{1}{n}\right)(x^{(k)} - \lambda_1).$$

□

Exercise 5.18. Consider the following iteration:

$$x^{t+1} = x^t - \frac{1}{n^{1/k}} \frac{g^{(k-1)}(x)}{g^{(k)}(x)}$$

where $g^{(k)}(x) = \sum_i \frac{1}{(x - \lambda_i)^k}$. For $k = 1$, this is exactly the Newton iteration as $g^{(0)}(x) = n$. Show that when applied to a degree n real-rooted polynomial, starting with $x^{(0)} > \lambda_1$, in each iteration the distance to the largest root decreases by a factor of $1 - \frac{1}{n^{1/k}}$.

Such a dependence of $\log \frac{1}{\epsilon}$ is called linear convergence. The convergence of the Newton method can be quadratic, when close enough to a root.

Theorem 5.19. *Assume that $|f'(x^*)| \geq \alpha$ at $f(x^*) = 0$ and f' is L -Lipschitz. Then, if $|x^0 - x^*| \leq \frac{\alpha}{2L}$,*

$$|x^{(k)} - x^*| \leq \frac{\alpha}{L} \left(\frac{L}{\alpha} |x^{(k)} - x^*| \right)^{2^{(k)}}.$$

Proof. The iteration is

$$x^{(k+1)} - x^* = x^{(k)} - x^* - \frac{f(x^{(k)})}{f'(x^{(k)})}.$$

$$f(x^*) = f(x^{(k)}) + \int_{x^{(k)}}^{x^*} f'(z) dz = f(x^{(k)}) + f'(x^{(k)})(x^* - x^{(k)}) + \int_{x^{(k)}}^{x^*} (f'(z) - f'(x^{(k)})) dz.$$

Therefore,

$$\begin{aligned} x^{(k+1)} - x^* &= \frac{1}{f'(x^{(k)})} \int_{x^{(k)}}^{x^*} (f'(z) - f'(x^{(k)})) dz \\ &\leq \frac{L}{|f'(x^{(k)})|} \int_{x^{(k)}}^{x^*} |z - x^{(k)}| dz \\ &= \frac{L|x^* - x^{(k)}|^2}{2|f'(x^{(k)})|}. \end{aligned}$$

Since $f'(x^{(k)}) \geq f'(x^*) - L|x^{(k)} - x^*|$

$$|x^{(k+1)} - x^*| \leq \frac{L}{2(\alpha - L|x^{(k)} - x^*|)} |x^{(k)} - x^*|^2.$$

So, if $|x^{(k)} - x^*| \leq \frac{\alpha}{2L}$,

$$|x^{(k+1)} - x^*| \leq \frac{L}{\alpha} |x^{(k)} - x^*|^2 \leq \frac{1}{2} |x^{(k)} - x^*|$$

and

$$\frac{L}{\alpha} |x^{(k+1)} - x^*| \leq \left(\frac{L}{\alpha} |x^{(k)} - x^*| \right)^2.$$

After t steps,

$$\frac{L}{\alpha} |x^{(k)} - x^*| \leq \left(\frac{L}{\alpha} \epsilon_0 \right)^{2^{(k)}}$$

implying $|x^{(k)} - x^*| < \epsilon$ after $\log \log \left(\frac{L\epsilon_0}{\alpha\epsilon} \right)$ steps. Note that f has not been assumed to be convex or polynomial. \square

Moving back to optimization, we can view the goal as finding a root of $\nabla f(x) = 0$. Newton's iteration is the update

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

By the above proof, Newton's iteration has quadratic convergence from points close enough to the optimal.

Quasi-Newton Method

When the Jacobian of g is not available, we can approximate it using the function itself. For one dimension, we can approximate the Newton method and get the following secant method

$$x^{(k+1)} = x^{(k)} - g(x^{(k)}) \frac{x^{(k)} - x^{(k-1)}}{g(x^{(k)}) - g(x^{(k-1)})}$$

where we approximated the $g'(x^{(k)})$ by $\frac{g(x^{(k)}) - g(x^{(k-1)})}{x^{(k)} - x^{(k-1)}}$. For nice enough function, the convergence rate satisfies $\epsilon_{k+1} \leq C \cdot \epsilon_k^{\frac{1+\sqrt{5}}{2}}$, which is super linearly but not quadratic.

For higher dimension, we need to approximate the Jacobian of g . Let $J^{(k)}$ be the approximate Jacobian we maintained in the k^{th} iteration. Similar to the secant method, we want to enforce

$$J^{(k+1)} \cdot (x^{(k)} - x^{(k-1)}) = g(x^{(k)}) - g(x^{(k-1)}).$$

In dimension higher than one, this does not uniquely define the $J^{(k+1)}$. One natural choice is to find $J^{(k+1)}$ that is closest to $J^{(k)}$ while satisfying the equation above. Solving the problem

$$\min_{J^{(k+1)} \cdot (x^{(k)} - x^{(k-1)}) = g(x^{(k)}) - g(x^{(k-1)})} \|J^{(k+1)} - J^{(k)}\|_F, \quad (5.2)$$

we have the update rule

$$J^{(k+1)} = J^{(k)} + \frac{y^{(k)} - J^{(k)} s^{(k)}}{\|s^{(k)}\|^2} s^{(k)\top} \quad (5.3)$$

where $s^{(k)} = x^{(k)} - x^{(k-1)}$ and $y^{(k)} = g(x^{(k)}) - g(x^{(k-1)})$.

Exercise 5.20. Prove that the equation (5.3) is indeed the minimizer of (5.2).

When g is given by the gradient of a convex function f , we know that the Jacobian of g satisfies $Dg = \nabla^2 f(x) \succeq 0$. Therefore, we should impose some conditions such that $J^{(k)} \succeq 0$ for all k .

BFGS algorithm

Broyden–Fletcher–Goldfarb–Shanno (BFGS) algorithm is one of the most popular quasi-Newton methods. The algorithm maintains an approximate Hessian $J^{(k)}$ such that

- $J^{(k+1)}(x^{(k)} - x^{(k-1)}) = \nabla f(x^{(k)}) - \nabla f(x^{(k-1)})$
- $J^{(k+1)}$ is close to $J^{(k)}$.
- $J^{(k)} \succ 0$.

To achieve all of these conditions, the natural optimization is

$$J^{(k+1)} \stackrel{\text{def}}{=} \arg \min_{J s = y, J = J^\top} \left\| W^{\frac{1}{2}} \left(J^{-1} - \left(J^{(k)} \right)^{-1} \right) W^{\frac{1}{2}} \right\|_F^2$$

where $s^{(k)} = x^{(k)} - x^{(k-1)}$, $y^{(k)} = \nabla f(x^{(k)}) - \nabla f(x^{(k-1)})$ and $W = \int_0^1 \nabla^2 f(x^{(k-1)} + s(x^{(k)} - x^{(k-1)})) ds$ (or any W such that $W y = s$). In some sense, the $W^{-\frac{1}{2}}$ is just a correct change of variables so that the algorithm is affine invariant. Solving the equation above [25], one obtain the update

$$\left(J^{(k+1)} \right)^{-1} = (I - \rho_k \cdot s^{(k)} y^{(k)\top}) \left(J^{(k)} \right)^{-1} (I - \rho_k \cdot y^{(k)} s^{(k)\top}) + \rho_k \cdot s^{(k)} s^{(k)\top} \quad (5.4)$$

where $\rho_k = \frac{1}{y^{(k)\top} s^{(k)}}$. Alternatively, one can also show that [26]

$$J^{(k+1)} = \arg \min_{J s = y, J = J^\top} D_{KL}(\mathcal{N}(0, J) \| \mathcal{N}(0, J^{(k)})).$$

To implement the BFGS algorithm, it suffices to compute $(J^{(k)})^{-1} \nabla f(x^{(k)})$. Therefore, we can directly use the recursive formula (5.4) to compute $(J^{(k)})^{-1} \nabla f(x^{(k)})$ instead of maintaining $J^{(k)}$ or $(J^{(k)})^{-1}$ explicitly.

In practice, the recursive formula $J^{(k)}$ becomes too expensive and hence one can stop the recursive formula after constant steps, which gives the limited-memory BFGS algorithm.

■ 5.5 Interior Point Method for Linear Programs

In this section, we study interior point methods. In practice, this method reduces the problem of optimizing a convex function to solving a small number (typically less than 30) linear systems. In theory, it reduces the problem to $\tilde{O}(\sqrt{n})$ linear systems.

We start by describing interior point method for linear programs. We establish a polynomial bound and then later discuss implementation details.

■ 5.5.1 Basic Properties

We first consider the primal problem

$$(P) : \quad \min_x c^\top x \text{ subject to } Ax = b, x \geq 0$$

where $A \in \mathbb{R}^{m \times n}$. The difficulty of linear programs is the constraint $x \geq 0$. Without this constraint, we can simply solve it as a linear system. One natural idea to solve linear programs is to replace the hard constraint $x \geq 0$ by some smooth function. So, let us consider the following “regularized” version of the linear program for some $t \geq 0$:

$$(P_t) : \quad \min_x c^\top x - t \sum_{i=1}^n \ln x_i \text{ subject to } Ax = b.$$

We will explain the reason of choosing $\ln x$ in more detail later. For now, we can think it as a nice function that blows up to ∞ as x approaches zero.

One can think that $-\ln x$ gives a force from every constraint $x \geq 0$ to make sure $x \geq 0$ is true. Since the gradient of $-\ln x$ blows up when $x = 0$, when x is close enough, the force is large enough to counter the cost c . When $t \rightarrow 0$, then the problem (P_t) is closer to the original problem (P) and hence the minimizer of (P_t) is closer to a minimizer of (P) .

First, we give a formula for the minimizer of (P_t) .

Lemma 5.21 (Existence and Uniqueness of central path). *If the polytope $\{Ax = b, x \geq 0\}$ has an interior, then the optimum of (P_t) is unique and is given by the solution of the following system:*

$$\begin{aligned} xs &= t, \\ Ax &= b, \\ A^\top y + s &= c, \\ (x, s) &\geq 0 \end{aligned}$$

where the variables s_i are additional “slack” variables, and $xs = t$ is shorthand of $x_i s_i = t$ for all i .

Proof. The optimality condition, using dual variables y for the Lagrangian of $Ax = b$ is given by

$$c - \frac{t}{x} = A^\top y.$$

Write $s_i = \frac{t}{x_i}$, to get the formula. The solution is unique because the function $-\ln x$ is strictly convex. \square

Definition 5.22. We define the central path $\mathcal{C}_t = (x^{(t)}, y^{(t)}, s^{(t)})$ as the sequence of points satisfying

$$\begin{aligned} x^{(t)} s^{(t)} &= t, \\ Ax^{(t)} &= b, \\ A^\top y^{(t)} + s^{(t)} &= c, \\ (x^{(t)}, s^{(t)}) &\geq 0. \end{aligned}$$

To give another interpretation of the central path, note that the dual problem is

$$(D) : \quad \max_{y, s} b^\top y \text{ subject to } A^\top y + s = c, s \geq 0.$$

Note that for any feasible x and y , we have that

$$0 \leq c^\top x - b^\top y = c^\top x - x^\top A^\top y = x^\top s.$$

Hence, (x, y, s) solves the linear program if it satisfies the central path equation with $t = 0$. Therefore, following the central path is a balanced way to decrease $x_i s_i$ uniformly to 0. We can formalize the intuition that for small t , $x^{(t)}$ is a good approximation of the primal solution. In fact t itself is a bound on the error of the current solution.

Lemma 5.23 (Duality Gap). *We have that*

$$\text{Duality Gap} = c^\top x^{(t)} - b^\top y^{(t)} = c^\top x^{(t)} - \left(x^{(t)}\right)^\top A^\top y^{(t)} = \left(x^{(t)}\right)^\top s^{(t)} = tn.$$

The interior point method follows the following framework:

1. Find \mathcal{C}_1
2. Until $t < \frac{\varepsilon}{n}$,
 - (a) Use \mathcal{C}_t to find $\mathcal{C}_{(1-h)t}$ for $h = \frac{1}{10\sqrt{n}}$.

Note that this algorithm only finds a solution with ε error. If the linear program is integral, we can simply stop at small enough ε and round it off to the closest integral point.

■ 5.5.2 Following the central path

During the algorithm, we maintain a point (x, y, s) such that $Ax = b$, $A^\top y + s = c$ and $x_i s_i$ is close to t for all i . We show how to find a feasible $(x + \delta_x, y + \delta_y, s + \delta_s)$ such that it is even closer to t . We can write the equation as follows:

$$\begin{aligned} (x + \delta_x)(s + \delta_s) &\approx t, \\ A(x + \delta_x) &= b, \\ A^\top(y + \delta_y) + (s + \delta_s) &= c. \end{aligned}$$

(Omitted the non-negative conditions.) Using our assumption on (x, y, s) and noting that $\delta_x \cdot \delta_s$ is small, the equation can be simplified as follows. We use the notation $X = \text{Diag}(x)$, $S = \text{Diag}(s)$.

$$\begin{bmatrix} 0 & A^\top & I \\ A & 0 & 0 \\ S & 0 & X \end{bmatrix} \begin{bmatrix} \delta_x \\ \delta_y \\ \delta_s \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ t - xs \end{bmatrix}.$$

This is a linear system and hence we can solve it exactly.

Exercise 5.24. Let $r = t - xs$. Prove that $S\delta_x = (I - \bar{P})r$ and $X\delta_s = \bar{P}r$ where $\bar{P} = XA^\top(AS^{-1}XA^\top)^{-1}AS^{-1}$.

First, we show that $x^{(\text{new})} = x + \delta_x$ and $s^{(\text{new})} = s + \delta_s$ are feasible.

Lemma 5.25. Suppose $\sum_i (x_i s_i - t)^2 \leq \varepsilon^2 t^2$ with $\varepsilon < \frac{1}{2}$. Then, $x_i^{(\text{new})} > 0$ and $s_i^{(\text{new})} > 0$ for all i .

Proof. Note that $P^2 = P$. However, in general $P \neq P^\top$, i.e. P might not be an orthogonal projection matrix. It will be convenient to consider the orthogonal projection matrix $P = S^{-\frac{1}{2}}X^{\frac{1}{2}}A^\top(AS^{-1}XA^\top)^{-1}AS^{-\frac{1}{2}}X^{\frac{1}{2}}$. Note that

$$X^{-1}\delta_x = S^{-\frac{1}{2}}X^{-\frac{1}{2}}(I - P)S^{-\frac{1}{2}}X^{-\frac{1}{2}}r.$$

By the assumption for each i , $x_i s_i \geq (1 - \varepsilon)t$. Therefore, we have

$$\begin{aligned} \|X^{-1}\delta_x\|_2 &\leq \frac{1}{\sqrt{(1 - \varepsilon)t}} \|(I - P)S^{-\frac{1}{2}}X^{-\frac{1}{2}}r\|_2 \\ &\leq \frac{1}{\sqrt{(1 - \varepsilon)t}} \|S^{-\frac{1}{2}}X^{-\frac{1}{2}}r\|_2 \\ &\leq \frac{1}{(1 - \varepsilon)t} \|r\|_2 \leq \frac{\varepsilon}{1 - \varepsilon}. \end{aligned}$$

Similarly, we have $S^{-1}\delta_s = S^{-\frac{1}{2}}X^{-\frac{1}{2}}PS^{-\frac{1}{2}}X^{-\frac{1}{2}}r$. Hence, we have $\|S^{-1}\delta_s\|_2 \leq \frac{\varepsilon}{1 - \varepsilon}$. Therefore, when $\varepsilon < \frac{1}{2}$, we have both $\|X^{-1}\delta_x\|_\infty$ and $\|S^{-1}\delta_s\|_\infty$ less than 1, which shows that both $x^{(\text{new})}$ and $s^{(\text{new})}$ are positive.

Next, we show that xs is closer to t after one Newton step. \square

Lemma 5.26. If $\sum_i (x_i s_i - t)^2 \leq \varepsilon^2 t^2$ with $\varepsilon < \frac{1}{4}$, we have that

$$\sum_i \left(x_i^{(\text{new})} s_i^{(\text{new})} - t \right)^2 \leq (\varepsilon^4 + 16\varepsilon^5) t^2.$$

Proof. We have that $x_i \delta_{s,i} + s_i \delta_{x,i} = t - x_i s_i$. Using this,

$$\text{LHS} = \sum_i \left(x_i^{(\text{new})} s_i^{(\text{new})} - t \right)^2 = \sum_i (x_i s_i + x_i \delta_{s,i} + s_i \delta_{x,i} + \delta_{x,i} \delta_{s,i} - t)^2 = \sum_i \delta_{x,i}^2 \delta_{s,i}^2 \leq ((1 + \epsilon)t)^2 \cdot \sum_i \left(\frac{\delta_{x,i}}{x_i} \right)^2 \left(\frac{\delta_{s,i}}{s_i} \right)^2$$

where in the last step we used $x_i^2 s_i^2 \leq (1 + \epsilon)^2 t^2$. Using the previous lemma, we have that

$$\begin{aligned} \text{LHS} &\leq ((1 + \epsilon)t)^2 \cdot \|X^{-1} \delta_x\|_4^2 \|S^{-1} \delta_s\|_4^2 \\ &\leq ((1 + \epsilon)t)^2 \cdot \|X^{-1} \delta_x\|_2^2 \|S^{-1} \delta_s\|_2^2 \\ &\leq ((1 + \epsilon)t)^2 \left(\frac{\epsilon}{1 - \epsilon} \right)^4 \\ &\leq (\epsilon^4 + 16\epsilon^5) t^2 \end{aligned}$$

□

Using this, we have the main theorem.

Theorem 5.27. *We can solve a linear program to within δ “error” (see Lemma 5.28) in $O(\sqrt{n} \log(\frac{1}{\delta}))$ iterations and each iteration only needs to solve a linear system.*

Proof. Let $\Phi = \sum_i (x_i s_i - t)^2$ be the error of the current iteration. We always maintain $\Phi \leq \frac{t^2}{16}$ for the current (x, y, s) and t . At each step, we use Lemma 5.26 which makes $\Phi \leq \frac{t^2}{50}$. Then, we decrease t to $t(1 - \frac{1}{10\sqrt{n}})$. Note that

$$\sum_i (x_i s_i - t(1 - h))^2 \leq 2\Phi + 2t^2 h^2 n \leq \frac{2t^2}{50} + \frac{2t^2}{100} \leq \frac{(t(1 - h))^2}{16}.$$

Therefore, the invariant is preserved after each step. Since t is decreased by a $(1 - \frac{1}{10\sqrt{n}})$ factor each step, it takes $O(\sqrt{n} \log(\frac{1}{\delta}))$ to decrease t from 1 to δ^2 . □

■ 5.5.3 Finding the initial point

The first question is to find C_1 . This can be handled by extending the problem to slightly higher dimension. To the reader familiar with the Simplex method, this might be reminiscent of the two phases of the simplex method, where the purpose of the first phase is to find a feasible initial solution.

Lemma 5.28. *Consider a linear program $\min_{Ax=b, x \geq 0} c^\top x$ with n variables and d constraints. Assume that*

1. *Diameter: For any $x \geq 0$ with $Ax = b$, we have that $\|x\|_\infty \leq R$.*
2. *Lipschitz constant of the objective: $\|c\|_\infty \leq L$.*

For any $0 < \delta \leq 1$, the modified linear program $\min_{\bar{A}\bar{x}=\bar{b}, \bar{x} \geq 0} \bar{c}^\top \bar{x}$ with

$$\bar{A} = \begin{bmatrix} A & 0 & \frac{1}{R}b - A1_n \\ 1_n^\top & 1 & 0 \end{bmatrix}, \bar{b} = \begin{bmatrix} \frac{1}{R}b \\ n+1 \end{bmatrix}, \text{ and } \bar{c} = \begin{bmatrix} \delta/L \cdot c \\ 0 \\ 1 \end{bmatrix}$$

satisfies the following:

1. $\bar{x} = \begin{bmatrix} 1_n \\ 1 \\ 1 \end{bmatrix}$, $\bar{y} = \begin{bmatrix} 0_d \\ -1 \end{bmatrix}$ and $\bar{s} = \begin{bmatrix} 1_n + \frac{\delta}{L} \cdot c \\ 1 \\ 1 \end{bmatrix}$ are feasible primal dual vectors.

2. *For any feasible primal dual vectors $(\bar{x}, \bar{y}, \bar{s})$ with duality gap at most δ^2 , the vector $\hat{x} = R \cdot \bar{x}_{1:n}$ ($\bar{x}_{1:n}$ are the first n coordinates of \bar{x}) is an approximate solution to the original linear program in the following*

sense

$$\begin{aligned} c^\top \hat{x} &\leq \min_{Ax=b, x \geq 0} c^\top x + LR \cdot \delta, \\ \|A\hat{x} - b\|_1 &\leq 4n\delta \cdot \left(R \sum_{i,j} |A_{i,j}| + \|b\|_1 \right), \\ \hat{x} &\geq 0. \end{aligned}$$

Part 1. For the first result, straightforward calculations show that $(\bar{x}, \bar{y}, \bar{s}) \in \mathbb{R}^{(n+2) \times (d+1) \times (n+2)}$ are feasible, i.e.,

$$\bar{A}\bar{x} = \begin{bmatrix} A & 0 & \frac{1}{R}b - A1_n \\ 1_n^\top & 1 & 0 \end{bmatrix} \cdot \begin{bmatrix} 1_n \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} \frac{1}{R}b \\ n+1 \end{bmatrix} = \bar{b}$$

and

$$\begin{aligned} \bar{A}^\top \bar{y} + \bar{s} &= \begin{bmatrix} A^\top & 1_n \\ \frac{1}{R}b^\top - 1_n^\top A^\top & 0 \end{bmatrix} \cdot \begin{bmatrix} 0_d \\ -1 \end{bmatrix} + \begin{bmatrix} 1_n + \frac{\delta}{L} \cdot c \\ 1 \\ 1 \end{bmatrix} \\ &= \begin{bmatrix} -1_n \\ -1 \\ 0 \end{bmatrix} + \begin{bmatrix} 1_n + \frac{\delta}{L} \cdot c \\ 1 \\ 1 \end{bmatrix} \\ &= \begin{bmatrix} \frac{\delta}{L} \cdot c \\ 0 \\ 1 \end{bmatrix} = \bar{c} \end{aligned}$$

Part 2. For the second result, we let

$$\text{OPT} = \min_{Ax=b, x \geq 0} c^\top x, \quad \text{and,} \quad \overline{\text{OPT}} = \min_{\bar{A}\bar{x}=\bar{b}, \bar{x} \geq 0} \bar{c}^\top \bar{x}$$

For any optimal $x \in \mathbb{R}^n$ in the original LP, we consider the following $\bar{x} \in \mathbb{R}^{n+2}$

$$\bar{x} = \begin{bmatrix} \frac{1}{R}x \\ n+1 - \frac{1}{R} \sum_{i=1}^n x_i \\ 0 \end{bmatrix} \quad (5.5)$$

and $\bar{c} \in \mathbb{R}^{n+2}$

$$\bar{c} = \begin{bmatrix} \frac{\delta}{L} \cdot c^\top \\ 0 \\ 1 \end{bmatrix} \quad (5.6)$$

We want to argue that $\bar{x} \in \mathbb{R}^{n+2}$ is feasible in the modified LP. It is obvious that $\bar{x} \geq 0$, it remains to show $\bar{A}\bar{x} = \bar{b} \in \mathbb{R}^{d+1}$. We have

$$\bar{A}\bar{x} = \begin{bmatrix} A & 0 & \frac{1}{R}b - A1_n \\ 1_n^\top & 1 & 0 \end{bmatrix} \cdot \begin{bmatrix} \frac{1}{R}x \\ n+1 - \frac{1}{R} \sum_{i=1}^n x_i \\ 0 \end{bmatrix} = \begin{bmatrix} \frac{1}{R}Ax \\ n+1 \end{bmatrix} = \begin{bmatrix} \frac{1}{R}b \\ n+1 \end{bmatrix} = \bar{b},$$

where the third step follows from $Ax = b$, and the last step follows from definition of \bar{b} .

Therefore, using the definition of \bar{x} in (5.5) we have that

$$\overline{\text{OPT}} \leq \bar{c}^\top \bar{x} = \begin{bmatrix} \frac{\delta}{L} \cdot c^\top & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} \frac{1}{R}x \\ n+1 - \frac{1}{R} \sum_{i=1}^n x_i \\ 0 \end{bmatrix} = \frac{\delta}{LR} \cdot c^\top x = \frac{\delta}{LR} \cdot \text{OPT}. \quad (5.7)$$

where the first step follows from modified program is solving a minimization problem, the second step follows from definition of $\bar{x} \in \mathbb{R}^{n+2}$ (5.5) and $\bar{c} \in \mathbb{R}^{n+2}$ (5.6), the last step follows from $x \in \mathbb{R}^n$ is an optimal solution in the original linear program.

Given a feasible $(\bar{x}, \bar{y}, \bar{s}) \in \mathbb{R}^{(n+2) \times (d+1) \times (n+2)}$ with duality gap δ^2 , we can write $\bar{x} = \begin{bmatrix} \bar{x}_{1:n} \\ \tau \\ \theta \end{bmatrix} \in \mathbb{R}^{n+2}$ for some $\tau \geq 0, \theta \geq 0$. We can compute $\bar{c}^\top \bar{x}$ which is $\frac{\delta}{L} \cdot c^\top \bar{x}_{1:n} + \theta$. Then, we have

$$\frac{\delta}{L} \cdot c^\top \bar{x}_{1:n} + \theta \leq \overline{\text{OPT}} + \delta^2 \leq \frac{\delta}{LR} \cdot \overline{\text{OPT}} + \delta^2, \quad (5.8)$$

where the first step follows from definition of duality gap, the last step follows from (5.7).

Hence, we can upper bound the $\overline{\text{OPT}}$ of the transformed program as follows:

$$c^\top \hat{x} = R \cdot c^\top \bar{x}_{1:n} = \frac{LR}{\delta} \cdot \frac{\delta}{L} c^\top \bar{x}_{1:n} \leq \frac{RL}{\delta} \left(\frac{\delta}{LR} \cdot \overline{\text{OPT}} + \delta^2 \right) = \overline{\text{OPT}} + LR \cdot \delta,$$

where the first step follows by $\hat{x} = R \cdot \bar{x}_{1:n}$, the third step follows by (5.8).

Note that

$$\frac{\delta}{L} c^\top \bar{x}_{1:n} \geq -\frac{\delta}{L} \|c\|_\infty \|\bar{x}_{1:n}\|_1 = -\frac{\delta}{L} \|c\|_\infty \left\| \frac{1}{R} x \right\|_1 \geq -\frac{\delta}{L} \|c\|_\infty \frac{n}{R} \|x\|_\infty \geq -\delta n, \quad (5.9)$$

where the second step follows from definition $\bar{x} \in \mathbb{R}^{n+2}$, and the last step follows from $\|c\|_\infty \leq L$ and $\|x\|_\infty \leq R$.

We can upper bound the θ in the following sense,

$$\theta \leq \frac{\delta}{LR} \cdot \overline{\text{OPT}} + \delta^2 + \delta n \leq 2n\delta + \delta^2 \leq 4n\delta \quad (5.10)$$

where the first step follows from (5.8) and (5.9), the second step follows by $\overline{\text{OPT}} = \min_{Ax=b, x \geq 0} c^\top x \leq nLR$ (because $\|c\|_\infty \leq L$ and $\|x\|_\infty \leq R$), and the last step follows from $\delta \leq 1 \leq n$.

The constraint in the new polytope shows that

$$A\bar{x}_{1:n} + \left(\frac{1}{R}b - A1_n \right) \theta = \frac{1}{R}b.$$

Using $\hat{x} = R\bar{x}_{1:n} \in \mathbb{R}^n$, we have

$$A \frac{1}{R} \hat{x} + \left(\frac{1}{R}b - A1_n \right) \theta = \frac{1}{R}b.$$

Rewriting it, we have $A\hat{x} - b = (RA1_n - b)\theta \in \mathbb{R}^d$ and hence

$$\|A\hat{x} - b\|_1 = \|(RA1_n - b)\theta\|_1 \leq \theta(\|RA1_n\|_1 + \|b\|_1) \leq \theta \cdot (R\|A\|_1 + \|b\|_1) \leq 4n\delta \cdot (R\|A\|_1 + \|b\|_1),$$

where the second step follows from triangle inequality, the third step follows from $\|A1_n\|_1 \leq \|A\|_1$ (because the definition of entry-wise ℓ_1 norm), and the last step follows from (5.10).

■ 5.5.4 Why \sqrt{n} ?

The central path is the solution to the following ODE

$$\begin{aligned} S_t \frac{d}{dt} x_t + X_t \frac{d}{dt} s_t &= 1, \\ A \frac{d}{dt} x_t &= 0, \\ A^\top \frac{d}{dt} y_t + \frac{d}{dt} s_t &= 0. \end{aligned}$$

Solving this linear system, we have that $S_t \frac{dx_t}{dt} = (I - P_t)1$ and $X_t \frac{ds_t}{dt} = P_t 1$ where $P_t = X_t A^\top (A S_t^{-1} X_t A^\top)^{-1} A S_t^{-1}$. Using that $x_t s_t = t$, we have that

$$P_t = X_t A^\top (A X_t^2 A^\top)^{-1} A X_t = S_t^{-1} A^\top (A S_t^{-2} A^\top)^{-1} A S_t^{-1}$$

and that $X_t^{-1} \frac{dx_t}{dt} = \frac{1}{t}(I - P_t)1$ and $S_t^{-1} \frac{ds_t}{dt} = \frac{1}{t} P_t 1$. Equivalently, we have

$$\frac{d \ln x_t}{d \ln t} = (I - P_t)1 \text{ and } \frac{d \ln s_t}{d \ln t} = P_t 1.$$

Note that

$$\|P_t 1\|_\infty \leq \|P_t 1\|_2 = \sqrt{n}.$$

Hence, x_t and s_t can change by at most a constant factor when we change t by a $1 \pm \frac{1}{\sqrt{n}}$ factor.

Exercise 5.29. If we are given x such that $\|\ln x - \ln x_t\|_\infty = O(1)$, then we can find x_t by solving $\tilde{O}(1)$ linear systems.

■ 5.6 Interior Point Method for Convex Programs

The interior point method can be used to optimize any convex function. For more in-depth treatment, please see the structural programming section in [57].

Recall that any convex optimization problem

$$\min_x f(x)$$

can be rewritten in the epigraph form as

$$\min_{\{(x,t): f(x) \leq t\}} t.$$

Hence, it suffices to study the problem $\min_{x \in K} c^\top x$. Similar to the case of linear programs, we replace the hard constraint $x \in K$ by a soft constraint as follows:

$$\min_x \phi_t(x) \text{ where } \phi_t(x) = t c^\top x + \phi(x).$$

where $\phi(x)$ is a convex function such that $\phi(x) \rightarrow +\infty$ as $x \rightarrow \partial K$. Note that we put the parameter t in front of the cost $c^\top x$ instead of ϕ as in the last lecture, it is slightly more convenient here. We say ϕ is a *barrier* for K . To be concrete, we can always keep in mind $\phi(x) = -\sum_{i=1}^n \ln x_i$. As before, we define the central path.

Definition 5.30. The central path $x_t = \arg \min_x \phi_t(x)$.

The interior point method follows the following framework:

1. Find x close to x_1 .
2. While t is not tiny,
 - (a) Move x closer to x_t
 - (b) $t \rightarrow (1 + h) \cdot t$.

■ 5.6.1 Self-concordance

In this section, we give a general analysis for the Newton method. In the next section, we will use this to show that interior point method can be generalized to convex optimization. A key property of the Newton method is that it is invariant under linear transformation. In general, whenever a method uses k^{th} order information, we need to assume the k^{th} derivative is continuous. Otherwise, the k^{th} derivative is not useful for algorithmic purposes. For the Newton method, it is convenient to assume that the Hessian is Lipschitz. Since the method is invariant under linear transformation, it only makes sense to impose an assumption that is invariant under linear transformation.

Definition 5.31. Given a convex function $f : \mathbb{R}^n \rightarrow \mathbb{R}$, and any point $x \in \mathbb{R}^n$, define the norm $\|\cdot\|_x$ as

$$\|v\|_x^2 = v^\top \nabla^2 f(x) v.$$

We call a function f self-concordant if for any $h \in \mathbb{R}^n$ and any x in $\text{dom} f$, we have

$$D^3 f(x)[h, h, h] \leq 2 \|h\|_x^3$$

where $D^k f(x)[h_1, h_2, \dots, h_k]$ is the directional k^{th} derivative of f along the directions h_1, h_2, \dots, h_k .

Remark. The constant 2 is chosen so that $-\ln(x)$ exactly satisfies the assumption and it is not very important, in that by scaling f , we can change any constant to any other constant.

Exercise 5.32. Show that the following property is equivalent to self-concordance as defined above: restricted on any straight line $g(t) = f(x + th)$, we have $g'''(t) \leq 2g''(t)^{3/2}$.

Exercise 5.33. Show that the functions $x^\top A x$, $-\ln x$, $-\ln(1 - \sum x_i^2)$, $-\ln \det X$ are self-concordant under suitable nonnegativity conditions.

The self-concordance condition says that locally, the Hessian does not change too fast, i.e., the change in the Hessian is bounded by its magnitude (to the power 1.5). We will skip the proof of the lemma below.

Lemma 5.34. Given a self-concordant function f , for any $h_1, h_2, h_3 \in \mathbb{R}^n$, we have

$$D^3 f(x)[h_1, h_2, h_3] \leq 2 \|h_1\|_x \|h_2\|_x \|h_3\|_x.$$

From the self-concordance condition, we have the following more directly usable property.

Lemma 5.35. For a self-concordant function f and any $x \in \text{dom} f$ and any $\|y - x\|_x < 1$, we have that

$$(1 - \|y - x\|_x)^2 \nabla^2 f(x) \preceq \nabla^2 f(y) \preceq \frac{1}{(1 - \|y - x\|_x)^2} \nabla^2 f(x).$$

Proof. Let $\alpha(t) = \langle \nabla^2 f(x + t(y - x))u, u \rangle$. Then, we have that

$$\alpha'(t) = D^3 f(x + t(y - x))[y - x, u, u].$$

By self-concordance, we have

$$|\alpha'(t)| \leq 2 \|y - x\|_{x+t(y-x)} \|u\|_{x+t(y-x)}^2. \quad (5.11)$$

For $u = y - x$, we have $|\alpha'(t)| \leq 2\alpha(t)^{3/2}$. Hence, we have $\frac{d}{dt} \frac{1}{\sqrt{\alpha(t)}} \geq -1$. Integrating both sides wrt t , we have

$$\frac{1}{\sqrt{\alpha(t)}} \geq \frac{1}{\sqrt{\alpha(0)}} - t = \frac{1}{\|x - y\|_x} - t.$$

Rearranging it gives

$$\|y - x\|_{x+t(y-x)}^2 = \alpha(t) \leq \frac{1}{(\frac{1}{\|x-y\|_x} - t)^2} = \frac{\|x - y\|_x^2}{(1 - t\|x - y\|_x)^2}.$$

For general u , (5.11) gives

$$|\alpha'(t)| \leq 2 \frac{\|x - y\|_x}{1 - t\|x - y\|_x} \alpha(t).$$

Rearranging,

$$\left| \frac{d}{dt} \ln \alpha(t) \right| \leq 2 \frac{\|x - y\|_x}{1 - t\|x - y\|_x} = -2 \frac{d}{dt} \ln(1 - t\|x - y\|_x)$$

Integrating both from $t = 0$ to 1 gives the result. \square

■ 5.6.2 Self-concordant barrier functions

To analyze the algorithm above, we need to assume that ϕ is well-behaved. We measure the quality of ϕ by $\|\nabla\phi\|_{\nabla^2\phi(x)^{-1}}$. One can think this as the Lipschitz constant of ϕ but measured in the local norm.

Definition 5.36. We call ϕ a ν -self-concordant barrier for K if ϕ is self-concordant, $\phi(x) \rightarrow +\infty$ as $x \rightarrow \partial K$ and that $\|\nabla\phi(x)\|_{\nabla^2\phi(x)^{-1}}^2 \leq \nu$ for all x .

Not all convex functions are self-concordant. However, for our purpose, it suffices to show that we can construct a self-concordant barrier for any convex set.

Theorem 5.37. *Any convex set has an n -self concordant barrier.*

Unfortunately, this is an existence result and the barrier function is expensive to compute. In practice, we construct self-concordant barriers out of simpler ones:

Lemma 5.38. *The following functions are self-concordant barriers. We use ν -sc as a short form for ν -self-concordant barrier.*

- $-\ln x$ is 1-sc for $\{x \geq 0\}$.
- $-\ln \cos(x)$ is 1-sc for $\{|x| \leq \frac{\pi}{2}\}$.
- $-\ln(t^2 - \|x\|^2)$ is 2-sc for $\{t \geq \|x\|_2\}$.
- $-\ln \det X$ is n -sc for $\{X \in \mathbb{R}^{n \times n}, X \succeq 0\}$.
- $-\ln x - \ln(\ln x + t)$ is 2-sc for $\{x \geq 0, t \geq -\ln x\}$.
- $-\ln t - \ln(\ln t - x)$ is 2-sc for $\{t \geq e^x\}$.
- $-\ln x - \ln(t - x \ln x)$ is 2-sc for $\{x \geq 0, t \geq x \ln x\}$.
- $-2 \ln t - \ln(t^{2/p} - x^2)$ is 4-sc for $\{t \geq |x|^p\}$ for $p \geq 1$.
- $-\ln x - \ln(t^p - x)$ is 2-sc for $\{t^p \geq x \geq 0\}$ for $0 < p \leq 1$.
- $-\ln t - \ln(x - t^{-1/p})$ is 2-sc for $\{x > 0, t \geq x^{-p}\}$ for $p \geq 1$.
- $-\ln x - \ln(t - x^{-p})$ is 2-sc for $\{x > 0, t \geq x^{-p}\}$ for $p \geq 1$.

The following lemma shows how we can combine barriers.

Lemma 5.39. *If ϕ_1 and ϕ_2 are ν_1 and ν_2 -self concordant barriers for K_1 and K_2 respectively, then $\phi_1 + \phi_2$ is a $\nu_1 + \nu_2$ self concordant barrier for $K_1 \cap K_2$.*

Lemma 5.40. *If ϕ is a ν -self concordant barrier for K , then $\phi(Ax + b)$ is ν -self concordant for $\{y : Ay + b \in K\}$.*

Exercise 5.41. Using the lemmas above, prove that $-\sum_{i=1}^m \ln(a_i^\top x - b_i)$ is an m -self concordant barrier for the convex set $\{Ax \geq b\}$.

■ 5.6.3 Convergence of Newton method for self-concordant functions

Now we are ready to study the convergence of Newton method.

Lemma 5.42. *Given a self-concordant convex function f , consider the iteration*

$$x' = x - (\nabla^2 f(x))^{-1} \nabla f(x).$$

Suppose that $r = \|\nabla f(x)\|_{\nabla^2 f(x)^{-1}} < 1$, then we have

$$\|\nabla f(x')\|_{\nabla^2 f(x')^{-1}} \leq \frac{r^2}{(1-r)^2}.$$

Remark 5.43. Note that $\|\nabla f(x)\|_{\nabla^2 f(x)^{-1}} = \|\nabla^2 f(x)^{-1} \nabla f(x)\|_x$ is the step size of the Newton method. This is a measurement of the error, since the goal is to find x with $\nabla f(x) = 0$.

Proof. Lemma 5.35 shows that

$$\nabla^2 f(x') \succeq (1-r)^2 \nabla^2 f(x).$$

and hence

$$\|\nabla f(x')\|_{\nabla^2 f(x')^{-1}} \leq \frac{\|\nabla f(x')\|_{\nabla^2 f(x)^{-1}}}{(1-r)}.$$

To bound $\nabla f(x')$, we calculate that

$$\begin{aligned} \nabla f(x') &= \nabla f(x) + \int_0^1 \nabla^2 f(x + t(x' - x))(x' - x) dt \\ &= \nabla f(x) - \int_0^1 \nabla^2 f(x + t(x' - x))(\nabla^2 f(x))^{-1} \nabla f(x) dt \\ &= \left(\nabla^2 f(x) - \int_0^1 \nabla^2 f(x + t(x' - x)) dt \right) (\nabla^2 f(x))^{-1} \nabla f(x). \end{aligned} \quad (5.12)$$

For the term in the bracket, we use Lemma 5.35 to get (note that $\int_0^1 (1-tr)^2 dt = 1-r + \frac{1}{3}r^2$):

$$(1-r + \frac{1}{3}r^2) \nabla^2 f(x) \preceq \int_0^1 \nabla^2 f(x + t(x' - x)) dt \preceq \frac{1}{1-r} \nabla^2 f(x).$$

Therefore, we have

$$\left\| (\nabla^2 f(x))^{-\frac{1}{2}} \left(\nabla^2 f(x) - \int_0^1 \nabla^2 f(x + t(x' - x)) dt \right) (\nabla^2 f(x))^{-\frac{1}{2}} \right\|_{\text{op}} \leq \max\left(\frac{r}{1-r}, r - \frac{1}{3}r^2\right) = \frac{r}{1-r}.$$

Putting it into (5.12) gives

$$\begin{aligned} \|\nabla f(x')\|_{\nabla^2 f(x)^{-1}} &= \left\| \nabla^2 f(x)^{-\frac{1}{2}} \nabla f(x') \right\|_2 \\ &\leq \left\| (\nabla^2 f(x))^{-\frac{1}{2}} \left(\nabla^2 f(x) - \int_0^1 \nabla^2 f(x + t(x' - x)) dt \right) (\nabla^2 f(x))^{-\frac{1}{2}} \right\|_{\text{op}} \left\| (\nabla^2 f(x))^{-\frac{1}{2}} \nabla f(x) \right\|_2 \\ &\leq \frac{r}{1-r} \cdot r \\ &= \frac{r^2}{1-r}. \end{aligned}$$

□

Finally, we bound the error of the current iterate in terms of $\|\nabla f(x)\|_{\nabla^2 f(x)^{-1}}$.

Lemma 5.44. *Given x such that $\|\nabla f(x)\|_{\nabla^2 f(x)^{-1}} \leq \frac{1}{6}$, we have that*

- $\|x - x^*\|_{x^*} \leq 2\|\nabla f(x)\|_{\nabla^2 f(x)^{-1}},$
- $\|x - x^*\|_x \leq \frac{4}{3}\|\nabla f(x)\|_{\nabla^2 f(x)^{-1}},$
- $f(x) \leq f(x^*) + \|\nabla f(x)\|_{\nabla^2 f(x)^{-1}}^2.$

Proof. Let $r = \|x - x^*\|_x$. Suppose that $r \leq \frac{1}{4}$. Note that

$$\nabla f(x) = \nabla f(x) - \nabla f(x^*) = \int_0^1 \nabla^2 f(x^* + t(x - x^*))(x - x^*) dt.$$

Using that $\nabla^2 f(x^* + t(x - x^*)) \succeq (1 - (1-t)r)^2 \nabla^2 f(x)$ (Lemma 5.35), we have

$$\begin{aligned} \|\nabla f(x)\|_{\nabla^2 f(x)^{-1}} &= \left\| \int_0^1 \nabla^2 f(x^* + t(x - x^*))(x - x^*) dt \right\|_{\nabla^2 f(x)^{-1}} \\ &\geq \int_0^1 (1 - (1-t)r)^2 \|x - x^*\|_x dt \\ &= \left(1 - r + \frac{r^2}{3}\right) r \geq \frac{3r}{4}. \end{aligned}$$

Using $\|\nabla f(x)\|_{\nabla^2 f(x)^{-1}} \leq \frac{1}{6}$, we have indeed $r \leq \frac{1}{4}$ (our lower bound above is a non-decreasing function) Using Lemma 5.35 again, we have

$$\|x - x^*\|_{x^*} \leq \frac{\|x - x^*\|_x}{1 - r} \leq \frac{4}{3} \frac{1}{1 - \frac{1}{4}} \|\nabla f(x)\|_{\nabla^2 f(x)^{-1}} \leq 2 \|\nabla f(x)\|_{\nabla^2 f(x)^{-1}}.$$

For the bound for $f(x)$, we have that

$$f(x) = f(x^*) + \langle \nabla f(x^*), x - x^* \rangle + \int_0^1 (1-t)(x - x^*)^\top \nabla^2 f(x^* + t(x - x^*)) (x - x^*) dt.$$

Using that $\nabla^2 f(x^* + t(x - x^*)) \preceq \frac{1}{(1-(1-t)r)^2} \nabla^2 f(x)$, we have

$$\begin{aligned} f(x) &\leq f(x^*) + \int_0^1 \frac{1-t}{(1-(1-t)r)^2} dt \cdot \|x - x^*\|_x^2 \\ &= f(x^*) + \frac{1}{r^2} \left(\frac{r}{1-r} + \log(1-r) \right) \|x - x^*\|_x^2 \\ &\leq f(x^*) + \left(\frac{1}{2} + r \right) \|x - x^*\|_x^2 \\ &\leq f(x^*) + \|\nabla f(x)\|_{\nabla^2 f(x)^{-1}}^2 \end{aligned}$$

where we used $r \leq \frac{1}{4}$ at the end. □

■ 5.6.4 Main Algorithm and Analysis

Algorithm 17: InteriorPointMethod

Input: A ν -self-concordant barrier ϕ for K , the minimizer x of ϕ .

Define $f_t(x) = tc^\top x + \phi(x)$. $t = \frac{1}{6} \|c\|_{\nabla^2 \phi(x)^{-1}}^{-1}$.

while $t \leq \frac{\nu + \sqrt{\nu}}{\epsilon}$ **do**
 $x \leftarrow x - \nabla^2 f_t(x)^{-1} \nabla f_t(x)$.
 $t \leftarrow (1+h)t$ with $h = \frac{1}{9\sqrt{\nu}}$.
end
return x .

We first explain the termination condition. Intuitively, we can see that $\min f_t(x_t)$ tends to optimality as $t \rightarrow \infty$. We first need a lemma showing that the gradient of ϕ is small.

Lemma 5.45 (Duality Gap). *Suppose that ϕ is a ν -self concordant barrier. For any $x, y \in K$, we have that*

$$\langle \nabla \phi(x), y - x \rangle \leq \nu.$$

Proof. Let $\alpha(t) = \langle \nabla \phi(z_t), y - x \rangle$ where $z_t = x + t(y - x)$. Then, we have

$$\alpha'(t) = \langle \nabla^2 \phi(z_t)(y - x), y - x \rangle.$$

Note that

$$\alpha(t) \leq \|\nabla \phi(z_t)\|_{\nabla^2 \phi(z_t)^{-1}} \|y - x\|_{\nabla^2 \phi(z_t)} \leq \sqrt{\nu} \|y - x\|_{\nabla^2 \phi(z_t)}.$$

Hence, we have $\alpha'(t) \geq \frac{1}{v} \alpha(t)^2$. If $\alpha(0) \leq 0$, then we are done. Otherwise, α is increasing and hence $\alpha(1) > 0$. Since $\frac{1}{\alpha(1)} \leq \frac{1}{\alpha(0)} - \frac{1}{v}$. So, $\alpha(0) \leq v$. □

Lemma 5.46 (Duality Gap). *Suppose that ϕ is a ν -self concordant barrier, we have that*

$$\langle c, x_t \rangle \leq \langle c, x^* \rangle + \frac{\nu}{t}.$$

More generally, for any x such that $\|tc + \nabla \phi(x)\|_{(\nabla^2 \phi(x))^{-1}} \leq \frac{1}{6}$, we have that

$$\langle c, x \rangle \leq \langle c, x^* \rangle + \frac{\nu + \sqrt{\nu}}{t}.$$

Proof. Let x^* be a minimizer of $c^\top x$ on K . By optimality, we have $tc + \nabla\phi(x) = 0$. Therefore, we have

$$\langle c, x_t \rangle - \langle c, x^* \rangle = \frac{1}{t} \langle \nabla\phi(x_t), x^* - x_t \rangle \leq \frac{\nu}{t}.$$

For the second result, let $f(x) = tc^\top x + \phi(x)$. Lemma 5.44 shows that

$$\|x - x_t\|_x \leq 2\|\nabla f(x)\|_{\nabla^2 f(x)^{-1}} \leq \frac{1}{3}.$$

Hence,

$$\langle c, x - x_t \rangle \leq \|c\|_{\nabla^2 \phi(x)^{-1}} \|x - x_t\|_x \leq \frac{1}{3} \|c\|_{\nabla^2 \phi(x)^{-1}}$$

Using $c = \frac{tc + \nabla\phi(x)}{t} - \frac{\nabla\phi(x)}{t}$, we have

$$\begin{aligned} \langle c, x - x_t \rangle &\leq \frac{1}{3t} (\|tc + \nabla\phi(x)\|_{\nabla^2 \phi(x)^{-1}} + \|\nabla\phi(x)\|_{\nabla^2 \phi(x)^{-1}}) \\ &\leq \frac{1}{3t} \left(\frac{1}{6} + \sqrt{\nu} \right) \leq \frac{\sqrt{\nu}}{t}. \end{aligned}$$

This gives the result. \square

Hence, it suffices to end with $t = (\nu + \sqrt{\nu})/\varepsilon$, which is exactly same as the previous lecture.

Theorem 5.47. *Given a ν -self concordant barrier ϕ and its minimizer. We can find $x \in K$ such that $c^\top x \leq c^\top x^* + \varepsilon$ in*

$$O(\sqrt{\nu} \log(\frac{\nu}{\varepsilon} \|c\|_{\nabla^2 \phi(x)^{-1}}))$$

iterations.

Proof. We prove by induction that $\|\nabla f_t(x)\|_{\nabla^2 f_t(x)^{-1}} \leq \frac{1}{6}$ at the beginning of each iteration. This is true at the beginning by the definition of initial t . By Lemma 5.42, after the Newton step, we have

$$\|\nabla f_t(x)\|_{\nabla^2 f_t(x)^{-1}} \leq \left(\frac{1/6}{1 - 1/6} \right)^2 = \frac{1}{25}.$$

Let $t' = (1+h)t$ with $h = \frac{1}{9\sqrt{\nu}}$. Note that $\nabla f_{t'}(x) = (1+h)tc + \nabla\phi(x)$ and hence $\nabla f_{t'}(x) = (1+h)\nabla f_t(x) - h\nabla\phi(x)$ and $\nabla^2 f_{t'}(x) = \nabla^2 f_t(x) = \nabla^2 \phi(x)$. Therefore, we have that

$$\begin{aligned} \|\nabla f_{t'}(x)\|_{\nabla^2 f_{t'}(x)^{-1}} &= \|(1+h)\nabla f_t(x) - h\nabla\phi(x)\|_{\nabla^2 f_t(x)^{-1}} \\ &\leq (1+h)\|\nabla f_t(x)\|_{\nabla^2 f_t(x)^{-1}} + h\|\nabla\phi(x)\|_{\nabla^2 \phi(x)^{-1}} \\ &\leq \frac{1+h}{25} + h\sqrt{\nu} \leq \frac{1}{6}. \end{aligned}$$

This completes the induction. \square

Chapter 6

Sparsification

In this chapter, we study some randomization techniques for faster convex optimization.

■ 6.1 Subspace embedding

In this section and the next section, we consider the least squares regression problem

$$\min_x \|Ax - b\|_2^2$$

where $A \in \mathbb{R}^{n \times d}$ with $n \geq d$ (we assume this throughout the chapter). The gradient of the function is $2A^\top Ax - 2A^\top b$. Setting it to zero, and assuming $A^\top A$ is invertible, the solution is given by

$$x = (A^\top A)^{-1} A^\top b.$$

If $A^\top A$ is not invertible, we use its pseudo-inverse. If the matrix $A^\top A \in \mathbb{R}^{d \times d}$ is given, then we can solve the equation above in time d^ω , the current complexity of matrix multiplication. If $n > d^\omega$, then the bottleneck is simply to compute $A^\top A$. The following lemma shows that it suffices to approximate $A^\top A$.

The simplest iteration is the Richardson iteration:

$$x^{(k+1)} = A^\top b + (I - A^\top A)x^{(k)} = x^{(k)} + A^\top b - A^\top Ax^{(k)}.$$

To ensure this converges, we scale down $A^\top A$ by its largest eigenvalue so that $A^\top A \prec I$. This gives a bound of $O(\kappa(A^\top A) \log(1/\epsilon))$ on the number of iterations to get ϵ error where $\kappa(A^\top A) = \lambda_{\max}(A^\top A)/\lambda_{\min}(A^\top A)$. More generally, one can use *pre-conditioning*. Recall that for a vector v , the norm $\|v\|_M$ is defined as $v^\top M v$.

Lemma 6.1. *Given a matrix M such that $A^\top A \preceq M \preceq \kappa \cdot A^\top A$ for some $\kappa \geq 1$. Consider the algorithm $x^{(k+1)} = x^{(k)} - M^{-1}(A^\top Ax^{(k)} - A^\top b)$. Then, we have that*

$$\|x^{(k)} - x^*\|_M \leq \left(1 - \frac{1}{\kappa}\right)^k \|x^{(0)} - x^*\|_M.$$

Remark 6.2. The proof also shows why the choice of norm above is the natural one. In this norm, the residual drops geometrically.

Proof. Using $x^* = (A^\top A)^{-1} A^\top b$, i.e., $A^\top b = (A^\top A)x^*$, and the formula of $x^{(k+1)}$, we have

$$\begin{aligned} x^{(k+1)} - x^* &= x^{(k)} - M^{-1}(A^\top Ax^{(k)} - A^\top b) - x^* \\ &= x^{(k)} - M^{-1}(A^\top Ax^{(k)} - A^\top Ax^*) - x^* \\ &= (I - M^{-1}A^\top A)(x^{(k)} - x^*). \end{aligned}$$

Therefore, the norm of error is

$$\begin{aligned} \|x^{(k+1)} - x^*\|_M^2 &= (x^{(k)} - x^*)^\top (I - A^\top A M^{-1}) M (I - M^{-1} A^\top A) (x^{(k)} - x^*) \\ &= (x^{(k)} - x^*)^\top M^{\frac{1}{2}} (I - H)^2 M^{\frac{1}{2}} (x^{(k)} - x^*) \end{aligned}$$

where $H = M^{-\frac{1}{2}} A^\top A M^{-\frac{1}{2}}$. Note that the eigenvalues of H lie between $1/\kappa$ and 1 and hence

$$\lambda_{\max}(I - H)^2 \leq \left(1 - \frac{1}{\kappa}\right)^2.$$

This gives the conclusion. \square

Note that $x^\top A^\top A x = \|Ax\|^2$. Alternatively, we can think that our goal is to approximate A by a smaller matrix B s.t. $\|Ax\|^2$ is close to $\|Bx\|^2$ for all x . In this section, we show that we can simply take $B = \Pi A$ for a random matrix Π with relatively few rows. With this choice of M , we can run the Richardson iteration. We need to see if this will make the entire procedure more efficient.

Definition 6.3. A matrix $\Pi \in \mathbb{R}^{m \times n}$ is an embedding for a set $S \subset \mathbb{R}^n$ with distortion ϵ if

$$(1 - \epsilon)\|y\|^2 \leq \|\Pi y\|^2 \leq (1 + \epsilon)\|y\|^2$$

for all $y \in S$.

In this section, we focus on the case that S is a d -dimensional subspace in \mathbb{R}^n , namely $S = \{Ax : x \in \mathbb{R}^d\}$. Consider the SVD $A = U\Sigma V^\top$. For any $y \in S$, we have that

$$\|U^\top y\|_2^2 = \|U^\top U \Sigma V^\top x\|_2^2 = x^\top V \Sigma^2 V^\top x = \|Ax\|^2.$$

Therefore, any d -dimensional subspace has a zero distortion embedding of size $d \times n$.

Exercise 6.4. For any d -dimensional subspace S , any embedding with distortion $\epsilon < 1$ must have at least d rows.

This embedding is not useful for solving the least squares problem because the solution of the least square problem is simply a closed form of the SVD decomposition $x = V\Sigma^{-1}U^\top b$ and finding the SVD is usually more expensive.

■ 6.1.1 Oblivious Subspace Embedding via Johnson-Lindenstrauss

Surprisingly, there are random embeddings that have small distortion without knowledge of the subspace.

Definition 6.5. A random matrix $\Pi \in \mathbb{R}^{m \times n}$ is a (d, ϵ, δ) -oblivious subspace embedding (OSE) if for any fixed d -dimensional subspace $S \subset \mathbb{R}^n$, Π is an embedding for S with distortion ϵ with probability at least $1 - \delta$.

The next lemma provides an equivalent definition.

Lemma 6.6. We call Π a (d, ϵ, δ) OSE if for any matrix $U \in \mathbb{R}^{n \times d}$ with orthonormal columns, we have that

$$\mathbf{P}(\|U^\top \Pi^\top \Pi U - I_d\|_{\text{op}} \leq \epsilon) \geq 1 - \delta.$$

Proof. Let S be the subspace with an orthonormal basis $U \in \mathbb{R}^{n \times d}$, namely $S = \{y : y = Uz\}$. Then, the condition

$$(1 - \epsilon)\|y\|^2 \leq \|\Pi y\|^2 \leq (1 + \epsilon)\|y\|^2$$

can be rewritten as

$$(1 - \epsilon)U^\top U \preceq U^\top \Pi^\top \Pi U \preceq (1 + \epsilon)U^\top U.$$

Using $U^\top U = I_d$, we have

$$(1 - \epsilon)I_d \preceq U^\top \Pi^\top \Pi U \preceq (1 + \epsilon)I_d.$$

\square

For the special case $d = 1$, the definition becomes

$$\mathbf{P} [||\Pi a||_2^2 - 1| \leq \epsilon] \geq 1 - \delta$$

for all unit vectors a . An OSE for $d = 1$ is given by the Johnson-Lindenstrauss Lemma. The original version was for a uniform random subspace of dimension d , but later versions extended this to Gaussian, Bernoulli and more general random matrices [74].

Lemma 6.7 (Johnson-Lindenstrauss Lemma). *Let $\Pi \in \mathbb{R}^{m \times n}$ be a random matrix with i.i.d entries from $N(0, \frac{1}{\sqrt{m}})$ or uniformly sampled from $\pm \frac{1}{\sqrt{m}}$ with $m = \Theta(\frac{1}{\epsilon^2} \log(\frac{1}{\delta}))$. Then, Π is a $(1, \epsilon, \delta)$ OSE.*

We will skip the proof for this as we will prove a more general result later. Next, we show that any OSE for $d = 1$ is a OSE for general d . Therefore, it suffices to focus on the case $d = 1$. First, we need a lemma about ϵ -net on S^{n-1} .

Lemma 6.8. *For any $\epsilon > 0$ and any $n \in \mathbb{N}$, there are at most $(1 + \frac{2}{\epsilon})^n$ unit vectors $x_i \in \mathbb{R}^n$ such that for any unit vector $x \in \mathbb{R}^n$, there is an i such that $\|x - x_i\|_2 \leq \epsilon$.*

Remark. We call the points $\{x_i\}_i$ the ϵ -net on S^{n-1} .

Proof. We consider the following algorithm:

1. $V = S^{n-1}$. $i \leftarrow 1$.
2. While there is $x_i \in V$
 - (a) $V \leftarrow V \setminus B(x_i, \epsilon)$.
 - (b) $i \leftarrow i + 1$.

Let $\{x_1, x_2, \dots, x_N\}$ be the points it found. By the construction, it is clear that $\|x - x_i\| \leq \epsilon$ for some i (else the procedure would continue). Now consider balls of radius $\epsilon/2$ centered at each x_i . To bound the number of points, we note that all $B(x_i, \frac{\epsilon}{2})$ are disjoint and that all balls lie in $B(0, 1 + \frac{\epsilon}{2})$. Therefore,

$$N \cdot \text{vol}(B(0, \frac{\epsilon}{2})) \leq \text{vol}(B(0, 1 + \frac{\epsilon}{2})).$$

and hence $N \leq (1 + \frac{2}{\epsilon})^n$. □

Lemma 6.9. *Suppose that Π is a $(1, \epsilon, \delta)$ OSE. Then, Π is a $(d, 4\epsilon, 5^d \delta)$ OSE.*

Proof. Let $N = \{x_i\}_{i=1}^N$ be a $\frac{1}{2}$ -net for S^{d-1} . Then, for any x , we have $x_1 \in N$ such that $\|x - x_1\|_2 \leq \frac{1}{2}$. Using the $\frac{1}{2}$ -net guarantee on the vector $x - x_1$, we can find $x_2 \in N$ and $0 \leq t_2 \leq \frac{1}{2}$ such that

$$\|x - x_1 - t_2 x_2\| \leq \frac{1}{4}.$$

Continuing similarly, we have $x = \sum_{i=1}^{\infty} t_i x_i$ with $0 \leq t_i \leq \frac{1}{2^{i-1}}$. Hence, we have that

$$\begin{aligned} x^\top (U^\top \Pi^\top \Pi U - I_d) x &= \sum_{i,j} t_i t_j x_i^\top (U^\top \Pi^\top \Pi U - I_d) x_j \\ &\leq \sum_{i,j} t_i t_j \cdot \max_{x \in N} |x^\top |U^\top \Pi^\top \Pi U - I_d| x| \\ &\leq 4 \max_{x \in N} |x^\top |U^\top \Pi^\top \Pi U - I_d| x| \\ &= 4 \max_{x \in UN} ||\Pi x||^2 - 1| \end{aligned}$$

Now, using that Π is $(1, \epsilon, \delta)$ OSE, we have that

$$\mathbf{P} (||\Pi x||^2 - 1| \leq \epsilon) \geq 1 - \delta.$$

Taking a union bound over all $x \in UN$, we have

$$\mathbf{P}(x^\top (U^\top \Pi^\top \Pi U - I_d) x \leq 4\epsilon) \geq 1 - 5^d \delta.$$

□

This reduction and the Johnson-Lindenstrauss Lemma shows that a random $\pm \frac{1}{\sqrt{m}}$ is a (d, ϵ, δ) OSE with

$$m = \Theta\left(\frac{1}{\epsilon^2}(d + \log(\frac{1}{\delta}))\right).$$

As we discussed before any (d, ϵ, δ) OSE should have at least d rows. Therefore, the number of rows of this OSE is tight for the regime $\epsilon = \Theta(1)$. We only need an OSE for $\epsilon = \Theta(1)$ because of Lemma 6.1; by iterating we can get any ϵ with an overhead of $\log(1/\epsilon)$. Unfortunately, computing ΠA is in fact more expensive than $A^\top A$. The first involves multiplying $\Theta(d) \times n$ and $n \times d$ matrix, the second one involves multiplying $d \times n$ and $n \times d$ matrix.

■ 6.1.2 Sparse Johnson-Lindenstrauss

We consider the sparse matrix $\Pi \in \mathbb{R}^{m \times n}$ where each entry is $\pm \frac{1}{\sqrt{s}}$ with probability $\frac{s}{m}$ and 0 otherwise. We will show that this random matrix is a (d, ϵ, δ) -OSE for $s = \Theta(\log^2(d/\delta)/\epsilon^2)$ and $m = \Theta(d \log(d/\delta)/\epsilon^2)$. When $n = d = 1$, $\|\Pi x\|^2$ is the number of non-zeros in the only column. Therefore, we indeed need that s scales like $1/\epsilon^2$. The advantage of a sparse embedding is that applying it can be much more efficient.

Remark 6.10. It turns out that one can select exactly s non-zeros for each column. This allows us to use $s = \Theta(\frac{\log(d/\delta)}{\epsilon})$. The proof of this is slightly more complicated due to the lack of independence [16].

To analyze $U^\top \Pi^\top \Pi U$, we note that

$$U^\top \Pi^\top \Pi U = \sum_{r=1}^m (\Pi U)_r^\top (\Pi U)_r.$$

Since each row of Π is independent, we can use matrix concentration bounds to analyze the sum above. See [70] for a survey on matrix concentration bounds.

Theorem 6.11 (Matrix Chernoff). *Suppose we have a sequence of independent, random, self-adjoint matrices $M_j \in \mathbb{R}^{n \times n}$ such that $\mathbf{E} M_j = I$ and $0 \preceq M_j \preceq R \cdot I$. Then, for $T = \frac{R}{\epsilon^2} \log \frac{n}{\delta}$,*

$$(1 - O(\epsilon))I \preceq \frac{1}{T} \sum_{j=1}^T M_j \preceq (1 + O(\epsilon))I$$

with probability at least $1 - \delta$.

Lemma 6.12 (Hanson-Wright Inequality). *For independent random variables $\sigma_1, \dots, \sigma_n$ with $\mathbf{E} \sigma_i = 0$, $|\sigma_i| \leq 1$ and $A \in \mathbb{R}^{n \times n}$, we have*

$$|\sigma^\top A \sigma - \mathbf{E} \sigma^\top A \sigma| \lesssim \|A\|_F \sqrt{\log(\frac{1}{\delta})} + \|A\|_{\text{op}} \log(\frac{1}{\delta})$$

with probability $1 - \delta$.

For our problem, we set $M_r = m \cdot U^\top \pi_r \pi_r^\top U$ where π_r is the r -th row of Π (as a column vector). One can check that $M_r \succeq 0$ and that $\mathbf{E} M_r = I$. Next, we note that

$$M_r \preceq m \cdot \pi_r^\top U U^\top \pi_r \cdot I. \tag{6.1}$$

With small probability, $\pi_r^\top U U^\top \pi_r$ can be huge. However, as long as $\pi_r^\top U U^\top \pi_r$ is bounded by R with probability $1 - \delta$, then we can still use the matrix Chernoff bound above. To bound $\pi_r^\top U U^\top \pi_r$, we will use the following large deviation inequality.

Lemma 6.13. *Assume that $s \gg \frac{m}{n} \log(\frac{1}{\delta}), \log^2(\frac{1}{\delta})/\epsilon^2$ and $m \gg d \log(\frac{1}{\delta})/\epsilon^2$. Then,*

$$\pi_r^\top U U^\top \pi_r \leq \frac{\epsilon^2}{\log(d/\delta)}$$

with probability $1 - \delta$. (Here \gg means greater by a sufficiently large constant factor).

Proof. Note that $\pi_r \in \mathbb{R}^n$ with each entry non-zero with probability $\frac{s}{m}$. By the Chernoff bound, one can show that π_r has at most $2sn/m$ non-zeros with probability $1 - \delta$ using that $sn/m \gg \log(\frac{1}{\delta})$. Let I be the set of indices for which π_r is non-zero. Conditional on the set I and that $|I| \leq 2sn/m$, note that $\sigma \stackrel{\text{def}}{=} \pi_r|_I$ is a random $\pm \frac{1}{\sqrt{s}}$ vector. Let $P = (UU^\top)|_{I \times I}$. Then, we have that

$$\pi_r^\top UU^\top \pi_r = \sigma^\top P \sigma.$$

The Hanson-Wright inequality shows that

$$|\sigma^\top P \sigma - \mathbf{E} \sigma^\top P \sigma| \lesssim \frac{1}{s} \|P\|_F \sqrt{\log(\frac{1}{\delta})} + \frac{1}{s} \|P\|_{\text{op}} \log(\frac{1}{\delta}).$$

Note that UU^\top is a projection matrix and hence $\|P\|_{\text{op}} \leq 1$. Since $P \succeq 0$, we have that

$$\|P\|_F = \sqrt{\text{tr} P^2} \leq \sqrt{\|P\|_{\text{op}} \cdot \text{tr} P} \leq \sqrt{\text{tr} P}.$$

Also, we have that $\mathbf{E} \sigma^\top P \sigma = \frac{1}{s} \text{tr} P$. Hence, we have

$$\sigma^\top P \sigma \leq \frac{1}{s} \left(\text{tr} P + O \left(\sqrt{\text{tr} P \cdot \log \frac{1}{\delta}} + \log \frac{1}{\delta} \right) \right)$$

with probability $1 - \delta$. Note that $\text{tr} UU^\top = \text{tr} U^\top U = d$ and that P is a random diagonal block of UU^\top of size at most $2sn/m$. By the Chernoff bound, one can show that

$$\text{tr} P \leq \frac{4sd}{m}.$$

Hence, we have

$$\sigma^\top P \sigma \leq \frac{4d}{m} + \frac{1}{s} O \left(\sqrt{\frac{sd}{m} \cdot \log \frac{1}{\delta}} + \log \frac{1}{\delta} \right)$$

with probability $1 - \delta$. Using $s \gg \log^2(\frac{d}{\delta})/\epsilon^2$ and $m \gg d \log(\frac{d}{\delta})/\epsilon^2$, we have $\sigma^\top P \sigma \leq \frac{\epsilon^2}{\log(d/\delta)}$ with probability $1 - \delta$. \square

Now we can prove the main theorem.

Theorem 6.14. *Consider a random sparse matrix $\Pi \in \mathbb{R}^{m \times n}$ where each entry is $\pm \frac{1}{\sqrt{s}}$ with probability $\frac{s}{m}$ and 0 otherwise. There exist constants c_1, c_2 such that for $m = c_1 \frac{d \log(\frac{d}{\delta})}{\epsilon^2}$ and $s = c_2 \frac{\log^2(\frac{d}{\delta})}{\epsilon^2}$ Π is an $O(d, \epsilon, \delta)$ -OSE.*

Proof. By the previous lemma, we have that

$$\pi_r^\top UU^\top \pi_r \leq \frac{\epsilon^2}{\log(d/\delta)}$$

with high probability. Under this event, using Theorem 6.11 and (6.1), we have that

$$(1 - O(\epsilon))I \preceq \sum_{r=1}^m \pi_r^\top UU^\top \pi_r \preceq (1 + O(\epsilon))I.$$

\square

■ 6.1.3 Back to Regression

In the last subsection, we presented a proof sketch of a suboptimal OSE. For completeness, we state a tighter version here:

Algorithm 18: RegressionUsingOSE

Input: a matrix $A \in \mathbb{R}^{n \times d}$, a vector $b \in \mathbb{R}^d$, success probability δ and target accuracy ϵ .
 Let Π be a $O(d, \frac{1}{4}, \delta)$ OSE constructed by Theorem 6.14.
 Compute $A' = 2\Pi A$, $M = A'^\top A'$ and M^{-1} .
 $x^{(1)} = 0$.
for $k = 1, 2, \dots, 4 \log(\frac{1}{\epsilon})$ **do**
 $x^{(k+1)} = x^{(k)} - M^{-1}(A'^\top A x^{(k)} - A'^\top b)$
end
return $x^{(\text{last})}$.

Theorem 6.15. *Given any matrix $A \in \mathbb{R}^{n \times d}$, any vector $b \in \mathbb{R}^d$, the algorithm RegressionUsingOSE returns a vector x such that*

$$\|A^\top A x - A^\top b\|_{(A^\top A)^{-1}} \leq \epsilon \|A^\top b\|_{(A^\top A)^{-1}}.$$

with probability $1 - \delta$ in $\tilde{O}(\text{nnz}(A) + d^\omega)$ time.

Proof. The guarantee of x follows from the definition of OSE and Lemma 6.1. We note that ΠA simply involves duplicating each row of A into roughly s many rows in ΠA . Hence, the cost of computing ΠA is $O(s \cdot \text{nnz}(A)) = \tilde{O}(\text{nnz}(A))$. The cost of computing M takes $\tilde{O}(d^\omega)$ time. Computing M^{-1} takes $\tilde{O}(d^\omega)$ time. The loop takes $\tilde{O}(\text{nnz}(A))$ time. This explain the total time. \square

Linear regression can also be solved in time $O(\text{nnz}(A) + d^{O(1)})$ via a very sparse embedding: each column of Π picks exactly one nonzero entry in a random location. This was analyzed by Clarkson and Woodruff [77]. See also [34] for a survey.

■ 6.2 Leverage Score Sampling

Here we give a way to reduce solving a tall linear regression system into a sequence of submatrices:

Theorem 6.16 ([17]). *Given a matrix $A \in \mathbb{R}^{n \times d}$. Let $T(m)$ be the cost of solving $B^\top B x = b$ among all m distinct subrows B of A . Then, we have that*

$$T(n) = O^*(\text{nnz}(A) + T(O(d \log d))).$$

Remark. Here we use O^* to emphasize there is some dependence on $\log(\frac{1}{\epsilon})$ suppressed for notational simplicity. Lemma 6.1 shows that once we can solve the system with constant approximation, we can repeat $\log(\frac{1}{\epsilon})$ times to get an ϵ -accurate solution.

■ 6.2.1 Leverage scores

The key concept in this reduction is leverage score.

Definition 6.17. Given a matrix $A \in \mathbb{R}^{n \times d}$, let a_i^\top be the i^{th} row of A . The leverage score of the i^{th} row of A is

$$\sigma_i(A) \stackrel{\text{def}}{=} a_i^\top (A^\top A)^+ a_i.$$

Note that $\sigma(A)$ is the diagonal of the projection matrix $A(A^\top A)^+ A^\top$. Since $0 \preceq A(A^\top A)^+ A^\top \preceq I$, we have that $0 \leq \sigma_i(A) \leq 1$. Moreover, since $A(A^\top A)^+ A^\top$ is a projection matrix, the sum of A 's leverage scores (its trace) is equal to the rank of A :

$$\sum_{i=1}^n \sigma_i(A) = \text{tr}(A(A^\top A)^+ A^\top) = \text{rank}(A(A^\top A)^+ A^\top) = \text{rank}(A) \leq d. \quad (6.2)$$

The leverage score measures the “importance” of a row in forming the row space of A . If a row has a component orthogonal to all other rows, its leverage score is 1. Removing it would decrease the rank of A , completely changing its row space. The *coherence* of A is $\|\sigma(A)\|_\infty$. If A has low coherence, no particular row is especially important. If A has high coherence, it contains at least one row whose removal would significantly affect the composition of A ’s row space. The following two characterizations help with this intuition.

Lemma 6.18. *For all $A \in \mathbb{R}^{n \times d}$ and $i \in [n]$ we have that*

$$\sigma_i(A) = \min_{A^\top x = a_i} \|x\|_2^2.$$

where a_i is the i^{th} row of A .

Lemma 6.19. *For all $A \in \mathbb{R}^{n \times d}$ and $i \in [n]$, we have that $\sigma_i(A)$ is the smallest t such that*

$$a_i a_i^\top \preceq t \cdot A^\top A. \quad (6.3)$$

Sampling rows from A according to their exact leverage scores gives a spectral approximation for A with high probability. Sampling by leverage score overestimates also suffices.

Lemma 6.20. *Given a vector u of leverage score overestimates, i.e., $\sigma_i(A) \leq u_i$ for all i , define*

$$X = \frac{1}{p_i} a_i a_i^\top \quad \text{with probability} \quad p_i = \frac{u_i}{\|u\|_1}.$$

For $T = \Omega(\frac{\|u\|_1 \log n}{\varepsilon^2})$, with probability $1 - \frac{1}{n^{O(1)}}$, we have that

$$(1 - \varepsilon) A^\top A \preceq \frac{1}{T} \sum_{i=1}^T X_i \preceq (1 + \varepsilon) A^\top A$$

where X_i are independent copies of X .

Proof. Note that $\mathbf{E}X = A^\top A$ and that

$$0 \preceq X = \frac{1}{p_i} a_i a_i^\top \preceq \frac{\|u\|_1}{\sigma_i} a_i a_i^\top \preceq \|u\|_1 \cdot A^\top A.$$

Now, the statement simply follows from the matrix Chernoff bound with $M_k = (A^\top A)^{-\frac{1}{2}} X_k (A^\top A)^{-\frac{1}{2}}$ and $R = \|u\|_1$. \square

Combining Lemma 6.20 and Lemma 6.1, we have that

$$T(n) = \text{cost of computing } \sigma_i + O^*(\text{nnz}(A) + T(d \log d)) \quad (6.4)$$

where we used that $\|\sigma\|_1 = O(d)$. However, computing σ exactly is too expensive for many purposes. In [67], they showed that we can compute leverage scores approximately by solving only polylogarithmically many regression problems. This result uses the fact that

$$\sigma_i(A) = \|A(A^\top A)^+ A^\top e_i\|_2^2$$

and that by the Johnson-Lindenstrauss Lemma these lengths are preserved up to a multiplicative error if we project these vectors to a random low-dimensional subspace.

In particular, this lemma shows that we can approximate $\sigma_i(A)$ via $\|\Pi A(A^\top A)^+ A^\top e_i\|_2^2$. The benefit of this is that we can compute $\Pi A(A^\top A)^+$ by solving $\frac{\log n}{\varepsilon^2}$ many linear systems. In other words, we have that

$$\text{cost of approximating } \sigma_i = O^*(\text{nnz}(A)) + O^*(T(n)).$$

Putting it into (6.4), we have this useless formula

$$T(n) = O^*(\text{nnz}(A) + T(n) + T(d \log d)).$$

This is a chicken and egg problem. To solve an overdetermined system faster, we want to use leverage score to sample the rows. And to approximate the leverage score, we need to solve the original overdetermined system. (Even worse, we need to solve it a few times.)

■ 6.2.2 Uniform Sampling

The key idea to break this chicken and egg problem is to use uniform sampling of the rows of A . We define

$$\sigma_{i,S} = a_i^\top (A_S^\top A_S)^{-1} a_i$$

where A_S is A restricted to rows in S . The set S will be a random sample of k rows of A . Note that $A_S^\top A_S$ is an overestimate of σ_i . Hence, it suffices to bound $\|\sigma_{i,S}\|_1$. The key lemma is the following:

Lemma 6.21. *We have that*

$$\mathbf{E}_{|S|=k} \sum_{i=1}^n \sigma_{i,S \cup \{i\}} \leq \frac{nd}{k}.$$

Proof. Note that

$$\mathbf{E}_{|S|=k} \sum_{i=1}^n \sigma_{i,S \cup \{i\}} = \mathbf{E}_{|S|=k} \sum_{i \notin S} \sigma_{i,S \cup \{i\}} + \mathbf{E}_{|S|=k} \sum_{i \in S} \sigma_{i,S \cup \{i\}}.$$

Note that $\sum_{i \in S} \sigma_{i,S \cup \{i\}} = \sum_{i \in S} \sigma_{i,S} \leq d$. Hence, the second term is bounded by n .

For the first term, we note that “sample a set S of size k , then sample $i \notin S$ ” is same as “sample a set T of size $k+1$, then sample $i \in T$ ”. Hence, we have

$$\begin{aligned} \mathbf{E}_{|S|=k} \mathbf{E}_{i \notin S} \sigma_{i,S \cup \{i\}} &= \mathbf{E}_{|T|=k+1} \mathbf{E}_{i \in T} \sigma_{i,T} \\ &\leq \mathbf{E}_{|T|=k+1} \frac{d}{k+1} = \frac{d}{k+1} \end{aligned}$$

Hence, we have that

$$\mathbf{E}_{|S|=k} \sum_{i=1}^n \sigma_{i,S \cup \{i\}} \leq \frac{d}{k+1} (n-k) + d = d \cdot \frac{n+1}{k+1}.$$

□

Next, using Sherman-Morrison formula, we have that

$$\sigma_{i,S \cup \{i\}} = \begin{cases} \sigma_{i,S} & \text{if } i \in S \\ \frac{1}{1 + \frac{1}{\sigma_{i,S}}} & \text{otherwise} \end{cases}.$$

Namely, we can compute $\sigma_{i,S \cup \{i\}}$ using $\sigma_{i,S}$. Therefore, we have that

$$\text{cost of approximating } \sigma_{i,S \cup \{i\}} = O^*(\text{nnz}(A)) + O^*(T(k)).$$

Using Lemma 6.21, we have now

$$T(n) = O^*(\text{nnz}(A) + T(k) + T(\frac{nd}{k} \log d)).$$

Picking $k = \sqrt{nd \log d}$, we have that

$$T(n) = O^*(\text{nnz}(A) + T(\sqrt{nd \log d})).$$

Repeating this process $\tilde{O}(1)$ times, we have

$$T(n) = O^*(\text{nnz}(A) + T(O(d \log d))).$$

■ 6.3 Stochastic Gradient Descent

In this section, we study problems of the form $\sum f_i$ where each f_i is convex and the sum can be either infinite or finite.

■ 6.3.1 Stochastic Problem

In this part, we discuss the problem

$$\min_x F(x), \text{ where } F(x) \stackrel{\text{def}}{=} \mathbf{E}_{f \sim \mathcal{D}} f(x)$$

where \mathcal{D} is a distribution of convex functions in \mathbb{R}^d . The goal is to find the minimizer $x^* = \operatorname{argmin}_x F(x)$. Suppose we observed samples f_1, f_2, \dots, f_T from \mathcal{D} . Ideally, we wish to approximate x^* by the empirical risk minimizer

$$x_{\text{ERM}}^{(T)} = \arg \min_x F_T(x) \stackrel{\text{def}}{=} \frac{1}{T} \sum_{i=1}^T f_i(x).$$

It is known that $x_{\text{ERM}}^{(T)}$ is optimal in a certain sense in spite of its computational cost. Therefore, to discuss the efficiency of an optimization algorithm for $F(x)$, it is helpful to consider the ratio

$$\frac{\mathbf{E}F(x_{\text{ERM}}^{(T)}) - F(x^*)}{\mathbf{E}F(x_{\text{ERM}}^{(T)}) - F(x^*)}.$$

We will first discuss the term $\mathbf{E}F(x_{\text{ERM}}^{(T)}) - F(x^*)$. As an example, consider the simplest one-dimensional problem $F(x) = \mathbf{E}_{b \sim N(0,1)} (x - b)^2$. Note that $x^{(T)}$ is simply the average of T standard normal variables and hence

$$\begin{aligned} \mathbf{E}F(x_{\text{ERM}}^{(T)}) - F(x^*) &= \mathbf{E}_{b_1, b_2, \dots, b_T} \mathbf{E}_b (x_{\text{ERM}}^{(T)} - b)^2 - b^2 \\ &= \mathbf{E}_{b_1, b_2, \dots, b_T} (x_{\text{ERM}}^{(T)})^2 \\ &= \mathbf{E}_{b_1, b_2, \dots, b_T} \left(\frac{1}{T} \sum_{i=1}^T b_i \right)^2 = \frac{1}{T}. \end{aligned}$$

In general, the following lemma shows that

$$\mathbf{E}F(x_{\text{ERM}}^{(T)}) - F(x^*) \rightarrow \frac{\sigma^2}{T} \quad \text{where } \sigma^2 = \frac{1}{2} \mathbf{E} \|\nabla f(x^*)\|_{(\nabla^2 F(x^*))^{-1}}^2.$$

where $\frac{\sigma^2}{T}$ is called the Cramer-Rao bound.

Lemma 6.22. *Suppose that f is μ -strongly convex with Lipschitz Hessian for all $f \sim \mathcal{D}$ for some $\mu > 0$. Suppose that $\mathbf{E}_{f \sim \mathcal{D}} \|\nabla f(x^*)\|^2 < +\infty$. Then, we have that*

$$\lim_{N \rightarrow +\infty} \frac{\mathbf{E}F(x_{\text{ERM}}^{(N)}) - F(x^*)}{\sigma^2/N} = 1.$$

Remark. The statement holds with weaker assumptions and the rate of convergence can be made quantitative.

Proof. We first prove $x_{\text{ERM}}^{(N)} \rightarrow x^*$ as $N \rightarrow +\infty$. By the optimality condition of $x_{\text{ERM}}^{(N)}$, and using Taylor's theorem, for some \tilde{x} , we have that

$$0 = \nabla F_N(x_{\text{ERM}}^{(N)}) = \nabla F_N(x^*) + \nabla^2 F_N(\tilde{x})(x_{\text{ERM}}^{(N)} - x^*). \quad (6.5)$$

By the μ -strongly convexity, we have

$$\|x_{\text{ERM}}^{(N)} - x^*\|_2^2 \leq \frac{1}{\mu} \|\nabla F_N(x^*)\|^2.$$

Since $\mathbf{E}_{f \sim \mathcal{D}} \nabla f(x^*) = \nabla F(x^*) = 0$, we have

$$\begin{aligned} \mathbf{E} \|x_{\text{ERM}}^{(N)} - x^*\|_2^2 &\leq \frac{1}{\mu} \mathbf{E} \frac{1}{N^2} \sum_i \|\nabla f_i(x^*)\|^2 \\ &= \frac{1}{\mu N} \mathbf{E}_{f \sim \mathcal{D}} \|\nabla f(x^*)\|^2 \end{aligned}$$

Therefore, $x_{\text{ERM}}^{(N)} \rightarrow x^*$ as $N \rightarrow +\infty$.

Now, to compute the error, Taylor expansion of F at x^* shows that

$$F(x_{\text{ERM}}^{(N)}) - F(x^*) = \frac{1}{2}(x_{\text{ERM}}^{(N)} - x^*)^\top \nabla^2 F(\bar{x})(x_{\text{ERM}}^{(N)} - x^*)$$

for some \bar{x} between x^* and $x_{\text{ERM}}^{(N)}$. Using this and (6.5) gives

$$F(x_{\text{ERM}}^{(N)}) - F(x^*) = \frac{1}{2} \nabla F_N(x^*)^\top (\nabla^2 F_N(\tilde{x}))^{-1} \nabla^2 F(\bar{x}) (\nabla^2 F_N(\tilde{x}))^{-1} \nabla F_N(x^*).$$

Since $x_{\text{ERM}}^{(N)} \rightarrow x^*$ and $\nabla^2 F_N \succeq \mu I$, we have $(\nabla^2 F_N(\tilde{x}))^{-1} \nabla^2 F(\bar{x}) (\nabla^2 F_N(\tilde{x}))^{-1} \rightarrow (\nabla^2 F(x^*))^{-1}$. Hence, we have

$$\begin{aligned} \lim_{N \rightarrow \infty} \mathbf{E} N \cdot (F(x_{\text{ERM}}^{(N)}) - F(x^*)) &= \lim_{N \rightarrow \infty} \frac{N}{2} \mathbf{E} \nabla F_N(x^*)^\top (\nabla^2 F(x^*))^{-1} \nabla F_N(x^*) \\ &= \frac{1}{2} \mathbf{E} \|\nabla f(x^*)\|_{(\nabla^2 F(x^*))^{-1}}^2. \end{aligned}$$

□

Now, we discuss how to achieve a bound similar to σ^2/T using stochastic gradient descent. Since gradient descent is a first order method, we can only achieve a bound related to the ℓ_2 norm, $\mathbf{E} \|\nabla f(x^*)\|_2^2$, instead of the inverse Hessian norm.

Lemma 6.23. *Suppose f has L -Lipschitz gradient for all $f \in \mathcal{D}$. Let x^* be the minimizer of F . Then, we have*

$$\mathbf{E}_{f \sim \mathcal{D}} \|\nabla f(x) - \nabla f(x^*)\|_2^2 \leq 2L \cdot (F(x) - F(x^*)).$$

Proof. Let $g(x) = f(x) - \nabla f(x^*)^\top (x - x^*)$. By construction, x^* is the minimizer of g and $f(x^*) = g(x^*)$. Hence, by the progress of gradient descent, we know

$$g(x^*) \leq g(x) - \frac{1}{2L} \|\nabla g(x)\|^2.$$

Rearranging the term, we have

$$\|\nabla g(x)\|^2 \leq 2L(g(x) - g(x^*))$$

and hence

$$\|\nabla f(x) - \nabla f(x^*)\|^2 \leq 2L \cdot (f(x) - f(x^*) - \nabla f(x^*)^\top (x - x^*)).$$

Taking expectation, we have the result. □

Algorithm 19: StochasticGradientDescent (SGD)

Input: Initial point $x^{(0)} \in \mathbb{R}^d$, step size $h > 0$. Access to \mathcal{D} , a distribution on convex functions.
for $k = 0, 1, \dots, T$ **do**
 Sample $f \sim \mathcal{D}$.
 $x^{(k+1)} \leftarrow x^{(k)} - h \cdot \nabla f(x^{(k)})$.
end

Theorem 6.24. *Suppose f has L -Lipschitz gradient for all $f \in \mathcal{D}$ and F is μ strongly convex. Let x^* be the minimizer of F and $\sigma^2 = \frac{1}{2} \mathbf{E} \|\nabla f(x^*)\|^2$. For step size $h \leq \frac{1}{4L}$, the sequence $x^{(k)}$ in StochasticGradientDescent satisfies*

$$\mathbf{E} \|x^{(k)} - x^*\|^2 \leq \frac{8h\sigma^2}{\mu} + (1 - \frac{h\mu}{2})^k \cdot \|x^{(0)} - x^*\|^2$$

and

$$\frac{1}{T} \sum_{k=0}^{T-1} \mathbf{E} F(x^{(k)}) - F(x^*) \leq 4h\sigma^2 + \frac{\|x^{(0)} - x^*\|^2}{hT}.$$

Proof. Note that

$$\|x^{(k+1)} - x^*\|^2 = \|x^{(k)} - x^*\|^2 - 2h \langle x^{(k)} - x^*, \nabla f(x^{(k)}) \rangle + h^2 \|\nabla f(x^{(k)})\|^2.$$

Taking expectation on f and using that

$$\begin{aligned} \mathbf{E}\|\nabla f(x^{(k)})\|^2 &\leq 2\mathbf{E}\|\nabla f(x^{(k)}) - \nabla f(x^*)\|^2 + 2\mathbf{E}\|\nabla f(x^*)\|^2 \\ &\leq 4L \cdot (F(x^{(k)}) - F(x^*)) + 4\sigma^2, \end{aligned}$$

we have

$$\begin{aligned} \mathbf{E}\|x^{(k+1)} - x^*\|^2 &= \|x^{(k)} - x^*\|^2 - 2h \langle x^{(k)} - x^*, \nabla F(x^{(k)}) \rangle + 4h^2\sigma^2 + 4Lh^2 \cdot (F(x^{(k)}) - F(x^*)) \\ &\leq \|x^{(k)} - x^*\|^2 - (2h - 4Lh^2)(F(x^{(k)}) - F(x^*)) + 4h^2\sigma^2. \end{aligned} \quad (6.6)$$

Using $h \leq \frac{1}{4L}$ and $F(x^{(k)}) - F(x^*) \leq \frac{1}{2\mu} \|\nabla F(x^{(k)})\|_2^2$, we have

$$\mathbf{E}\|x^{(k+1)} - x^*\|^2 \leq 4h^2\sigma^2 + \left(1 - \frac{h\mu}{2}\right) \cdot \|x^{(k)} - x^*\|^2.$$

The first conclusion follows.

For the second conclusion, (6.6) shows that

$$\mathbf{E}F(x^{(k)}) - F(x^*) \leq \frac{\mathbf{E}\|x^{(k)} - x^*\|^2 - \mathbf{E}\|x^{(k+1)} - x^*\|^2}{h} + 4h\sigma^2.$$

Hence, we have

$$\frac{1}{T} \sum_{k=0}^{T-1} \mathbf{E}F(x^{(k)}) - F(x^*) \leq 4h\sigma^2 + \frac{\|x^{(0)} - x^*\|^2}{hT}$$

□

Exercise 6.25. Applying the theorem above twice, show that one can achieve error $\tilde{O}(\frac{\sigma^2}{\mu T})$, which is roughly same as the Cramer-Rao bound.

We note that for many algorithms in this book, such as mirror descent, the stochastic version is obtained by replacing the gradient ∇F by the gradient of a sample, ∇f .

■ 6.3.2 Finite Sum Problem

When $\nabla f(x^*) = 0$ for all $f \sim \mathcal{D}$, stochastic gradient descent converges exponentially. When the function is given by a finite sum $F = \frac{1}{n} \sum f_i$, we can reduce the variance at x^* by replacing

$$\nabla \tilde{f}_i(x) = \nabla f_i(x) - \nabla f_i(x^{(0)}) + \nabla F(x^{(0)}).$$

Note that if $x^{(0)}$ is close to x^* , then $\nabla \tilde{f}_i(x^*)$ is small because both $\nabla f_i(x^*) - \nabla f_i(x^{(0)})$ and $\nabla F(x^{(0)})$ are small. Formally, the variance for \tilde{f} is bounded as follows:

Lemma 6.26. *Suppose f has L -Lipschitz gradient for all $f \in \mathcal{D}$. For any $f \in \mathcal{D}$, let $\nabla \tilde{f}(x) = \nabla f(x) - \nabla f(x^{(0)}) + \nabla F(x^{(0)})$ for some fixed $x^{(0)}$. Then, we have*

$$\mathbf{E}\|\nabla \tilde{f}(x^*)\|^2 \leq 8L \cdot (F(x^{(0)}) - F(x^*)).$$

Proof. Note that

$$\begin{aligned} \mathbf{E}\|\nabla \tilde{f}(x^*)\|^2 &\leq 2\mathbf{E}\|\nabla f(x^*) - \nabla f(x^{(0)})\|^2 + 2\|\nabla F(x^{(0)}) - \nabla F(x^*)\|^2 \\ &= 2\mathbf{E}\|\nabla f(x^*) - \nabla f(x^{(0)})\|^2 + 2\mathbf{E}\|\nabla f(x^{(0)}) - \nabla f(x^*)\|^2 \\ &\leq 4L(F(x^{(0)}) - F(x^*)) + 4L(F(x^{(0)}) - F(x^*)) \end{aligned}$$

where we used Lemma 6.23 at the end. □

Algorithm 20: StochasticVarianceReducedGradient (SVRG)

Input: Initial point $x^{(0)} \in \mathbb{R}^d$, step size $h > 0$, restart time m .
 $\tilde{x} = x^{(0)}$.
for $k = 0, 1, \dots, T$ **do**
 if k is a multiple of m and $k \neq 0$ **then**
 $x^{(k)} = \frac{1}{m} \sum_{j=1}^m x^{(k-j)}$.
 $\tilde{x} = x^{(k)}$.
 end
 Sample f_i for $i \in [n]$
 $x^{(k+1)} \leftarrow x^{(k)} - h \cdot (\nabla f(x^{(k)}) - \nabla f(\tilde{x}) + \nabla F(\tilde{x}))$.
end

Theorem 6.27. Suppose f has L -Lipschitz gradient for all f_i and F is μ strongly convex. Let x^* be the minimizer of F . For step size $h = \frac{1}{64L}$ and $m = \frac{256L}{\mu}$, the sequence $x^{(km)}$ in StochasticVarianceReducedGradient satisfies

$$\mathbf{E}F(x^{(km)}) - F(x^*) \leq \frac{1}{2^k} \cdot (F(x^{(0)}) - F(x^*)).$$

In particular, it takes $O((n + \frac{L}{\mu}) \log(\frac{1}{\epsilon}))$ gradient computations to find x such that $\mathbf{E}F(x) - F(x^*) \leq \epsilon \cdot (F(x^{(0)}) - F(x^*))$.

Remark. Gradient descent gives $O(n \frac{L}{\mu} \log(\frac{1}{\epsilon}))$ instead because computing ∇F involves computing n gradients ∇f .

Proof. The algorithm consists of $\frac{T}{m}$ phases. For the first phase, we compute $\nabla F(x^{(0)})$. Lemma 6.26 shows that

$$\mathbf{E}\|\nabla f(x^{(k)}) - \nabla f(x^{(0)}) + \nabla F(x^{(0)})\|^2 \leq 8L \cdot (F(x^{(0)}) - F(x^*)).$$

Hence, Theorem 6.24 shows that

$$\begin{aligned} \frac{1}{m} \sum_{k=0}^{m-1} \mathbf{E}F(x^{(k)}) - F(x^*) &\leq 16hL \cdot (F(x^{(0)}) - F(x^*)) + \frac{F(x^{(0)}) - F(x^*)}{\mu hm} \\ &\leq \frac{1}{2} (F(x^{(0)}) - F(x^*)). \end{aligned}$$

Hence, the error decreases by half each phase. This shows the result. \square

■ 6.4 Coordinate Descent

If some of the coordinates are more important than others for optimization, it makes sense to update the important coordinates more often.

Lemma 6.28. Given a convex function f , suppose that $\frac{\partial^2}{\partial x_i^2} f(x) \leq L_i$ for all x and let $L = \sum L_i$. If we sample coordinate i with probability $p_i = \frac{L_i}{L}$, then,

$$\mathbf{E}_i f(x - \frac{1}{L_i} \frac{\partial}{\partial x_i} f(x) e_i) \leq f(x) - \frac{1}{2L} \|\nabla f(x)\|_2^2.$$

Proof. Note that the function $\zeta(t) = f(x + te_i)$ is L_i smooth. Hence, we have that

$$f(x - \frac{1}{L_i} \frac{\partial}{\partial x_i} f(x) e_i) \leq f(x) - \frac{1}{2L_i} \frac{\partial}{\partial x_i} f(x)^2.$$

Since we sample coordinate i with probability $p_i = \frac{L_i}{L}$, we have that

$$\begin{aligned} \mathbf{E}f(x - \frac{1}{L_i} \frac{\partial}{\partial x_i} f(x) e_i) &\leq f(x) - \sum_i \frac{L_i}{L} \frac{1}{2L_i} \frac{\partial}{\partial x_i} f(x)^2 \\ &= f(x) - \frac{1}{2L} \sum_i \frac{\partial}{\partial x_i} f(x)^2 \\ &= f(x) - \frac{1}{2L} \|\nabla f(x)\|_2^2. \end{aligned}$$

□

By the same proof as Theorem 2.9, we have the following:

Algorithm 21: CoordinateDescent (CD)

Input: Initial point $x^{(0)} \in \mathbb{R}^d$, step size $h > 0$.
for $k = 0, 1, \dots, T$ **do**
 Sample i with probability proportional to L_i .
 $x^{(k+1)} \leftarrow x^{(k)} - \frac{1}{L_i} \frac{\partial}{\partial x_i} f(x^{(k)}) e_i$.
end

Theorem 6.29 (Coordinate Descent Convergence). *Given a convex function f , suppose that $\frac{\partial^2}{\partial x_i^2} f(x) \leq L_i$ for all x and let $L = \sum L_i$. Consider the algorithm $x^{(k+1)} \leftarrow x^{(k)} - \frac{1}{L_i} \frac{\partial}{\partial x_i} f(x^{(k)}) e_i$. Then, we have that*

$$\mathbf{E}f(x^{(k)}) - f(x^*) \leq \frac{2LR^2}{k+4} \quad \text{with} \quad R = \max_{f(x) \leq f(x^{(0)})} \|x - x^*\|_2$$

for any minimizer x^* of f . If f is μ strongly convex, then we also have

$$\mathbf{E}f(x^{(k)}) - f(x^*) \leq (1 - \frac{\mu}{L})^{\Omega(k)} (f(x^{(0)}) - f(x^*)).$$

Remark. Note that $\frac{L}{d} \leq \text{Lip}(\nabla f) \leq L$. Therefore gradient descent takes at least $\frac{1}{d}$ times as many steps as coordinate descent while each step takes d times longer (usually).

■ 7.1 Chebyshev Polynomials

The goal of this section is to introduce some basic results in approximation theory. Suppose magically there was a polynomial $q(x)$ such that $q(0) = 1$ and $q(x) = 0$ for all $x > 0$. By assumption, we know that the constant term in q is 1 and hence we can write

$$q(x) = 1 - xp(x)$$

for some $p(x)$. Therefore, for any positive definite matrix A , we have that

$$I - Ap(A) = 0$$

and hence $A^{-1} = p(A)$. Therefore, we could compute $A^{-1}b$ by calculating $p(A)b$ which takes $\deg(p) \cdot \text{nnz}(A)$ time. Unfortunately, there is no such polynomial q . In this section, we will discuss if there is such polynomial that satisfies the condition above approximately.

We will bound $\inf_{q(0)=1} (\max_i |q(\lambda_i)|)$ for matrices A satisfying $\mu \cdot I \preceq A \preceq L \cdot I$. First, we note that we can choose $q(x) = (1 - \frac{x}{L})^k$ and get

$$\inf_{q(0)=1} \max_{\mu \leq x \leq L} |q(x)| \leq \left(1 - \frac{\mu}{L}\right)^k.$$

This corresponds to the Richardson iteration, and the above bound shows that it takes $O(\frac{L}{\mu} \log(\frac{1}{\epsilon}))$ degree to make the error bounded by ϵ . The key fact we will use is that we can in general approximate a polynomial of degree k by a polynomial of degree $\tilde{O}(\sqrt{k})$. The construction uses Chebyshev polynomials. This will imply an $\tilde{O}(\sqrt{\frac{L}{\mu}})$ iteration bound for the conjugate gradient method of the next section.

Definition 7.1. For any integer d , the d 'th Chebyshev polynomial is defined as the unique polynomial that satisfies

$$T_d(\cos \theta) = \cos(d\theta).$$

Exercise 7.2. Show that $T_d(x)$ is a degree $|d|$ polynomial in x and that

$$xT_d(x) = \frac{T_{d+1}(x) + T_{d-1}(x)}{2}. \quad (7.1)$$

Theorem 7.3 (Chernoff Bound). For independent random variables Y_1, \dots, Y_s such that $\mathbf{P}(Y_i = 1) = \mathbf{P}(Y_i = -1) = \frac{1}{2}$, for any $a \geq 0$, we have

$$\mathbf{P}\left(\left|\sum_{i=1}^s Y_i\right| \geq a\right) \leq 2 \exp\left(-\frac{a^2}{2s}\right).$$

Now we are ready to show that there is a degree $\tilde{O}(\sqrt{s})$ polynomial that estimates x^s .

Theorem 7.4. For any positive integers s and d , there is a polynomial p of degree d such that

$$\max_{x \in [-1, 1]} |p(x) - x^s| \leq 2 \exp\left(-\frac{d^2}{2s}\right).$$

Proof. Let Y_i are i.i.d. random variable uniform on $\{-1, 1\}$. Let $Z_s = \sum_{i=1}^s Y_i$. Note that

$$\mathbf{E}_{z \sim Z_s} T_z = \mathbf{E}_{z \sim Z_{s-1}} \frac{1}{2} (T_{z+1} + T_{z-1})$$

Now, (7.1) shows that $\mathbf{E}_{z \sim Z_s} T_z(x) = \mathbf{E}_{z \sim Z_{s-1}} x T_z(x)$. By induction, we have

$$\mathbf{E}_{z \sim Z_s} T_z(x) = x^s T_0(x) = x^s. \quad (7.2)$$

Now, we define the polynomial $p(x) = \mathbf{E}_{z \sim Z_s} T_z(x) 1_{|z| \leq d}$. The error of the polynomial can be bounded as follows

$$\begin{aligned} \max_{x \in [-1, 1]} |p(x) - x^s| &= \max_{x \in [-1, 1]} |\mathbf{E}_{z \sim Z_s} T_z(x) 1_{|z| > d}| \\ &\leq \max_{x \in [-1, 1]} \mathbf{E}_{z \sim Z_s} |T_z(x)| 1_{|z| > d} \\ &\leq \mathbf{P}_{z \sim Z_s} (|z| > d) \\ &\leq 2 \exp\left(-\frac{d^2}{2s}\right) \end{aligned}$$

where we used (7.2) on the first line, $|T_z(x)| \leq 1$ for all $x \in [-1, 1]$ on the third line and Chernoff bound (Theorem 7.3) on the last line. \square

Remark. This proof comes from [64]. Please see [64] for the approximation of other functions.

By scaling and translating Theorem 7.4, we have the following guarantee.

Theorem 7.5. For any $0 < \mu \leq L$ and any $0 \leq \epsilon \leq 1$, there is a polynomial q of degree $O(\sqrt{\frac{L}{\mu}} \log(\frac{1}{\epsilon}))$ such that

$$\inf_{q(0)=1} \max_{\mu \leq x \leq L} |q(x)| \leq \epsilon.$$

Proof. Theorem 7.4 shows that there is q such that

$$\max_{x \in [0, L]} \left| q(x) - \left(1 - \frac{x}{L}\right)^s \right| \leq 2 \exp\left(-\frac{d^2}{2s}\right).$$

Hence, we have that $|q(0) - 1| \leq 2 \exp\left(-\frac{d^2}{2s}\right)$ and that

$$\max_{x \in [\mu, L]} |q(x)| \leq \left(1 - \frac{\mu}{L}\right)^s + 2 \exp\left(-\frac{d^2}{2s}\right).$$

To make both $|q(0) - 1| \leq \frac{\epsilon}{3}$ and $\max_{x \in [\mu, L]} |q(x)| \leq \frac{\epsilon}{3}$, we set $d = O(\sqrt{s} \log \frac{1}{\epsilon})$ and $s = O(\frac{L}{\mu} \log(\frac{1}{\epsilon}))$. By rescaling q , we have $q(0) = 1$. \square

■ 7.2 Conjugate Gradient

Consider any algorithm that starts with $x^{(0)} = 0$ and satisfies the invariant

$$x^{(k+1)} \in x^{(0)} + \text{span}\{\nabla f(x^{(0)}), \nabla f(x^{(1)}), \dots, \nabla f(x^{(k)})\}.$$

For $f(x) = \frac{1}{2} x^\top A x - b^\top x$, it is easy to see that $x^{(k)} \in \mathcal{K}_k$ defined as follows:

Definition 7.6. Define the Krylov subspaces $\mathcal{K}_0 = \{0\}$, $\mathcal{K}_k = \text{span}\{b, Ab, \dots, A^{k-1}b\}$.

Therefore, the best such an algorithm can do is to solve $\min_{x \in \mathcal{K}_k} f(x)$. For the quadratic function $f(x) \stackrel{\text{def}}{=} \frac{1}{2} x^\top A x - b^\top x$, one can compute $\min_{x \in \mathcal{K}_k} f(x)$ efficiently using the conjugate gradient method. Note that

$$\arg \min_{x \in \mathcal{K}_k} f(x) = \arg \min_{x \in \mathcal{K}_k} \|x - x^*\|_A^2$$

where $Ax^* = b$.

Throughout this section, we assume A is positive definite. For a given linear system $Ax = b$, we can always go to $A^\top A x = A^\top b$ to satisfy the assumption.

Lemma 7.7. Let $x^{(k)} = \operatorname{argmin}_{x \in \mathcal{K}_k} f(x)$ be the Krylov sequence. . Then, the steps $v^{(k)} = x^{(k)} - x^{(k-1)}$ are “conjugate”, namely,

$$v^{(i)\top} A v^{(j)} = 0 \text{ for all } i \neq j.$$

Proof. Assume that $i < j$. The optimality of $x^{(j)}$ shows that $\nabla f(x^{(j)}) \in \mathcal{K}_j^\perp \subset \mathcal{K}_{j-1}^\perp$ and that $\nabla f(x^{(j-1)}) \in \mathcal{K}_{j-1}^\perp$. Hence, we have

$$A v^{(j)} = \nabla f(x^{(j)}) - \nabla f(x^{(j-1)}) \in \mathcal{K}_{j-1}^\perp.$$

Next, we note that $v^{(i)} = x^{(i)} - x^{(i-1)} \in \mathcal{K}_i \subset \mathcal{K}_{j-1}$. Hence, we have $v^{(i)\top} A v^{(j)} = 0$. \square

Since the steps are conjugate, $v^{(i)}$ forms a conjugate basis for the Krylov subspaces:

$$\mathcal{K}_k = \operatorname{span}\{v^{(1)}, v^{(2)}, \dots, v^{(k)}\}.$$

Note that $x^{(k)} = x^{(k-1)} + v^{(k)}$. Hence, it suffices to find a formula for $v^{(k)}$.

Lemma 7.8. We have

$$v^{(k)} = \frac{v^{(k)\top} r^{(k-1)}}{\|r^{(k-1)}\|^2} \left(r^{(k-1)} - \frac{r^{(k-1)\top} A v^{(k-1)}}{v^{(k-1)\top} A v^{(k-1)}} v^{(k-1)} \right).$$

Proof. Again, the optimality condition shows that $\nabla f(x^{(k-1)}) \in \mathcal{K}_{k-1}^\perp$ and that $\nabla f(x^{(k-1)}) \in \mathcal{K}_k$ by the definition of \mathcal{K} . Hence, we have

$$\mathcal{K}_k = \operatorname{span}\{v^{(1)}, \dots, v^{(k-1)}, r^{(k-1)}\}$$

where $r^{(k-1)} = b - A x^{(k-1)}$. Therefore, we have

$$v^{(k)} = c_0 r^{(k-1)} + \sum_{i=1}^{k-1} c_i v^{(i)}$$

for some c_0 .

For c_0 , we use that $r^{(k-1)} \in \mathcal{K}_{k-1}^\perp$. This gives $v^{(k)\top} r^{(k-1)} = c_0 \|r^{(k-1)}\|^2$.

For c_{k-1} , since $v^{(i)\top} A v^{(k-1)} = 0$ for any $i \neq k-1$, we have

$$0 = v^{(k)\top} A v^{(k-1)} = c_0 r^{(k-1)\top} A v^{(k-1)} + c_{k-1} v^{(k-1)\top} A v^{(k-1)}$$

and $c_{k-1} = -c_0 \cdot \frac{r^{(k-1)\top} A v^{(k-1)}}{v^{(k-1)\top} A v^{(k-1)}}$.

For other c_i , we note that $A v^{(j)} \in \mathcal{K}_{j+1}$ and $r^{(k-1)} \in \mathcal{K}_{k-1}^\perp$. Hence, $c_i = 0$ for all $i \notin \{0, k-1\}$.

Substitute the c_i , we get

$$v^{(k)} = \frac{v^{(k)\top} r^{(k-1)}}{\|r^{(k-1)}\|^2} \left(r^{(k-1)} - \frac{r^{(k-1)\top} A v^{(k-1)}}{v^{(k-1)\top} A v^{(k-1)}} v^{(k-1)} \right).$$

\square

To make the formula simpler, we define $p^{(k)} = \frac{\|r^{(k-1)}\|_2^2}{v^{(k)\top} r^{(k-1)}} v^{(k)}$.

Lemma 7.9. We have that $x^{(k)} = x^{(k-1)} + \frac{\|r^{(k-1)}\|_2^2}{p^{(k)\top} A p^{(k)}} p^{(k)}$ and $p^{(k)} = r^{(k-1)} - \frac{\|r^{(k-1)}\|_2^2}{\|r^{(k-2)}\|_2^2} p^{(k-1)}$.

Proof. For the first formula, note that

$$x^{(k)} = x^{(k-1)} + v^{(k)} = x^{(k-1)} + \frac{v^{(k)\top} r^{(k-1)}}{\|r^{(k-1)}\|_2^2} p^{(k)}.$$

For the quantity $v^{(k)\top} r^{(k-1)}$, we note that $f(x^{(k-1)} + t v^{(k)})$ is minimized at $t = 1$ and hence

$$\begin{aligned} v^{(k)\top} r^{(k-1)} &= v^{(k)\top} A v^{(k)} \\ &= \frac{v^{(k)\top} r^{(k-1)}}{\|r^{(k-1)}\|_2^2} \frac{v^{(k)\top} r^{(k-1)}}{\|r^{(k-1)}\|_2^2} p^{(k)\top} A p^{(k)} \end{aligned}$$

where we used the definition of $p^{(k)}$. Simplifying gives

$$\frac{v^{(k)\top} r^{(k-1)}}{\|r^{(k-1)}\|_2^2} = \frac{\|r^{(k-1)}\|_2^2}{p^{(k)\top} A p^{(k)}}$$

and hence the first formula.

For the second formula, we use Lemma 7.8 and substitute $p^{(k)} = \frac{\|r^{(k-1)}\|_2^2}{v^{(k)\top} r^{(k-1)}} v^{(k)}$. This gives

$$p^{(k)} = r^{(k-1)} - \frac{r^{(k-1)\top} A v^{(k-1)}}{\|r^{(k-2)}\|_2^2} p^{(k-1)}. \quad (7.3)$$

Note that

$$r^{(k-1)} = b - Ax^{(k-1)} = r^{(k-2)} - Av^{(k-1)}.$$

Taking inner product with $r^{(k-1)}$ and using $r^{(k-1)} \perp r^{(k-2)}$ gives $\|r^{(k-1)}\|^2 = r^{(k-1)\top} A v^{(k-1)}$. Put this into (7.3) gives the result. \square

Algorithm 22: ConjugateGradient (CG)

```

 $r^{(0)} = b - Ax^{(0)}, p^{(0)} = r^{(0)}.$ 
for  $k = 1, 2, \dots$  do
     $\alpha = \frac{\|r^{(k-1)}\|_2^2}{p^{(k-1)\top} A p^{(k-1)}}.$ 
     $x^{(k)} \leftarrow x^{(k-1)} + \alpha p^{(k-1)}.$ 
     $r^{(k)} \leftarrow r^{(k-1)} - \alpha A p^{(k-1)}.$ 
    if  $\|r^{(k)}\|_2 \leq \epsilon$  then return  $x^{(k)};$ 
     $p^{(k)} = r^{(k)} - \frac{\|r^{(k)}\|_2^2}{\|r^{(k-1)}\|_2^2} p^{(k-1)}.$ 
end

```

Theorem 7.10. Let $f(x) = \frac{1}{2}x^\top Ax - b^\top x$ for some positive definite matrix A and some vector b . Let $x^{(k)}$ be the sequence produced by ConjugateGradient. Then, we have

$$f(x^{(k)}) - f(x^*) \leq \frac{1}{2} \inf_{q(0)=1} \max_i q(\lambda_i)^2 \cdot \|b\|_{A^{-1}}^2$$

where q searches over polynomials of degree at most k and λ_i are eigenvalues of A .

Proof. Note that $\mathcal{K}_k = \{p(A) : \deg p < k\}$. Hence, we have

$$\begin{aligned}
 2(f(x^{(k)}) - f(x^*)) &= \min_{x \in \mathcal{K}_k} \|x - x^*\|_A^2 \\
 &= \inf_{\deg p < k} \|(p(A) - A^{-1})b\|_A^2 \\
 &= \inf_{\deg p < k} \|A^{-\frac{1}{2}}(Ap(A) - I)A^{-\frac{1}{2}}b\|_2^2 \\
 &= \inf_{\deg p < k} \|(Ap(A) - I)A^{-\frac{1}{2}}b\|_2^2
 \end{aligned}$$

Let $q(x) = 1 - xp(x)$. Note that $q(0) = 1$ and $\deg q \leq k$ and any such q is of the form $1 - xp$. Hence, we have

$$\begin{aligned}
 2(f(x^{(k)}) - f(x^*)) &= \inf_{\deg q \leq k, q(0)=1} \|q(A)A^{-\frac{1}{2}}b\|_2^2 \\
 &\leq \inf_{q(0)=1} \|q(A)\|_{\text{op}}^2 \cdot \|b\|_{A^{-1}}^2.
 \end{aligned}$$

The result follows from the fact that $\|q(A)\|_{\text{op}}^2 = \max_i q(\lambda_i)^2$. \square

It is known that for any $0 < \mu \leq L$, there is a degree k polynomial q with $q(0) = 1$ such that

$$\max_i q(\lambda_i)^2 \leq 2 \left(1 - \frac{2}{\sqrt{\frac{L}{\mu}} + 1} \right)^k$$

Therefore, it takes $O(\sqrt{\frac{L}{\mu}} \log(\frac{1}{\epsilon}))$ iterations to find x such that $f(x) - f(x^*) \leq \epsilon \cdot \|b\|_{A^{-1}}^2$.

Also, we note that if there are only s distinct eigenvalues in A , then conjugate gradient finds the exact solution in s iterations.

■ 7.3 Accelerated Gradient Descent via Plane Search

According to legend, the first proof for accelerated gradient descent is due to Nemirovski in the 70s. The first proof involves a 2-dimensional plane search subroutine. Later on this was improved to line search and finally Nesterov showed how to get rid of line search in 1982. We change the proof slightly to get rid of all uses of parameters.

Algorithm 23: NemAGD

Input: Initial point $x^{(1)} \in \mathbb{R}^n$.
for $k = 1, 2, \dots$ **do**
 $x^{(k)+} \leftarrow \operatorname{argmin}_{x=x^{(k)}+t\nabla f(x^{(k)})} f(x)$.
 $P^{(k)} \leftarrow x^{(1)} + \operatorname{span}(x^{(k)+} - x^{(1)}, \sum_{s=1}^k \frac{\nabla f(x^{(s)})}{\|\nabla f(x^{(s)})\|})$.
 // Alternatively, one can use $P^{(k)} \leftarrow x^{(k)} + \operatorname{span}(x^{(k)} - x^{(1)}, \nabla f(x^{(k)}), \sum_{s=1}^k \frac{\nabla f(x^{(s)})}{\|\nabla f(x^{(s)})\|})$
 without defining $x^{(k)+}$.
 $x^{(k+1)} = \arg \min_{x \in P^{(k)}} f(x)$.
end

Theorem 7.11. Assume that f is convex with $\nabla^2 f(x) \preceq L \cdot I$ for all x . Then, we have that

$$f(x^{(k)}) - f(x^*) \lesssim \frac{L \|x^* - x^{(1)}\|^2}{k^2}.$$

Proof. Let $\delta_k = f(x^{(k)}) - f(x^*)$. By the convexity of f , we have

$$\begin{aligned} \delta_k &\leq \nabla f(x^{(k)})^\top (x^{(k)} - x^*) \\ &= \nabla f(x^{(k)})^\top (x^{(k)} - x^{(1)}) + \nabla f(x^{(k)})^\top (x^{(1)} - x^*). \end{aligned}$$

Since $x^{(k)}$ is the minimizer on $P^{(k-1)}$ which contains $x^{(1)}$, we have $\nabla f(x^{(k)})^\top (x^{(k)} - x^{(1)}) = 0$ and hence

$$\delta_k \leq \nabla f(x^{(k)})^\top (x^{(1)} - x^*).$$

Let $\lambda_t = \frac{1}{\|\nabla f(x^{(t)})\|}$. Note that

$$\sum_{k=1}^T \lambda_k \delta_k \leq \left\langle \sum_{k=1}^T \frac{\nabla f(x^{(k)})}{\|\nabla f(x^{(k)})\|}, x^{(1)} - x^* \right\rangle \leq \|x^* - x^{(1)}\|_2 \cdot \left\| \sum_{k=1}^T \frac{\nabla f(x^{(k)})}{\|\nabla f(x^{(k)})\|} \right\|_2.$$

Finally, we note that $\nabla f(x^{(k+1)}) \perp P^{(k)}$ and hence $\nabla f(x^{(k+1)}) \perp \sum_{s=1}^k \frac{\nabla f(x^{(s)})}{\|\nabla f(x^{(s)})\|}$. Therefore, we have

$$\left\| \sum_{k=1}^T \frac{\nabla f(x^{(k)})}{\|\nabla f(x^{(k)})\|} \right\|_2^2 = \sum_{k=1}^T \left\| \frac{\nabla f(x^{(k)})}{\|\nabla f(x^{(k)})\|} \right\|_2^2 = T.$$

Hence, we have

$$\sum_{k=1}^T \lambda_k \delta_k \leq \sqrt{T} \cdot \|x^* - x^{(1)}\|_2.$$

Since $x^{(k)+} \in P$, we have that

$$\delta_{k+1} = f(x^{(k+1)}) - f(x^*) \leq f(x^{(k)+}) - f(x^*) \leq \delta_k - \frac{1}{2L} \|\nabla f(x^{(k)})\|_2^2.$$

Hence, we have $\|\nabla f(x^{(k)})\|_2^2 \leq 2L(\delta_k - \delta_{k+1})$. This gives

$$\sum_{k=1}^T \frac{\delta_k}{\sqrt{\delta_k - \delta_{k+1}}} \leq \sqrt{2LT} \cdot \|x^* - x^{(1)}\|_2$$

for all T . Solving this recursion gives the result. \square

Exercise 7.12. Solve the recursion omitted at the end of the proof.

Note that the proof above used only the fact that $\{x^{(1)}, x^{(k)+}, \sum_{s=1}^k \frac{\nabla f(x^{(s)})}{\|\nabla f(x^{(s)})\|}\} \subset P$. Therefore, one can put extra vectors in P to obtain extra features. For example, if we use the subspace

$$P = x^{(k)} + \text{span}(x^{(k)} - x^{(1)}, \nabla f(x^{(k)}), \sum_{s=1}^k \frac{\nabla f(x^{(s)})}{\|\nabla f(x^{(s)})\|}, x^{(k)} - x^{(k-1)}),$$

then one can prove that this algorithm is equivalently to conjugate gradient when f is a quadratic function.

■ 7.4 Accelerated Gradient Descent

■ 7.4.1 Gradient Mapping

To give a general version of acceleration, we consider problem of the form

$$\min_x \phi(x) \stackrel{\text{def}}{=} f(x) + h(x)$$

where $f(x)$ is strongly convex and smooth and $h(x)$ is convex. We assume that we access the function f and h differently via:

1. Let \mathcal{T}_f be the cost of computing $\nabla f(x)$.
2. Let $\mathcal{T}_{h,\lambda}$ be the cost of minimizing $h(x) + \frac{\lambda}{2} \|x - c\|_2^2$ exactly.

The idea is to move whatever we can optimize in ϕ to h and hopefully this makes the remaining part of ϕ , f , as smooth and strongly convex as possible. To make the statement general, we only assume h is convex and hence h may not be differentiable. To handle this issue, we need to define an approximate derivative of h that we can compute.

Definition 7.13. We define the gradient step

$$p_x = \operatorname{argmin}_y f(x) + \nabla f(x)^\top (y - x) + \frac{L}{2} \|y - x\|^2 + h(y)$$

and the gradient mapping

$$g_x = L(x - p_x).$$

Note that if $h = 0$, then $p_x = x - \frac{1}{L} \nabla f(x)$ and $g_x = \nabla f(x)$. In general, if $\phi \in \mathcal{C}^2$, then we have that

$$p_x = x - \frac{1}{L} \nabla \phi(x) + O\left(\frac{1}{L^2}\right).$$

Therefore, we have that $g_x = \nabla\phi(x) + O(\frac{1}{L})$. Hence, the gradient mapping is an approximation of the gradient of ϕ that is computable in time $\mathcal{T}_g + \mathcal{T}_{h,L}$.

The key lemma we use here is that ϕ satisfies a lower bound defining using g_x . Ideally, we would love to get a lower bound as follows:

$$\phi(z) \geq \phi(x) + g_x^\top(z - x) + \frac{\mu}{2} \|z - x\|_2^2.$$

But it is WRONG. If that was true for all z , then we would have $g_x = \nabla\phi(x)$. However, if $\phi \in \mathcal{C}^2$ is μ strongly convex, then we have

$$\begin{aligned} \phi(z) &\geq \phi(x) + \nabla\phi(x)^\top(z - x) + \frac{\mu}{2} \|z - x\|_2^2 \\ &\geq \phi(x) - \frac{1}{L} \nabla\phi(x)^\top(z - x) + \frac{1}{2L} \|\nabla\phi(x)\|^2 + \nabla\phi(x)^\top(z - x) + \frac{\mu}{2} \|z - x\|_2^2. \end{aligned} \quad (7.4)$$

It turns out that this is true and is exactly what we need for proving gradient descent, mirror descent and accelerated gradient descent.

Theorem 7.14. *Given $\phi = f + h$. Suppose that f is μ strongly convex with L -Lipschitz gradient. Then, for any z , we have that*

$$\phi(z) \geq \phi(p_x) + g_x^\top(z - p_x) + \frac{1}{2L} \|g_x\|_2^2 + \frac{\mu}{2} \|z - p_x\|_2^2.$$

Proof. Let $\bar{f}(y) = f(x) + \nabla f(x)^\top(y - x) + \frac{L}{2} \|y - x\|_2^2$ and $p_t = p_x + t(z - p_x)$. Using that p_0 is the minimizer of $\bar{f} + h$, we have that

$$\bar{f}(p_0) + h(p_0) \leq \bar{f}(p_t) + h(p_t) \leq \bar{f}(p_0) + \nabla\bar{f}(p_0)^\top(p_t - p_0) + \frac{L}{2} \|p_t - p_0\|^2 + h(p_t).$$

Hence, we have that

$$\begin{aligned} 0 &\leq \nabla\bar{f}(p_0)^\top(p_t - p_0) + \frac{L}{2} \|p_t - p_0\|^2 + h(p_t) - h(p_0) \\ &\leq t \cdot (\nabla\bar{f}(p_0)^\top(z - p_0) + h(z) - h(p_0)) + \frac{Lt^2}{2} \|z - p_0\|^2. \end{aligned}$$

Taking $t \rightarrow 0^+$, we have

$$\nabla\bar{f}(p_x)^\top(z - p_x) + h(z) - h(p_x) \geq 0$$

Expanding the term $\nabla\bar{f}(p_x)$, we have

$$\nabla f(x)^\top(z - p_x) + L(p_x - x)^\top(z - p_x) + h(z) - h(p_x) \geq 0.$$

Equivalently,

$$\begin{aligned} h(z) &\geq h(p_x) + \nabla f(x)^\top(p_x - z) + L(p_x - x)^\top(p_x - z) \\ &= h(p_x) + \nabla f(x)^\top(p_x - z) + \frac{1}{L} \|g_x\|^2 + L(p_x - x)^\top(x - z) \\ &= h(p_x) + \nabla f(x)^\top(p_x - z) + \frac{1}{L} \|g_x\|^2 + g_x^\top(z - x). \end{aligned}$$

Using that

$$f(z) \geq f(x) + \nabla f(x)^\top(z - x) + \frac{\mu}{2} \|z - x\|^2$$

and that

$$f(p_x) \leq f(x) + \nabla f(x)^\top(p_x - x) + \frac{1}{2L} \|g_x\|^2,$$

we have the result:

$$\begin{aligned} \phi(z) &\geq h(p_x) + f(x) + \nabla f(x)^\top(p_x - x) + \frac{1}{L} \|g_x\|^2 + g_x^\top(z - x) + \frac{\mu}{2} \|z - x\|^2 \\ &\geq \phi(p_x) + \frac{1}{2L} \|g_x\|^2 + g_x^\top(z - x) + \frac{\mu}{2} \|z - x\|^2. \end{aligned}$$

□

The next lemma shows that $\|g_x\|_2 \leq 2G$ if ϕ is G -Lipschitz.

Lemma 7.15. *If ϕ is G -Lipschitz, then $\|g_x\|_2 \leq 2G$ for all x .*

Proof. By the definition of gradient mapping (namely, p_x is the minimizer of a function), we have that

$$f(x) + \nabla f(x)^\top (p_x - x) + \frac{L}{2} \|p_x - x\|^2 + h(p_x) \leq f(x) + h(x).$$

Using $h(p_x) \geq h(x) + \nabla h(x)^\top (p_x - x)$, we have that

$$0 \geq \nabla \phi(x)^\top (p_x - x) + \frac{L}{2} \|p_x - x\|^2 \geq -G \|p_x - x\|_2 + \frac{L}{2} \|p_x - x\|^2.$$

Hence, we have that $\|p_x - x\|_2 \leq \frac{2}{L}G$ and hence $\|g_x\|_2 \leq 2G$. \square

■ 7.4.2 Gradient Descent Using Gradient Mapping

Putting $z = x$ in Theorem 7.14, we have the following:

Lemma 7.16 (Gradient Descent Lemma). *We have that*

$$\phi(p_x) \leq \phi(x) - \frac{1}{2L} \|g_x\|_2^2.$$

This shows that each step of the gradient step decreases the function value by $\frac{1}{2L} \|g_x\|_2^2$. Therefore, if the gradient is large, then we decrease the function value by a lot. On the other hand, Putting $z = x^*$ for Theorem 7.14 shows that

$$\phi(x^*) \geq \phi(p_x) + g_x^\top (x^* - x).$$

If the gradient is small and domain is bounded, this shows that we are close to the optimal. Combining these two facts, we can get the gradient descent.

■ 7.4.3 Mirror Descent Using Gradient Mapping

Consider the mirror descent as

$$x^{(k+1)} = x^{(k)} - \eta g_{x^{(k)}}. \quad (7.5)$$

The main difference between this and gradient descent is that we will take a larger step size η . To analyze the mirror descent, we use Theorem 7.14 and the convexity of ϕ to get that

$$\phi\left(\frac{1}{k} \sum_{i=1}^k p_{x^{(i)}}\right) - \phi(x^*) \leq \frac{1}{k} \sum_{i=1}^k (\phi(p_{x^{(i)}}) - \phi(x^*)) \leq \frac{1}{k} \sum_{i=1}^k g_{x^{(i)}}^\top (x^{(i)} - x^*). \quad (7.6)$$

Therefore, it suffices to upper bound $g_{x^{(i)}}^\top (x^{(i)} - x^*)$. The following lemma shows that if $g_{x^{(i)}}^\top (x^{(i)} - x^*)$ is large, then either the gradient is large or the distance to optimum moves a lot. It turns out this holds for any vector g , not necessarily an approximate gradient.

Lemma 7.17 (Mirror Descent Lemma). *Let $p = x - \eta g$. Then, we have that*

$$g^\top (x - u) = \frac{\eta}{2} \|g\|_2^2 + \frac{1}{2\eta} \left(\|x - u\|_2^2 - \|p - u\|_2^2 \right)$$

for any u .

■ 7.4.4 Algorithm and Analysis

Recall Lemma 7.16 shows that if the gradient is large, gradient descent makes a large progress. On the other hand, if the gradient is small, (7.6) shows that mirror descent makes a large progress. Therefore, it is natural to combine two approaches.

Algorithm 24: AGD

Input: Initial point $x^{(1)} \in \mathbb{R}^n$.

$y^{(1)} \leftarrow x^{(1)}, z^{(1)} \leftarrow x^{(1)}$.

for $k = 1, 2, \dots, T$ **do**

$x^{(k+1)} \leftarrow \tau z^{(k)} + (1 - \tau)y^{(k)}$.

 Perform a gradient step: $y^{(k+1)} = x^{(k+1)} - \frac{1}{L}g_{x^{(k+1)}}$.

 Perform a mirror step: $z^{(k+1)} = z^{(k)} - \eta g_{x^{(k+1)}}$.

end

Return $\frac{1}{T} \sum_{k=1}^T p_{x^{(k+1)}}$.

Note that if $\tau = 1$, the algorithm is simply mirror descent and if $\tau = 0$, the algorithm is gradient descent.

Theorem 7.18. *Setting $\frac{1-\tau}{\tau} = \eta L$ and $\eta = \frac{1}{\sqrt{\mu L}}$, we have that*

$$\phi\left(\frac{1}{T} \sum_{k=1}^T p_{x^{(k+1)}}\right) - \phi(x^*) \leq \frac{2}{T} \sqrt{\frac{L}{\mu}} \left(\phi(x^{(1)}) - \phi(x^*) \right).$$

In particular, if we restart the algorithm every $4\sqrt{\frac{L}{\mu}}$ iterations, we can find x such that

$$\phi(x) - \phi(x^*) \leq 2\left(1 - \sqrt{\frac{\mu}{L}}\right)^{\Omega(T)} \left(\phi(x^{(1)}) - \phi(x^*) \right)$$

in T steps. Furthermore, each step takes $\mathcal{T}_f + \mathcal{T}_{h,L}$

Proof. Lemma 7.17 showed that

$$g_{x^{(k+1)}}^\top (z^{(k)} - x^*) \leq \frac{\eta}{2} \|g_{x^{(k+1)}}\|_2^2 + \frac{1}{2\eta} \left(\|z^{(k)} - x^*\|_2^2 - \|z^{(k+1)} - x^*\|_2^2 \right) \quad (7.7)$$

This shows that if the mirror descent has large error $g_{x^{(k+1)}}^\top (z^{(k)} - x^*)$, then the gradient descent makes a large progress $(\frac{\eta}{2} \|g_{x^{(k+1)}}\|_2^2)$.

To make the left-hand side usable, note that $x^{(k+1)} = z^{(k)} + \frac{1-\tau}{\tau} \cdot (y^{(k)} - x^{(k+1)})$ and hence

$$\begin{aligned} g_{x^{(k+1)}}^\top (x^{(k+1)} - x^*) &= g_{x^{(k+1)}}^\top (z^{(k)} - x^*) + \frac{1-\tau}{\tau} \cdot g_{x^{(k+1)}}^\top (y^{(k)} - x^{(k+1)}) \\ &\leq g_{x^{(k+1)}}^\top (z^{(k)} - x^*) + \frac{1-\tau}{\tau} (\phi(y^{(k)}) - \phi(y^{(k+1)})) - \frac{1}{2L} \|g_{x^{(k+1)}}\|_2^2 \\ &\leq \frac{\eta}{2} \|g_{x^{(k+1)}}\|_2^2 + \frac{1}{2\eta} \left(\|z^{(k)} - x^*\|_2^2 - \|z^{(k+1)} - x^*\|_2^2 \right) + \frac{1-\tau}{\tau} (\phi(y^{(k)}) - \phi(y^{(k+1)})) - \frac{1}{2L} \|g_{x^{(k+1)}}\|_2^2. \end{aligned}$$

where we used Theorem 7.14 in the middle and (7.7) at the end.

Now, we set $\frac{1-\tau}{\tau} = \eta L$ and get

$$g_{x^{(k+1)}}^\top (x^{(k+1)} - x^*) \leq \eta L (\phi(y^{(k)}) - \phi(y^{(k+1)})) + \frac{1}{2\eta} \left(\|z^{(k)} - x^*\|_2^2 - \|z^{(k+1)} - x^*\|_2^2 \right).$$

Taking a sum on both side and let $\bar{x} = \frac{1}{T} \sum_{k=1}^T p_{x^{(k+1)}}$, we have that

$$\begin{aligned}
 \phi(\bar{x}) - \phi(x^*) &\leq \frac{1}{T} \sum_{k=1}^T (\phi(p_{x^{(k+1)}}) - \phi(x^*)) \\
 &\leq \frac{1}{T} \sum_{k=1}^T g_{x^{(k+1)}}^\top (x^{(k+1)} - x^*) \\
 &\leq \frac{\eta L}{T} (\phi(y^{(1)}) - \phi(y^{(T+1)})) + \frac{1}{2\eta T} \|z^{(1)} - x^*\|_2^2 \\
 &\leq \left(\frac{\eta L}{T} + \frac{1}{2\eta T \mu} \right) (\phi(x^{(1)}) - \phi(x^*))
 \end{aligned}$$

The conclusion follows from our setting of η . \square

■ 7.5 Accelerated Coordinate Descent

Recall from Theorem 6.29 that if $\frac{\partial^2}{\partial x_i^2} \ell(x) \leq L_i$ for all x and that ℓ is μ strongly convex, then we can find $x^{(k)}$ in k coordinate steps such that

$$\mathbf{E} \ell(x^{(k)}) - \ell(x^*) \leq (1 - \frac{\mu}{L})^{\Omega(k)} (\ell(x^{(0)}) - f(x^*))$$

where $L = \sum_i L_i$. Now, the really fun part is here. Consider the function

$$\phi(x) = f(x) + h(x) \quad \text{with} \quad f(x) = \frac{\mu}{2} \|x\|_2^2 \quad \text{and} \quad h(x) = \ell(x) - \frac{\mu}{2} \|x\|_2^2.$$

Since f is $\mu + \frac{L}{n}$ smooth (YES!, I know this is also μ smooth) and μ strongly convex and since h is convex, we apply Theorem 7.18 and get an algorithm that takes $O^*(\sqrt{\frac{L}{n\mu}})$ steps. Note that each step involves $\mathcal{T}_f + \mathcal{T}_{h, \mu + \frac{L}{n}}$. Obviously, $\mathcal{T}_f = 0$. Next, note that $\mathcal{T}_{h, \mu + \frac{L}{n}}$ involves solving a problem of the form

$$\begin{aligned}
 y_x &= \operatorname{argmin}_y \left(\frac{\mu}{2} + \frac{L}{2n} \right) \|y - x\|^2 + (\ell(y) - \frac{\mu}{2} \|x\|^2) \\
 &= \operatorname{argmin}_y \ell(y) - \mu y^\top x + \frac{L}{2n} \|y - x\|^2.
 \end{aligned}$$

Now, we can apply Theorem 6.29 to solve this problem. It takes

$$O^*\left(\frac{L + (L/n) \cdot n}{L/n}\right) = O^*(n) \text{ coordinate steps.}$$

Therefore, in total it takes

$$O^*\left(\sqrt{\frac{L}{n\mu}}\right) \cdot O^*(n) = O^*\left(\sqrt{\frac{Ln}{\mu}}\right) \text{ coordinate steps.}$$

Hence, we have the following theorem

Theorem 7.19 (Accelerated Coordinate Descent Convergence). *Given an μ strongly-convex function ℓ . Suppose that $\frac{\partial^2}{\partial x_i^2} \ell(x) \leq L_i$ for all x and let $L = \sum L_i$. We can minimize ℓ in $O^*(\sqrt{\frac{Ln}{\mu}})$ coordinate steps.*

Remark 7.20. It is known how to do it in $O^*(\sum_i \sqrt{\frac{L_i}{\mu}})$ steps [4].

■ 7.6 Accelerated Stochastic Descent

Recall from Theorem 6.27 that if $\nabla^2 \ell_i(x) \leq L$ for all x and i and that $\ell(x) = \frac{1}{n} \sum_{i=1}^n \ell_i(x)$ is μ strongly convex, then we can find x in $O((n + \frac{L}{\mu}) \log(\frac{1}{\epsilon}))$ stochastic steps such that

$$\mathbf{E} \ell(x) - \ell(x^*) \leq \epsilon (\ell(x^{(0)}) - \ell(x^*)).$$

Similar to the coordinate descent, we can accelerate it using the accelerated gradient descent (Theorem 7.18). To apply Theorem 7.18, we consider the function

$$\phi(x) = f(x) + h(x) \quad \text{with} \quad f(x) = \frac{\mu}{2} \|x\|_2^2 \quad \text{and} \quad h(x) = \ell(x) - \frac{\mu}{2} \|x\|_2^2.$$

Since f is $\mu + \frac{L}{n}$ smooth (YES!, I know this is also μ smooth) and μ strongly convex and since h is convex, we apply Theorem 7.18 and get an algorithm that takes $O^*(1 + \sqrt{\frac{L}{n\mu}})$ steps. Note that each step involves $\mathcal{T}_f + \mathcal{T}_{h, \mu + \frac{L}{n}}$. Obviously, $\mathcal{T}_f = 0$. Next, note that $\mathcal{T}_{h, \mu + \frac{L}{n}}$ involves solving a problem of the form

$$\begin{aligned} y_x &= \operatorname{argmin}_y \left(\frac{\mu}{2} + \frac{L}{2n} \right) \|y - x\|^2 + (\ell(y) - \frac{\mu}{2} \|x\|^2) \\ &= \operatorname{argmin}_y \ell(y) - \mu y^\top x + \frac{L}{2n} \|y - x\|^2 \\ &= \operatorname{argmin}_y \frac{1}{n} \sum_i (\ell_i(y) + \frac{L}{2n} \|y - x\|^2 - \mu y^\top x) \end{aligned}$$

Now, we can apply Theorem 6.27 to solve this problem. It takes

$$O^*\left(n + \frac{L + \frac{L}{n}}{\mu + \frac{L}{n}}\right) = O^*(n)$$

Therefore, in total it takes

$$O^*\left(1 + \sqrt{\frac{L}{n\mu}}\right) \cdot O^*(n) = O^*\left(n + \sqrt{n \frac{L}{\mu}}\right).$$

Theorem 7.21. *Given a convex function $\ell = \frac{1}{n} \sum \ell_i$. Suppose that $\nabla^2 \ell_i(x) \leq L$ for all i and x and that ℓ is μ strongly convex. Suppose we can compute $\nabla \ell_i$ in $O(1)$ time. We have an algorithm that outputs an x such that*

$$\mathbf{E} \ell(x) - \ell(x^*) \leq \epsilon (\ell(x^{(0)}) - \ell(x^*))$$

in $O^(n + \sqrt{n \frac{L}{\mu}})$ stochastic steps.*

Part II

Sampling

Chapter 8

Gradient-based Sampling

Sampling in high dimension is a fundamental problem. Informally, given access to a function $f : \mathbb{R}^n \rightarrow \mathbb{R} \cup \{\infty\}$, the sampling problem is to generate a point $x \in \mathbb{R}^n$ from the distribution with density proportional to $e^{-f(x)}$. Note that any density can be written in this form, so this is completely general. To make the problem precise, we also have to specify a starting point with positive density, and an error parameter ϵ that measures the distance of the distribution of the output from the desired target.

Unfortunately, in this generality, just like optimization, sampling is also intractable. To see this, consider the following function:

$$f(x) = \begin{cases} 0 & x \in S \\ M & x \notin S \end{cases}$$

for some closed set S . Then sampling according to e^{-f} for a sufficiently large M would allow us to find an element of S , which could, e.g., be the minimizer of a hard-to-optimize function.

Consider a second example, which might appear more tractable:

$$g(x) = e^{-\frac{1}{2}x^\top Ax} \mathbf{1}_{x \geq 0}.$$

Without the restriction to the nonnegative orthant, the target density is the Gaussian $N(0, A^{-1})$, and can be sampled by first sampling the standard Gaussian $N(0, I)$ and applying the linear transformation $A^{-1/2}$. To sample from the standard Gaussian in \mathbb{R}^n , we can sample each coordinate independently from $N(0, 1)$, a problem which has many (efficient) numerical recipes. But how can we handle the restriction? In the course of forthcoming chapters, we will see that this problem and its generalization to sampling logconcave densities, i.e., when f is convex, can be solved in polynomial time. It is remarkable that the polynomial-time frontier for both optimization and sampling is essentially determined by convexity.

We begin with gradient-based sampling methods. These rely on access to ∇f . These methods will in fact be natural algorithmic versions of continuous processes on random variables, a particularly pleasing connection. Later we will see methods that only use access to f , and others that utilize higher derivatives, notably the Hessian. The parallels to optimization will be pervasive and striking.

■ 8.1 Gradient-based methods: Langevin Dynamics

Here we study a simple stochastic process for generating samples from a desired distribution $e^{-f(x)}$. As we will see later in this chapter, it can also be viewed as a stochastic version of gradient descent *in the space of measures*. While gradient descent corresponds to an ordinary differential equation (ODE), stochastic gradient descent corresponds to a stochastic differential equation (SDE).

Algorithm 25: LangevinDiffusion (LD)

Input: Initial point $x_0 \in \mathbb{R}^n$.

Solve the stochastic differential equation

$$dx_t = -\nabla f(x_t)dt + \sqrt{2}dW_t$$

Output: x_t .

Here $f : \mathbb{R}^n \rightarrow \mathbb{R}$ is a function, x_t is the random variable at time t and dW_t is infinitesimal Brownian motion also known as a Wiener process. We can view it as the continuous version of the following discrete process

$$x_{t+1} = x_t - h\nabla f(x_t) + \sqrt{2h}\zeta_t$$

with ζ_t sampled independently from $N(0, I)$. When we take the step size $h \rightarrow 0$, this discrete process converges to the continuous one in distribution. We discuss the continuous version first.

A more general form of an SDE is

$$dx_t = \mu(x_t, t)dt + \sigma(x_t, t)dW_t$$

where $x_t \in \mathbb{R}^n$, $\mu(x_t, t) \in \mathbb{R}^n$ is a time-varying vector field and $\sigma(x_t, t) \in \mathbb{R}^{n \times m}$ is a time-varying linear transformation. The simplest such process is the Wiener process: $dx_t = dW_t$ which finds many applications in applied mathematics, finance, biology and physics. Another useful process is the Ornstein-Uhlenbeck Process:

$$dx_t = -ax_tdt + \sigma dW_t$$

This represents a particle moving in a fluid, the first term being the force of friction exerted on the particle and the second term being the movement caused by other particles colliding in our particle, which is modeled using Brownian motion.

A crucial difference between ordinary differentials and stochastic differentials is in the chain rule. Unlike classical differentials where we have $df(x) = \nabla f(x)dx$, we have the following chain rule for stochastic calculus.

Lemma 8.1 (Itô's lemma). *For any process $x_t \in \mathbb{R}^n$ satisfying $dx_t = \mu(x_t)dt + \sigma(x_t)dW_t$ where $\mu(x_t) \in \mathbb{R}^n$ and $\sigma(x_t) \in \mathbb{R}^{n \times m}$, we have that*

$$\begin{aligned} df(x_t) &= \nabla f(x_t)^\top dx_t + \frac{1}{2}(dx_t)^\top \nabla^2 f(x_t)(dx_t) \\ &= \nabla f(x_t)^\top \mu(x_t)dt + \nabla f(x_t)^\top \sigma(x_t)dW_t + \frac{1}{2}\text{tr}(\sigma(x_t)^\top \nabla^2 f(x_t)\sigma(x_t))dt. \end{aligned}$$

The usual chain rule comes from using Taylor expansion and taking a limit, i.e.,

$$\nabla f(x) = \lim_{h \rightarrow 0} \frac{(f(x) + h\nabla f(x)^\top y + \frac{1}{2}h^2 \dots) - f(x)}{h} = \lim_{h \rightarrow 0} \frac{h\nabla f(x)^\top y + \frac{1}{2}h^2 \dots}{h}$$

and only the first term survives, as the second and later terms goes to zero. But with the stochastic component, roughly speaking, $(dW_t)^2 = dt$ ¹, and we need to keep track of the second term in the Taylor expansion as well. For a detailed treatment of stochastic calculus, we refer the reader to a standard textbook such as [60].

First, we will see that e^{-f} is a stationary density for the Langevin SDE in continuous time. The proof relies on the following general theorem about the distribution induced by an SDE.

Theorem 8.2 (Fokker-Planck equation). *For any process $x_t \in \mathbb{R}^n$ satisfying $dx_t = \mu(x_t)dt + \sigma(x_t)dW_t$ where $\mu(x_t) \in \mathbb{R}^n$ and $\sigma(x_t) \in \mathbb{R}^{n \times m}$ with the initial point x_0 drawn from p_0 . Then the density p_t of x_t satisfies the equation*

$$\frac{dp_t}{dt} = - \sum_i \frac{\partial}{\partial x_i} (\mu(x)_i p_t(x)) + \frac{1}{2} \sum_{i,j} \frac{\partial^2}{\partial x_i \partial x_j} [(D(x))_{ij} p_t(x)]$$

where $D(x) = \sigma(x)\sigma(x)^\top$.

Proof. For any smooth function ϕ , we have that

$$\mathbf{E}_{x \sim p_t} \phi(x) = \mathbf{E} \phi(x_t).$$

¹By definition, $W_t \sim N(0, t)$, so the variance of W_t is t . Thus, $(dW_t)^2 = dt$ may seem to make sense. This can be justified rigorously through *quadratic variations*.

Taking derivatives on the both sides with respect to t , using Itô's lemma (Lemma 8.1), and noting that $\mathbf{E}dW_t = 0$, we have that

$$\begin{aligned} \int \phi(x) dp_t(x) dx &= \mathbf{E} \left(\nabla \phi(x_t)^\top \mu(x_t) dt + \nabla \phi(x_t)^\top \sigma(x_t) dW_t + \frac{1}{2} \text{tr}(\sigma(x_t)^\top \nabla^2 \phi(x_t) \sigma(x_t)) dt \right) \\ &= \mathbf{E} \left(\nabla \phi(x_t)^\top \mu(x_t) dt + \frac{1}{2} \text{tr}(\nabla^2 \phi(x_t) D(x_t)) dt \right). \end{aligned}$$

Using $x_t \sim p_t$, we have that

$$\int \phi(x) \frac{dp_t}{dt} dx = \int \nabla \phi(x)^\top \mu(x) p_t(x) + \frac{1}{2} \text{tr}(\nabla^2 \phi(x) D(x)) p_t(x) dx.$$

Integrating by parts,

$$\int \nabla \phi(x)^\top \mu(x) p_t(x) dx = - \int \phi(x) \sum_i \frac{\partial}{\partial x_i} (\mu_i(x) p_t(x)) dx.$$

Similarly, integrating by parts twice gives

$$\begin{aligned} \int \text{tr}(\sigma(x)^\top \nabla^2 \phi(x) \sigma(x)) p_t(x) dx &= \int \text{tr}(\nabla^2 \phi(x) \sigma(x) \sigma(x)^\top) p_t(x) dx \\ &= - \int \langle \nabla \phi(x), \sum_i \frac{\partial}{\partial x_i} (p_t(x) D(x)_i) \rangle dx \\ &= \sum_{i,j} \int \phi(x) \frac{\partial^2}{\partial x_i \partial x_j} [(D(x))_{ij} p_t(x)] dx. \end{aligned}$$

Hence,

$$\int \phi(x) \left[\frac{dp_t}{dt} + \sum_i \frac{\partial}{\partial x_i} (\mu_i(x) p_t(x)) - \frac{1}{2} \sum_{i,j} \frac{\partial^2}{\partial x_i \partial x_j} [(D(x))_{ij} p_t(x)] \right] dx = 0$$

for any smooth ϕ . Therefore, we have the conclusion of the theorem.

We apply the Fokker–Planck equation to the Langevin dynamics. \square

Theorem 8.3. *For any smooth function f , the density proportional to $F = e^{-f}$ is stationary for the Langevin dynamics.*

Proof. The Fokker–Planck equation (Theorem 8.2) shows that the distribution p_t of x_t satisfies

$$\frac{dp_t}{dt} = \sum_i \frac{\partial}{\partial x_i} \left(\frac{\partial f(x)}{\partial x_i} p_t(x) \right) + \sum_i \frac{\partial^2}{\partial x_i^2} [p_t(x)]. \quad (8.1)$$

Now since p_t is stationary the LHS is zero and we can rewrite the above as

$$\begin{aligned} \frac{dp_t}{dt} = 0 &= \sum_i \frac{\partial}{\partial x_i} \left(p_t(x) \frac{\partial f(x)}{\partial x_i} + \frac{\partial}{\partial x_i} p_t(x) \right) \\ &= \sum_i \frac{\partial}{\partial x_i} \left(p_t(x) \left(\frac{\partial f(x)}{\partial x_i} + \frac{\partial}{\partial x_i} \log p_t(x) \right) \right) \\ &= \sum_i \frac{\partial}{\partial x_i} \left(p_t(x) \left(\frac{\partial}{\partial x_i} \left[\log \frac{p_t(x)}{e^{-f(x)}} \right] \right) \right). \end{aligned}$$

We can verify that $p_t(x) \propto e^{-f(x)}$ is a solution. \square

Exercise 8.4. Consider the equation

$$\frac{d}{dt}p_t(x) = \frac{1}{2} \frac{d^2}{dx^2}p_t(x)$$

for $x \in \mathbb{R}, t > 0$. Show that the density of $\mathcal{N}(0, t)$, i.e.

$$\phi_t(x) = \frac{1}{\sqrt{2\pi t}} \exp\left(-\frac{x^2}{2t}\right)$$

satisfies this equation. Then generalize the process to \mathbb{R}^n .

Exercise 8.5. Consider the SDE with $X_t \in \mathbb{R}^n$:

$$dX_t = -X_t dt + \sqrt{2}dW_t.$$

Use the Fokker-Planck equation to derive a corresponding stationary density. Use Itô's lemma to derive $\mathbf{E}(\|X_t\|_4^4)$. (Hint: Take expectation on both sides of Itô's lemma for appropriate $f(X_t)$, and use $\mathbf{E}df(X_t) = d\mathbf{E}f(X_t)$ for continuous f and df).

■ 8.1.1 Convergence via Coupling in Wasserstein distance

Next we turn to the rate of convergence, which will also prove uniqueness of the stationary distribution for the stochastic process. For this, we assume that f is strongly convex. The proof is via the classical coupling technique [3].

Our goal is to bound the rate at which the distribution of the current point approaches the stationary distribution, in some chosen measure of distance between distributions (for example, the TV distance). To do this, in the coupling technique, we consider two points which are both following the random process. One of them is already in the stationary distribution, and therefore will stay there. The other is our point. We will show that there is a coupling of the two distributions, i.e., a joint distribution over the two points, whose marginals are identical to the single point processes, such that the expected distance between the two points decreases at a certain rate. More formally, we couple two copies x_t, y_t of the random process with different starting points (the coupling is a joint distribution $D(x_t, y_t)$ with the property that its marginal for each of x_t, y_t is exactly the process) and show that their distributions get closer over time.

While the challenge usually is to find a good coupling, in the present case, the simple identity coupling (i.e., the same Wiener process is used for both x_t and y_t) works well. The distance measure we will use here is the Wasserstein distance (in Euclidean norm, see Definition 0.12).

Exercise 8.6. Show that for two distributions with the same finite support, computing their Wasserstein distance reduces to a bipartite matching problem.

Lemma 8.7. Let x_t, y_t evolve according to the Langevin diffusion for a μ -strongly convex function $f : \mathbb{R}^n \rightarrow \mathbb{R}$. Then, there is a coupling γ between x_t and y_t s.t.

$$\mathbf{E}_{x_t, y_t \sim \gamma} \|x_t - y_t\|^2 \leq e^{-2\mu t} \|x_0 - y_0\|^2.$$

Proof. From the definition of LD, and by using the identity coupling, i.e., the same Gaussian dW_t for both processes x_t and y_t , we have that

$$\frac{d}{dt}(x_t - y_t) = \nabla f(y_t) - \nabla f(x_t).$$

Hence,

$$\frac{1}{2} \frac{d}{dt} \|x_t - y_t\|^2 = \langle \nabla f(y_t) - \nabla f(x_t), x_t - y_t \rangle.$$

Next, from the strong convexity of f , we have

$$\begin{aligned} f(y_t) - f(x_t) &\geq \nabla f(x_t)^\top (y_t - x_t) + \frac{\mu}{2} \|x_t - y_t\|^2, \\ f(x_t) - f(y_t) &\geq \nabla f(y_t)^\top (x_t - y_t) + \frac{\mu}{2} \|x_t - y_t\|^2. \end{aligned}$$

Adding two equations together, we have

$$(\nabla f(x_t) - \nabla f(y_t))^\top (x_t - y_t) \geq \mu \|x_t - y_t\|^2.$$

Therefore,

$$\frac{1}{2} \frac{d}{dt} \|x_t - y_t\|^2 \leq -\mu \|x_t - y_t\|^2.$$

Hence,

$$\begin{aligned} \frac{d}{dt} \log \|x_t - y_t\|^2 &= \frac{\frac{d}{dt} \|x_t - y_t\|^2}{\|x_t - y_t\|^2} \\ &\leq -2\mu. \end{aligned}$$

Integrating both sides from 0 to t , we get

$$\log \|x_t - y_t\|^2 - \log \|x_0 - y_0\|^2 \leq -2\mu t$$

which proves the result. \square

Exercise 8.8. Give an example of a function f for which the density proportional to e^{-f} is *not* stationary for the following discretized Langevin algorithm

$$x^{(k+1)} = x^{(k)} - \epsilon \nabla f(x^{(k)}) + \sqrt{2\epsilon} Z^{(k)}$$

where $Z^{(k)} \sim \mathcal{N}(0, 1)$ are independent and the distribution of $x^{(0)}$ is Gaussian.

■ 8.1.2 Convergence in χ^2 and KL divergences

Next we analyze the convergence of Langevin dynamics in the two most commonly used divergence metrics. The rate of mixing will depend on a fundamental functional constants of the target density, which we define next. These constants will play an important role in later algorithms and analysis, and we will also see equivalent geometric formulations of them.

Definition 8.9. We say that a probability measure ν on \mathbb{R}^n satisfies a *Poincaré inequality* (PI) with parameter $C_{PI}(\nu)$ if for all smooth functions $g : \mathbb{R}^n \rightarrow \mathbb{R}$,

$$\text{Var}_\nu g \leq C_{PI}(\nu) \mathbf{E}_\nu \left(\|\nabla g\|^2 \right) \quad (8.2)$$

where $\text{Var}_\nu g = \mathbf{E}_\nu |g - \mathbf{E}_\nu g|^2$.

The Poincaré inequality is implied by the generally stronger log-Sobolev inequality.

Definition 8.10. We say that a probability measure ν on \mathbb{R}^n satisfies a *log-Sobolev inequality* (LSI) with parameter $C_{LSI}(\nu)$ if for all smooth functions $g : \mathbb{R}^n \rightarrow \mathbb{R}$,

$$\text{Ent}_\nu(g^2) \leq 2C_{LSI}(\nu) \mathbf{E}_\nu \left(\|\nabla g\|^2 \right) \quad (8.3)$$

where $\text{Ent}_\nu(g^2) := \mathbf{E}_\nu(g^2 \log g^2) - \mathbf{E}_\nu(g^2) \log \mathbf{E}_\nu(g^2)$.

Theorem 8.11. Let f be a smooth function with log-Sobolev constant C_{LSI} . Then the Langevin dynamics

$$dx_t = -\nabla f(x)dt + \sqrt{2}dW_t$$

converges exponentially in KL-divergence (Definition 0.10) to the density $\nu(x) \propto e^{-f(x)}$ with mixing rate $O(C_{LSI})$, i.e., the distribution ρ_t of x_t satisfies

$$d_{KL}(\rho_t, \nu) \leq e^{-\frac{2}{C_{LSI}}t} d_{KL}(\rho_0, \nu).$$

The theorem will follow from the following lemma and the log-Sobolev inequality.

Lemma 8.12. *For a target distribution ν , with ρ_t being the distribution attained by Langevin dynamics at time t , starting at ρ_0 , we have*

$$\frac{d}{dt}d_{KL}(\rho_t, \nu) = -J_\nu(\rho_t)$$

where $J_\nu(\rho)$ is the relative Fisher information of ρ wrt ν , defined as $\mathbf{E}_\rho(\|\nabla \log(\rho/\nu)\|^2)$.

Proof. We compute the time derivative of the distribution of LD at time t with $\rho = \rho_t$:

$$\begin{aligned} \frac{d}{dt}d_{KL}(\rho_t, \nu) &= \frac{d}{dt} \int_{\mathbb{R}^n} \rho \log \frac{\rho}{\nu} \\ &= \int \frac{d\rho}{dt} \left(\log \frac{\rho}{\nu} + 1 \right) \\ &= - \int \nabla \cdot \left(\rho \nabla \log \frac{\rho}{\nu} \right) \\ &= - \int \langle \rho \nabla \log \frac{\rho}{\nu}, \nabla \log \frac{\rho}{\nu} \rangle \\ &= - \int \rho \left\| \nabla \log \frac{\rho}{\nu} \right\|_2^2 \\ &= \mathbf{E}_\rho \left(\left\| \nabla \log \frac{\rho}{\nu} \right\|_2^2 \right) = -J_\nu(\rho_t). \end{aligned}$$

□

The next lemma shows that the log-Sobolev constant can be equivalently formulated in terms of distributions in place of smooth functions.

Lemma 8.13. *The log-Sobolev constant of a distribution ν on \mathbb{R}^n can be equivalently defined as follows: for any distribution ρ on \mathbb{R}^n , we have*

$$d_{KL}(\rho, \nu) \leq \frac{C_{LSI}}{2} J_\nu(\rho).$$

Proof. To go one way, we use $g = \sqrt{\frac{\rho}{\nu}}$; to go the other way, define $\rho = \frac{g^2}{\mathbf{E}_\nu(g^2)}$.

□

We are now ready to prove Theorem 8.11.

Proof. We use Lemmas and to obtain

$$\frac{d}{dt}d_{KL}(\rho_t, \nu) = -J_\nu(\rho_t) \leq -\frac{2}{C_{LSI}}d_{KL}(\rho_t, \nu).$$

Integrating over time gives the theorem.

□

Exercise 8.14. Show that for Langevin Dynamics applied to a target density ν with Poincaré constant C_{PI} satisfies

$$\chi^2(\rho_t, \nu) \leq e^{-\frac{2}{C_{PI}}t} \chi^2(\rho_0, \nu).$$

■ 8.2 Langevin Dynamics is Gradient Descent in Density Space*²

Here we show that Langevin dynamics is simply gradient descent for the function $F(\rho) = d_{KL}(\rho||\nu)$ for two densities ρ, ν on the Wasserstein space where $\nu = e^{-f(x)} / \int e^{-f(y)} dy$ is the target and ρ is the current density. For this, we first define the Wasserstein space.

²Sections marked with * are more mathematical and can be skipped.

Definition 8.15. The Wasserstein space $P_2(\mathbb{R}^n)$ on \mathbb{R}^n is the manifold on the set of probability measures on \mathbb{R}^n such that the shortest path distance of two measures x, y in this manifold is exactly equal to the Wasserstein distance between x and y .

We let $T_p(\mathcal{M})$ refer to the tangent space at a point p in a manifold \mathcal{M} .

Lemma 8.16. For any $p \in P_2(\mathbb{R}^n)$ and $v \in T_p P_2(\mathbb{R}^n)$, we can write $v(x) = \nabla \cdot (p(x) \nabla \lambda(x))$ for some function λ on \mathbb{R}^n . Furthermore, the local norm of v in this metric is given by

$$\|v\|_p^2 = \mathbf{E}_{x \sim p} \|\nabla \lambda(x)\|^2.$$

Proof. Let $p \in P_2(\mathbb{R}^n)$ and $v \in T_p P_2(\mathbb{R}^n)$. We will show that any change of density v can be represented by a vector field c on \mathbb{R}^n as follows: Consider the process $x_0 \sim p$ and $\frac{d}{dt}x_t = c(x_t)$. Let p_t be the density of the distribution of x_t . To compute $\frac{d}{dt}p_t$, we follow the same idea as in the proof as Theorem 8.2. For any smooth function ϕ , we have that $\mathbf{E}_{x \sim p_t} \phi(x) = \mathbf{E} \phi(x_t)$. Taking derivatives on the both sides with respect to t , we have that

$$\int \phi(x) \frac{d}{dt} p_t(x) dx = \int \nabla \phi(x)^\top c(x) p_t(x) dx = - \int \nabla \cdot (c(x) p_t(x)) \phi(x) dx$$

where we used integration by parts at the end. Since this holds for all ϕ , we have that

$$\frac{dp_t(x)}{dt} = -\nabla \cdot (p_t(x) c(x)).$$

Since we are interested only in vector fields that generate the minimum movement in Wasserstein distance, we consider the optimization problem

$$\min_{-\nabla \cdot (pc) = v} \frac{1}{2} \int p(x) \|c(x)\|^2 dx$$

where we can think v is the change of p_t . Let $\lambda(x)$ be the Lagrangian multiplier of the constraint $-\nabla \cdot (pc) = v$. Then, the problem becomes

$$\begin{aligned} & \min_c \frac{1}{2} \int p(x) \|c(x)\|^2 dx - \int \lambda(x) \nabla \cdot (p(x) c(x)) dx. \\ &= \min_c \frac{1}{2} \int p(x) \|c(x)\|^2 dx + \int \nabla \lambda(x)^\top c(x) \cdot p(x) dx. \end{aligned}$$

Now, we note that the problem is a pointwise optimization problem whose minimizer is given by

$$c(x) = -\nabla \lambda(x).$$

This proves that any vector field that generates minimum movement in Wasserstein distance is a gradient field. Also, we have that $v(x) = \nabla \cdot (p(x) \nabla \lambda(x))$. Note that the right hand side is an elliptical differential equation and hence for any v with $\int v(x) dx = 0$, there is a unique solution $\lambda(x)$. Therefore, we can write $v(x) = \nabla \cdot (p(x) \nabla \lambda(x))$ for some $\lambda(x)$.

Next, we note that the movement is given by

$$\|v\|_p^2 = \int p(x) \|c(x)\|^2 dx = \mathbf{E}_{x \sim p} \|\nabla \lambda(x)\|^2.$$

□

As we discussed in the gradient descent section, one can use norms other than ℓ_2 norm. For the Wasserstein space, we should use the local norm as given in Lemma 8.16.

Theorem 8.17. Let ρ_t be the density of the distribution produced by Langevin Dynamics for the target distribution $\nu = e^{-f(x)} / \int e^{-f(y)} dy$. Then, we have that

$$\frac{d\rho}{dt} = \operatorname{argmin}_{v \in T_p P_2(\mathbb{R}^n)} \langle \nabla F(\rho), v \rangle_p + \frac{1}{2} \|v\|_p^2.$$

Namely, ρ_t follows continuous gradient descent in the density space for the function $F(\rho) = d_{\text{KL}}(\rho \| \nu)$ under the Wasserstein metric.

Proof. For any function c , the optimization problem of interest satisfies

$$\min_{\delta = \nabla \cdot (\rho \nabla \lambda)} \langle c, \delta \rangle + \frac{1}{2} \int \rho(x) \|\nabla \lambda(x)\|^2 dx = \min_{\nabla \lambda} - \int \rho(x) \cdot \nabla c(x)^\top \nabla \lambda(x) dx + \frac{1}{2} \int \rho(x) \|\nabla \lambda(x)\|^2 dx.$$

Solving the right hand side, we have $\nabla c = \nabla \lambda$ and hence $\delta = \nabla \cdot (\rho \nabla c)$. Now, we note that $\nabla F(\rho) = \log \frac{\rho}{\nu} - 1$. Therefore,

$$\begin{aligned} \frac{d\rho}{dt} &= \nabla \cdot (\rho \nabla (\log \frac{\rho}{\nu} - 1)) \\ &= \nabla \cdot (\rho \nabla \log \frac{\rho}{\nu}) \\ &= \nabla \cdot (\rho \nabla f) + \Delta \rho \end{aligned}$$

which is exactly equal to (8.1). \square

To analyze this continuous descent in Wasserstein space, we first prove that continuous gradient descent converges exponentially whenever F is strongly convex.

Lemma 8.18. *Let F be a function satisfying “Gradient Dominance”:*

$$\|\nabla F(x)\|_x^2 \geq \alpha \cdot (F(x) - \min_y F(y)) \quad \text{for all } x \quad (8.4)$$

on the manifold with the metric $\|\cdot\|_x$ where ∇ is the gradient on the manifold. Then, the process $dx_t = -\nabla F(x_t)dt$ converges exponentially, i.e., $F(x_t) - \min_y F(y) \leq e^{-\alpha t}(F(x_0) - \min_y F(y))$.

Proof. We write

$$\frac{d}{dt}(F(x) - \min_y F(y)) = \langle \nabla F(x_t), \frac{dx_t}{dt} \rangle_{x_t} = -\|\nabla F(x_t)\|_{x_t}^2 \leq -\alpha(F(x) - \min_y F(y)).$$

The conclusion follows. \square

Finally, we note that the log-Sobolev inequality for the density ν can be re-stated as the condition (8.4).

Lemma 8.19. *Fix a density ν . Then the log-Sobolev inequality, namely, for every smooth function g ,*

$$\frac{C_{LSI}}{2} \int \|\nabla g\|^2 d\nu \geq \int g(x)^2 \log g(x)^2 d\nu$$

implies the condition (8.4) with $\alpha = 1/C_{LSI}$.

Proof. Take $g(x) = \sqrt{\frac{\rho(x)}{\nu(x)}}$, the log-Sobolev inequality shows that

$$\frac{C_{LSI}}{2} \int \rho(x) \left\| \nabla \log \frac{\rho(x)}{\nu(x)} \right\|^2 dx \geq \int \rho(x) \log \frac{\rho(x)}{\nu(x)} dx \quad \text{for all } \rho.$$

As we calculate in Theorem 8.17, we have that

$$\|\nabla F(\rho)\|_\rho^2 = \int \rho(x) \left\| \nabla \log \frac{\rho(x)}{\nu(x)} \right\|^2 dx.$$

Therefore, this is exactly the condition (8.4) with coefficient $2/C_{LSI}$. \square

Combining Lemma 8.19 and Lemma 8.18, we obtain another proof of Theorem 8.11.

■ 8.2.1 Discussion

Langevin dynamics converges quickly in continuous time for isoperimetric distributions. Turning this into an efficient algorithm typically needs more assumptions and there is much room for choosing discretizations. This is similar to the situation with gradient descent for optimization. As we saw in Section 8.2, it turns out that Langevin dynamics is in fact gradient descent in the space of probability measures under the Wasserstein metric, where the function being minimized is the KL-divergence of the current density from the target stationary density. For more on this view of sampling as optimization over measures, see [76]. See [44] for a tight estimate of log-Sobolev constant for logconcave measures. In particular for a logconcave measure with support of diameter D , the log-Sobolev constant is $\Omega(1/D)$.

Elimination and Reduction

■ 9.1 Cutting Plane method for Volume Computation

The cutting plane method gives a simple algorithm for computing the volume of a bounded set, or the integral of a function. The algorithm relies crucially on the ability to compute the center of gravity of the original set/function restricted by halfspaces. For simplicity we describe it here for the case when the input object is a convex body.

Algorithm 26: CuttingPlaneVolume

Input: A body $K \subset \mathbb{R}^n$, $r \in R$, and an oracle for computing centroid.

Fix an ordering on the axes: e_1, e_2, \dots, e_n

$K^{(0)} = K$, $z^{(0)} = \text{centroid}(K^{(0)})$, $V = 1$, $k = 0$.

for $k = 0, \dots$ **do**

 Let e_i be an axis vector so that the width of $K^{(k)}$ along e_i is greater than $r/2$.

if *There is no such e_i* **then Break.;**

 Let a be e_i or $-e_i$ with sign chosen so that $H^{(k)} \stackrel{\text{def}}{=} \{x : a^\top x \leq a^\top z^{(k)}\}$ contains $z^{(0)}$.

$K^{(k+1)} \leftarrow K^{(k)} \cap H^{(k)}$.

$z^{(k+1)} \leftarrow \text{centroid}(K^{(k+1)})$.

$\hat{z} \leftarrow \text{centroid}(K^{(k)} \setminus K^{(k+1)})$.

$V \leftarrow V \cdot \frac{\|\hat{z} - z^{(k+1)}\|}{\|\hat{z} - z^{(k)}\|}$.

end

Return $V \cdot \prod_{i=1}^n w_i(K^{(k+1)})$ where $w_i(\cdot)$ is the width along e_i .

The idea behind the algorithm is simple: when we cut a set with a hyperplane through its centroid, the line joining the centroids of the two sides passes through the original centroid; moreover, the ratio of the two segments is exactly the ratio of the volumes of the two halfspaces.

Lemma 9.1. *For any measurable bounded set S in \mathbb{R}^n and any halfspace H with bounding hyperplane containing the centroid of S , we have*

$$\text{centroid}(S) = \frac{\text{vol}(S \cap H)}{\text{vol}(S)} \text{centroid}(S \cap H) + \frac{\text{vol}(S \cap \overline{H})}{\text{vol}(S)} \text{centroid}(S \cap \overline{H}).$$

The following lemma has a proof similar to that of the Grunbaum theorem.

Lemma 9.2. *Let $K \subseteq \mathbb{R}^n$ be a convex body with centroid at the origin. Suppose that for some unit vector θ , the support of K along θ is $[a, b]$. Then,*

$$|a| \geq \frac{b}{n}.$$

Exercise 9.3. Prove Lemma 9.2. [Hint: Use Theorem 1.27.]

Using the above property, we can show that the algorithm reaches a cuboid in a small number of iterations.

Theorem 9.4. *Let K be a convex body in \mathbb{R}^n containing a cube of side length r around its centroid and contained in a cube of side length R . Algorithm CuttingPlaneVolume correctly computes the volume of K using $O(n \log \frac{nR}{r})$ centroid computations.*

Proof. By Lemma 3.14, at each iteration, the volume of the remaining set $K^{(k)}$ decreases by a factor of at most $(1 - \frac{1}{e})$. When the directional width along any axis is less than $r/2$ (namely $\max_{x \in K} |e_i^\top x| \leq \frac{r}{2}$), the algorithm stops cutting along that axis. So, just before the last cut along any axis, the width in that direction is at least $r/2$. Then, we use the center of gravity to cut. By Lemma 9.2, the directional width along every axis of the surviving set is at least $r/2(n+1)$. Since the set always contains the origin, and the original set contains a cube of side length r , when the algorithm stops, it must be an axis-parallel cuboid with each side of length in the range $[r/2(n+1), r/2]$. So the final volume is at least $(r/2(n+1))^n$. The initial volume is at most R^n . Therefore the number of iterations is at most

$$\log_{(1-\frac{1}{e})} \left(\frac{R^n}{(r/2(n+1))^n} \right) = O(n \log(nR/r)).$$

In each iteration, by Lemma 9.1, the algorithm maintains the ratio of the volume of the original K to the current $K^{(k)}$. \square

The above algorithm shows that computing the volume is polytime reducible to computing the centroid. Since volume is known to be #P-hard for explicit polytopes, this means that centroid computation is also #P-hard for polytopes [62]. In later chapters we will see randomized polytime algorithms for sampling and hence for approximating centroid and volume.

Exercise 9.5. [12] Given a partial order P on an n -element set, it is of interest to count the number of linear extensions, i.e., total orders on the set that are consistent with P . We can define an associated polyhedron,

$$Q = \{x \in [0, 1]^n : x_i < x_j \text{ if } (i, j) \in P\}.$$

Show that the number of linear extensions of P is exactly $\text{vol}(Q)n!$.

■ 9.2 Optimization from Membership via Sampling

In this chapter, we assumed the oracle can be computed exactly. However, it is still open to determine the best runtime for reductions between *noisy* oracles, where the oracle provides answers to within some bounded error. In particular, the question about minimizing (approximately) convex functions under noisy oracles is an active research area, and the gaps between the lower bound and upper bound for many problems are still quite large ([8, 24, 13] based on [31]). We will see these methods in detail later. For now, to put them in the context of oracles, we just discuss the following theorem.

Theorem 9.6 (OPT via sampling). *Let $F(x) = e^{-\alpha c^T x} 1_K(x)$ for some convex set K in \mathbb{R}^n and vector $c \in \mathbb{R}^n$. Suppose $\min_{x \in K} c^T x$ is bounded. Let x be a random sample from the distribution with density proportional to $F(x)$. Then,*

$$\mathbf{E}(c^T x) \leq \min_K c^T x + \frac{n}{\alpha}.$$

Proof. We will show that the worst case is when the convex set K is an infinite cone. WLOG assume that the minimum is at $x = 0$. Replace every cross-section of K along c with an $(n-1)$ -dimensional ball of the same volume as the cross-section. This does not affect the expectation. Suppose the expectation is $\mathbf{E}(c^T x) = a$. Next, replace the subset of K with $c^T x \leq a$ with a cone whose base is the cross-section at a and apex is at zero. This only makes the expectation larger. Next, replace the subset of K on the right of a with the infinite conical extension of the cone to the left of a . Again, this expectation can only be higher.

Now for this infinite cone, we compute, using $y = c^T x$,

$$\begin{aligned} \mathbf{E}(c^T x) &= \frac{\int_0^\infty y e^{-\alpha y} y^{n-1} dy}{\int_0^\infty e^{-\alpha y} y^{n-1} dy} \\ &= \frac{1}{\alpha} \frac{\int_0^\infty e^{-y} y^n dy}{\int_0^\infty e^{-y} y^{n-1} dy} \\ &= \frac{1}{\alpha} \frac{n!}{(n-1)!} = \frac{n}{\alpha}. \end{aligned}$$

\square

The theorem says that if we sample according to $e^{-\alpha c^T x}$ for $\alpha = n/\varepsilon$, we will get an ε -approximation to the optimum. However, sampling from such a density is not trivial. Instead, we will have to go through a sequence of overlapping distributions, starting with one that is easy to sample and ending with a distribution that is focused close to the minimum. This method is known as *simulated annealing* and is the subject of Chapter 11. The complexity of sampling is polynomial in the dimension and logarithmic in a suitable notion of probabilistic distance between the starting distribution and the target distribution. The sampling algorithm only uses a membership (EVAL) oracle.

Exercise 9.7. Extend Theorem 9.6 by replacing $c^T x$ with any convex function $f(x)$.

Open Problem. Given an approximately convex function F on unit ball such that $\max_{\|x\|_2 \leq 1} |f(x) - F(x)| \leq \varepsilon/n$ for some convex function f , how efficiently can we find x in the unit ball such that $F(x) \leq \min_{\|x\|_2 \leq 1} F(x) + O(\varepsilon)$? The current fastest algorithm takes $O(n^4 \log^{O(1)}(n/\varepsilon))$ calls to the noisy EVAL oracle for F .

Chapter 10

Geometrization

In this chapter, we study polynomial-time sampling algorithms.

The Ball Walk

The simplest continuous algorithm for exploring space is Brownian motion with the ODE $dx_t = dW_t$. To turn this into a sampling algorithm, for a convex function f , we saw an extension using the gradient of f , namely

$$dx_t = -\nabla f(x_t) + \sqrt{2}dW_t$$

which can be used to sample according to the density proportional to e^{-f} . In this chapter we will begin with an even simpler method, which does not need access to the gradient or assume differentiability, only an oracle that can evaluate F .

Algorithm 27: BallWalk

Input: Step-size δ , number of steps T , starting point x_0 in the support of target density Q .

Repeat T times: at a point x ,

1. Pick a random point y in the δ -ball centered at x .

2. Go to y with probability $\min\left\{1, \frac{Q(y)}{Q(x)}\right\}$.

return x .

Exercise 10.1. Show that the distribution with density Q is *stationary* for the ball walk in a connected, compact full-dimensional set, i.e., if the distribution of the current point x has density Q , it remains Q .

Under mild conditions, the distribution of the current point approaches the target density Q . The main question is the rate of convergence, which would allow us to bound the number of steps. Note that each step involves only a function evaluation, to an oracle that outputs the value of a function proportional to the desired density. To bound the rate of convergence (and as a result the uniqueness of the stationary distribution), we first develop some general tools.

■ 10.1 Basics of Markov chains

For more detailed reading, including additional properties, see Section 1 of [52].

A Markov chain is defined using a σ -algebra (K, \mathcal{A}) , where K is the state space and \mathcal{A} is a set of subsets of K that is closed under complements and countable unions. For each element u of K , we have a probability measure P_u on (K, \mathcal{A}) , i.e., each set $A \in \mathcal{A}$ has a probability $P_u(A)$. Informally, P_u is the distribution obtained upon taking one step from u . The triple $(K, \mathcal{A}, \{P_u : u \in K\})$ along with a starting distribution Q_0 defines a Markov chain, i.e., a sequence of elements of K , w_0, w_1, \dots , where w_0 is chosen from Q_0 and each subsequent w_i is chosen from $P_{w_{i-1}}$. The choice of w_{i+1} depends only on w_i and is independent of w_0, \dots, w_{i-1} .

A distribution Q on (K, \mathcal{A}) is called *stationary* if taking one step from it maintains the distribution, i.e., for any $A \in \mathcal{A}$,

$$\int_K P_u(A) dQ(u) = Q(A).$$

A distribution Q is *atom-free* if there is no $x \in K$ with $Q(x) > 0$.

Example. For the ball walk in a convex body, the state space K is the convex body, and A is the set of all measurable subsets of K . The next step distribution is

$$P_u(\{u\}) = 1 - \frac{\text{vol}(K \cap (u + \delta B_n))}{\text{vol}(\delta B_n)}$$

and for any measurable subset A ,

$$P_u(A) = \frac{\text{vol}(A \cap (u + \delta B_n))}{\text{vol}(\delta B_n)} + 1_{u \in A}(u)P_u(\{u\})$$

The uniform distribution is stationary, i.e., $Q(A) = \frac{\text{vol}(A)}{\text{vol}(K)}$.

The *ergodic flow* of a subset A w.r.t. the distribution Q is defined as

$$\Phi(A) = \int_A P_u(K \setminus A) dQ(u).$$

A distribution Q is stationary if and only if $\Phi(A) = \Phi(K \setminus A)$. The existence and uniqueness of the stationary distribution Q for general Markov chains is a subject on its own. One way to ensure uniqueness of a stationary distribution is to use *lazy* Markov chains. In a lazy version of a given Markov chain, at each step, with probability $1/2$, we do nothing; with the rest we take a step according to the Markov chain. The next theorem is folklore.

Exercise 10.2. If Q is stationary w.r.t. a lazy ergodic Markov chain, then it is the unique stationary distribution for that Markov chain.

Informally, the mixing rate of a random walk is the number of steps required to reduce some measure of the distance of the current distribution to the stationary distribution by a constant factor. The following notions will be useful for comparing two distributions P, Q .

1. Total variation distance is $d_{tv}(P, Q) = \sup_{A \in \mathcal{A}} |P(A) - Q(A)|$.
2. L_2 or χ^2 -distance of P with respect to Q is

$$\chi^2(P, Q) = \int_K \left(\frac{dP(u)}{dQ(u)} - 1 \right)^2 dQ(u) = \int_K \left(\frac{dP(u)}{dQ(u)} \right)^2 dQ(u) - 1 = \int_K \frac{dP(u)}{dQ(u)} dP(u) - 1.$$

3. Warmth: P is said to be M -warm w.r.t. Q if $M = \sup_{A \in \mathcal{A}} \frac{P(A)}{Q(A)}$.

Convergence via Conductance

Now we introduce an important tool to bound the rate of convergence of Q_t , the distribution after t steps to Q . Assume that Q is the unique stationary distribution. The *conductance* of a subset A is defined as

$$\phi(A) = \frac{\Phi(A)}{\min\{Q(A), Q(K \setminus A)\}}$$

and the conductance of the Markov chain is

$$\phi = \min_A \phi(A) = \min_{0 < Q(A) \leq \frac{1}{2}} \frac{\int_A P_u(K \setminus A) dQ(u)}{Q(A)}.$$

The *local* conductance of an element u is $\ell(u) = 1 - P_u(\{u\})$.

For any $0 \leq s < \frac{1}{2}$, the s -conductance of a Markov chain is defined as

$$\phi_s = \min_{A: s < Q(A) \leq \frac{1}{2}} \frac{\phi(A)}{Q(A) - s}.$$

Ideally we would like to show that $d(Q_t, Q)$, the distance between the distribution after t steps and the target Q is monotonically (and rapidly) decreasing. We consider

$$\sup_{A: Q(A)=x} Q_t(A) - Q(A)$$

for each $x \in [0, 1]$. To prove inductively that this quantity decreases, Let \mathcal{G}_x be the set of functions defined as

$$\mathcal{G}_x = \left\{ g : K \rightarrow [0, 1] : \int_{u \in K} g(u) dQ(u) = x \right\}.$$

Using this, define

$$h_t(x) = \sup_{g \in \mathcal{G}_x} \int_{u \in K} g(u) (dQ_t(u) - dQ(u)) = \sup_{g \in \mathcal{G}_x} \int_{u \in K} g(u) dQ_t(u) - x.$$

This function is strongly concave.

Exercise 10.3. Show that the function h_t is concave, and if Q is atom-free, then $h_t(x) = \sup_{A: Q(A)=x} Q_t(A) - Q(A)$ and the supremum is achieved by some subset.

If the target density Q has atoms, i.e., points of positive probability, then the function g achieving h might have a fractional value at one atom.

Lemma 10.4. Let Q be atom-free and $t \geq 1$. For any $0 \leq x \leq 1$, let $y = \min\{x, 1 - x\}$. Then,

$$h_t(x) \leq \frac{1}{2} h_{t-1}(x - 2\phi y) + \frac{1}{2} h_{t-1}(x + 2\phi y).$$

Proof. Assume that $0 \leq x \leq \frac{1}{2}$. We construct two functions, g_1 and g_2 , and use these to bound $h_t(x)$. Let A be a subset that achieves $h_t(x)$. Define

$$g_1(u) = \begin{cases} 2P_u(A) - 1 & \text{if } u \in A, \\ 0 & \text{if } u \notin A, \end{cases} \quad \text{and} \quad g_2(u) = \begin{cases} 1 & \text{if } u \in A, \\ 2P_u(A) & \text{if } u \notin A. \end{cases}$$

Note that $\frac{1}{2}(g_1 + g_2)(u) = P_u(A)$ for all $u \in K$, which means that

$$\frac{1}{2} \int_{u \in K} g_1(u) dQ_{t-1}(u) + \frac{1}{2} \int_{u \in K} g_2(u) dQ_{t-1}(u) = \int_{u \in K} P_u(A) dQ_{t-1}(u) = Q_t(A).$$

Since the walk is lazy, $P_u(A) \geq \frac{1}{2}$ iff $u \in A$, the range of the functions g_1, g_2 is $[0, 1]$. We let

$$x_1 = \int_{u \in K} g_1(u) dQ(u) \quad \text{and} \quad x_2 = \int_{u \in K} g_2(u) dQ(u),$$

then $g_1 \in \mathcal{G}_{x_1}$ and $g_2 \in \mathcal{G}_{x_2}$. Moreover,

$$\frac{1}{2}(x_1 + x_2) = \frac{1}{2} \int_{u \in K} g_1(u) dQ(u) + \frac{1}{2} \int_{u \in K} g_2(u) dQ(u) = \int_{u \in K} P_u(A) dQ(u) = Q(A) = x.$$

since Q is stationary.

$$\begin{aligned} h_t(x) &= Q_t(A) - Q(A) \\ &= \frac{1}{2} \int_{u \in K} g_1(u) dQ_{t-1}(u) + \frac{1}{2} \int_{u \in K} g_2(u) dQ_{t-1}(u) - Q(A) \\ &= \frac{1}{2} \int_{u \in K} g_1(u) (dQ_{t-1}(u) - dQ(u)) + \frac{1}{2} \int_{u \in K} g_2(u) (dQ_{t-1}(u) - dQ(u)) \\ &\leq \frac{1}{2} h_{t-1}(x_1) + \frac{1}{2} h_{t-1}(x_2). \end{aligned}$$

Next,

$$\begin{aligned}
x_1 &= \int_{u \in K} g_1(u) dQ(u) \\
&= 2 \int_{u \in A} P_u(A) dQ(u) - \int_{u \in A} dQ(u) \\
&= 2 \int_{u \in A} (1 - P_u(K \setminus A)) dQ(u) - x \\
&= x - 2 \int_{u \in A} P_u(K \setminus A) dQ(u) \\
&= x - 2\Phi(A) \\
&\leq x - 2\phi x \\
&= x(1 - 2\phi).
\end{aligned}$$

Thus we have, $x_1 \leq x(1 - 2\phi) \leq x \leq x(1 + 2\phi) \leq x_2$. Since h_{t-1} is concave, the chord from x_1 to x_2 on h_{t-1} lies below the chord from $[x(1 - 2\phi), x(1 + 2\phi)]$. Therefore,

$$h_t(x) \leq \frac{1}{2}h_{t-1}(x(1 - 2\phi)) + \frac{1}{2}h_{t-1}(x(1 + 2\phi)).$$

□

A proof along the same lines implies the following generalization.

Lemma 10.5. *Let Q be atom-free and $0 \leq s \leq 1$. For any $s \leq x \leq 1 - s$, let $y = \min\{x - s, 1 - x - s\}$. Then for any integer $t > 0$,*

$$h_t(x) \leq \frac{1}{2}h_{t-1}(x - 2\phi_s y) + \frac{1}{2}h_{t-1}(x + 2\phi_s y).$$

These results can be extended to the case when Q has atoms with slightly weaker bounds [52].

Theorem 10.6. *Let $0 \leq s \leq 1$ and C_0 and C_1 be such that*

$$h_0(x) \leq C_0 + C_1 \min\{\sqrt{x - s}, \sqrt{1 - x - s}\}.$$

Then

$$h_t(x) \leq C_0 + C_1 \min\{\sqrt{x - s}, \sqrt{1 - x - s}\} \left(1 - \frac{\phi_s^2}{2}\right)^t.$$

The proof is by induction on t .

Corollary 10.7. *We have*

1. *Let $M = \sup_A Q_0(A)/Q(A)$. Then,*

$$d_{TV}(Q_t, Q) \leq \sqrt{M} \left(1 - \frac{\phi^2}{2}\right)^t.$$

2. *Let $0 < s \leq \frac{1}{2}$ and $H_s = \sup\{|Q_0(A) - Q(A)| : Q(A) \leq s\}$. Then,*

$$d_{TV}(Q_t, Q) \leq H_s + \frac{H_s}{s} \left(1 - \frac{\phi_s^2}{2}\right)^t.$$

3. *Let $M = \chi^2(Q_0, Q)$. Then for any $\varepsilon > 0$,*

$$d_{TV}(Q_t, Q) \leq \varepsilon + \sqrt{\frac{M}{\varepsilon}} \left(1 - \frac{\phi^2}{2}\right)^t.$$

Convergence via Log-Sobolev

For a warm start, the convergence rate established by conductance is asymptotically optimal in many cases of interest, including the ball walk for convex body. However, when the starting distribution is more focused, e.g., a single point, then there is a significant starting penalty usually a factor of the dimension or larger. One way to avoid this is to observe that the conductance of smaller subsets is in fact even higher and that one does not need to pay this large starting penalty. A classical technique in this regard is the log-Sobolev constant. For a Markov chain with stationary density Q and transition operator P , we can define it as follows.

$$\rho = \inf_{g: \text{smooth}, \int g(x)^2 dQ(x) = 1} \frac{\int_{x,y \in K} (f(x) - f(y))^2 P(x,y) dQ(x)}{\int f(x)^2 \log f(x)^2 dQ(x)}.$$

This parameter allows us to show convergence of the current distribution to the target in relative entropy. Recall that the relative entropy of a distribution P with respect to a distribution Q is

$$H_Q(P) = \int_K P(x) \log \frac{P(x)}{Q(x)} dQ(x).$$

Theorem 10.8. *For a Markov chain with distribution Q_t at time t , and log-Sobolev parameter ρ , we have*

$$H_Q(Q_t) \leq e^{-2\rho t} H_Q(Q_0).$$

■ 10.2 Conductance of the Ball Walk

In the section we bound the conductance of the ball walk when applied to the indicator function of a convex body. At first glance, the ball walk is not an efficient algorithm, even for uniformly sampling a convex body. The reason is simply that the local conductance could be exponentially small (consider a point close to the vertex of a polyhedron). We can get around this in two ways. The first, which is simpler, but less efficient is to “smoothen” the convex body by taking the Minkowski sum with a small Euclidean ball, i.e., replace K with $K + \alpha B^n$.

Exercise 10.9. Let K be a convex body in \mathbb{R}^n containing the unit ball. Show that (a) $\text{vol}(K + \alpha B^n) \leq (1 + \alpha)^n \text{vol}(K)$ and (b) with $\delta = \alpha/\sqrt{n}$ the local conductance of every point in $K + \alpha B^n$ is at least an absolute constant.

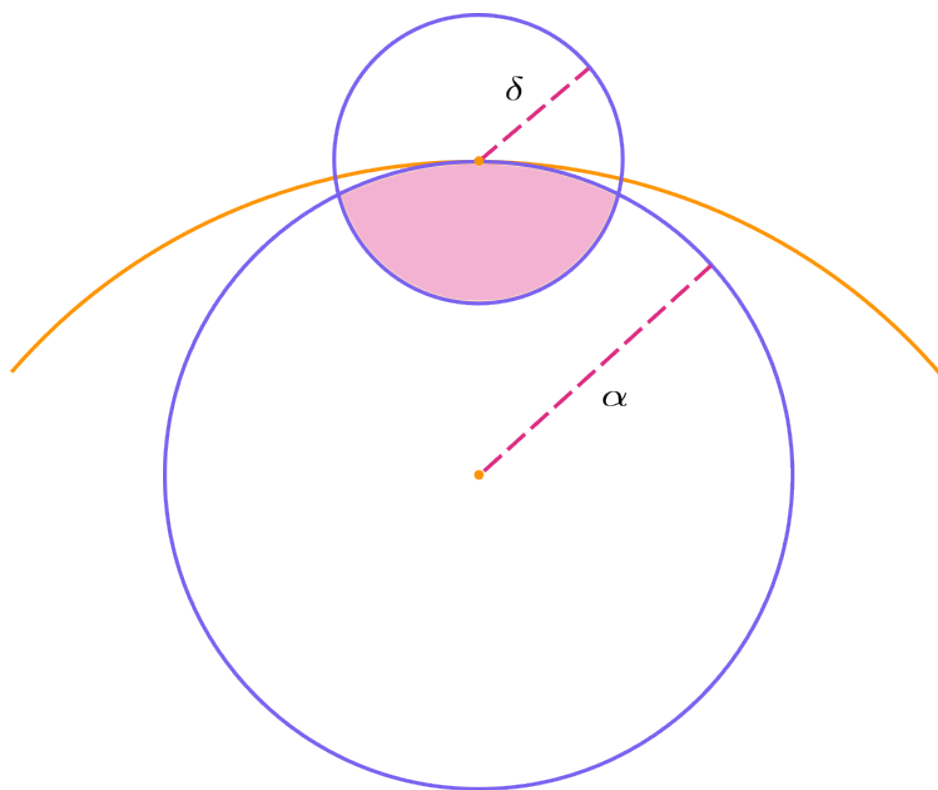
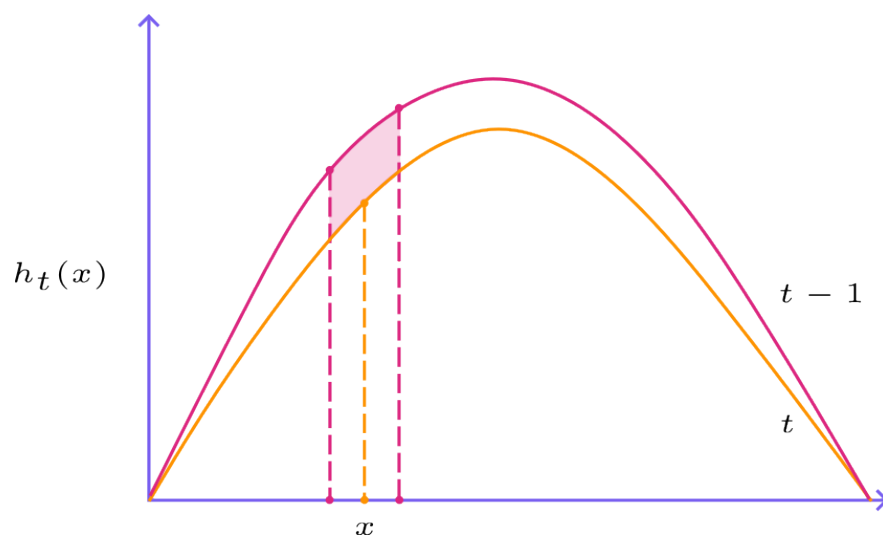
Using the exercise, it suffices to set $\alpha = 1/n$, so that a sample from $K + \alpha B^n$ has a large probability of being in K and then $\delta = 1/n^{3/2}$.

The second approach is to show that the local conductance is in fact large almost everywhere, and if the starting distribution is “warm” then these points can effectively be ignored. This will allow us to make δ much larger, namely $\delta = 1/\sqrt{n}$. Larger step sizes should allow us to prove faster mixing.

To convey the main ideas of the analysis, we focus on the first approach here. The goal is to show that the conductance of any subset is large, i.e., the probability of crossing over in one step is at least proportional to the measure of the set or its complement, whichever is smaller. First, we argue that the one-step distributions of two points will have a significant overlap if the points are sufficient close.

Lemma 10.10 (One-step overlap). *Let $u, v \in K$ s.t. $\ell(u), \ell(v) \geq \ell$ and $\|u - v\| \leq \frac{t\delta}{\sqrt{n}}$. Then the one-step distributions from them satisfy $d_{TV}(P_u, P_v) \leq 1 + t - \ell$.*

Proof. First assume that $\ell = 1$. This means that the balls of radius δ centered at u and v are fully contained in K . The TV distance between these distributions is bounded by $\text{vol}(u + \delta B^n \setminus v + \delta B^n) = \text{vol}(v + \delta B^n \setminus u + \delta B^n)$ divided by $\text{vol}(\delta B^n)$. This is exactly the volume of a band of thickness $\|u - v\|$ centered at the center of δB^n (see Fig.). This has relative volume at most t , proving the lemma under the assumption that $\ell = 1$. For the general case, we note that when the balls are intersected with a convex body, the increase in the TV distance is at most the probability that there is no proper move at u (or v), i.e., $1 - \ell$. This completes the proof. □



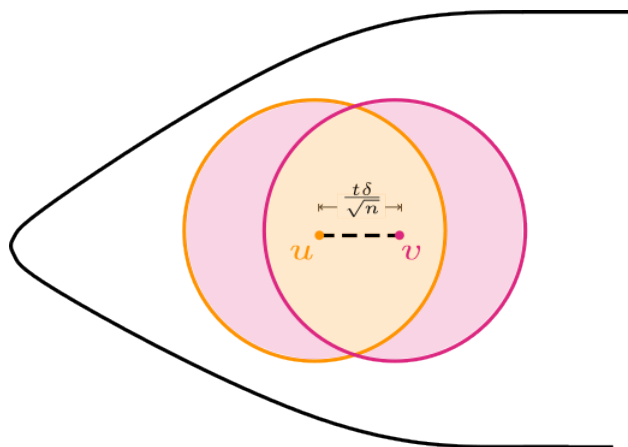


Figure 10.1: One-step overlap fully contained in K

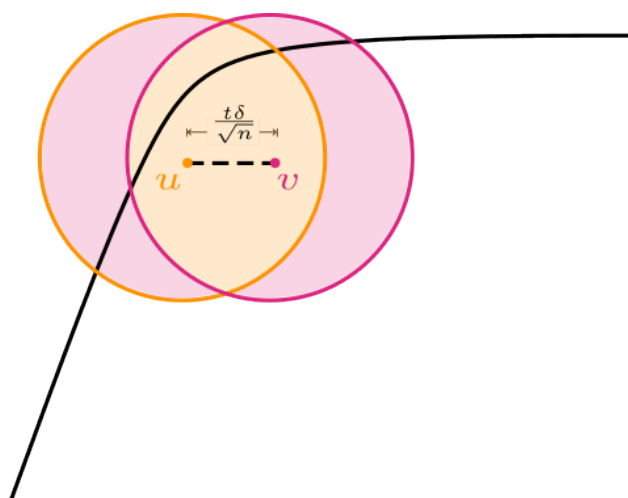


Figure 10.2: One-step overlap intersected by K

Setting $t = \ell/2$, this says that if the total variation distance between the one-step distributions from u, v is greater than $1 - \ell/2$, then the distance between them is at least $\frac{\ell\delta}{2\sqrt{n}}$. What this effectively says is that points close to the internal boundary of a subset are likely to cross over to the other side. To complete a proof we would need to show that the internal boundary of any subset is large if the subset (or its complement) is large, a purely geometric property.

Theorem 10.11 (Isoperimetry). *Let S_1, S_2, S_3 be a partition of a convex body K of diameter D . Then,*

$$\text{vol}(S_3) \geq \frac{2}{D} d(S_1, S_2) \min\{\text{vol}(S_1), \text{vol}(S_2)\}.$$

This can be generalized to any logconcave measure. We will discuss this and other extensions in detail later. But first we bound the conductance.

Theorem 10.12. *Let K be a convex body in \mathbb{R}^n of diameter D containing the unit ball and with every $u \in K$ having $\ell(u) \geq \ell$. Then the conductance of the ball walk on K with step size δ is*

$$\Omega\left(\frac{\ell^2\delta}{\sqrt{n}D}\right).$$

Proof. Let $K = S_1 \cup S_2$ be a partition into measurable sets. We will prove that

$$\int_{S_1} P_x(S_2) dx \geq \frac{\ell^2\delta}{16\sqrt{n}D} \min\{\text{vol}(S_1), \text{vol}(S_2)\} \quad (10.1)$$

Note that since the uniform distribution is stationary,

$$\int_{S_1} P_x(S_2) dx = \int_{S_2} P_x(S_1) dx.$$

Consider the points that are “deep” inside these sets, i.e., unlikely to jump out of the set:

$$S'_1 = \left\{x \in S_1 : P_x(S_2) < \frac{\ell}{4}\right\} \text{ and } S'_2 = \left\{x \in S_2 : P_x(S_1) < \frac{\ell}{4}\right\}.$$

Let S'_3 be the rest i.e., $S'_3 = K \setminus S'_1 \setminus S'_2$.

Suppose $\text{vol}(S'_1) < \text{vol}(S_1)/2$. Then

$$\int_{S_1} P_x(S_2) dx \geq \frac{\ell}{4} \text{vol}(S_1 \setminus S'_1) \geq \frac{\ell}{8} \text{vol}(S_1)$$

which proves (10.1).

So we can assume that $\text{vol}(S'_1) \geq \text{vol}(S_1)/2$ and similarly $\text{vol}(S'_2) \geq \text{vol}(S_2)/2$. Now, for any $u \in S'_1$ and $v \in S'_2$,

$$\|P_u - P_v\|_{tv} \geq 1 - P_u(S_2) - P_v(S_1) > 1 - \frac{\ell}{2}.$$

Applying Lemma 10.10 with $t = \ell/2$, we get that

$$|u - v| \geq \frac{\ell\delta}{2\sqrt{n}}.$$

Thus $d(S_1, S_2) \geq \ell\delta/2\sqrt{n}$. Applying Theorem 10.11 to the partition S'_1, S'_2, S'_3 , we have

$$\begin{aligned} \text{vol}(S'_3) &\geq \frac{\ell\delta}{\sqrt{n}D} \min\{\text{vol}(S'_1), \text{vol}(S'_2)\} \\ &\geq \frac{\ell\delta}{2\sqrt{n}D} \min\{\text{vol}(S_1), \text{vol}(S_2)\}. \end{aligned}$$

We can now prove (10.1) as follows:

$$\begin{aligned}
 \int_{S_1} P_x(S_2) dx &= \frac{1}{2} \int_{S_1} P_x(S_2) dx + \frac{1}{2} \int_{S_2} P_x(S_1) dx \\
 &\geq \frac{1}{2} \text{vol}(S'_3) \frac{\ell}{4} \\
 &\geq \frac{\ell^2 \delta}{16\sqrt{n}D} \min\{\text{vol}(S_1), \text{vol}(S_2)\}.
 \end{aligned}$$

□

Corollary 10.13. *The ball walk in a convex body with local conductance at least ℓ everywhere has mixing rate $O(nD^2\delta^2/\ell^4)$.*

Using the construction above of adding a small ball to every point of K gives a lower bound of $\delta = 1/n^{3/2}$ and $\ell = \Omega(1)$ and thus a polynomial bound of $O(n^4D^2)$ on the mixing time. As we will see presently, this can be improved to n^2D^2 by avoiding the blow-up, and analyzing the *average* local conductance. The example of starting near a corner (say of a hypercube) shows that this cannot work in general; however, from a *warm* start, it will suffice to bound the average local conductance rather than the minimum.

Warm Start and s -Conductance

In this section we give a better bound for the conductance of sufficiently large subsets resulting in the following bound on the mixing rate of the ball walk.

Theorem 10.14. *From a warm start, the ball walk in a convex body of diameter D containing a unit ball has a mixing rate of $O(n^2D^2)$ steps.*

This is based on two ideas: (1) most points of a convex body containing a unit ball have large local conductance and we can use $\delta = 1/\sqrt{n}$ instead of $1/n^{3/2}$, (2) the s -conductance is large and hence the walk mixes from a suitably warm start.

Lemma 10.15. *Let K be a convex body containing a unit ball. For the ball walk with δ step size, let $K_\delta = \{u \in K : \ell(u) \geq \frac{3}{4}\}$. Then K_δ is a convex set and $\text{vol}(K_\delta) \geq (1 - 2\delta\sqrt{n})\text{vol}(K)$.*

Exercise 10.16. Prove the first part of the previous lemma.

The proof of the above lemma will use the following bound on crossing the boundary of K .

Lemma 10.17. *Let L be any measurable subset of the boundary of a convex body K and $S_L = \{(x, y) : x \in K, y \notin K, \|x - y\| \leq \delta\}$. Then, we have*

$$\text{vol}_{2n}(S_L) \leq \frac{\delta}{(n+1)} \frac{\text{vol}(B^{n-1})}{\text{vol}(B^n)} \text{vol}_{n-1}(L) \text{vol}(\delta B^n).$$

Proof. It suffices to consider the case when L is infinitesimally small; and then we can assume that the surface of K is locally a hyperplane and compute the measure of S_L explicitly. □

Theorem 10.18. *The s -conductance of the ball walk with $\delta = \frac{s}{4\sqrt{n}}$ step size in a convex body K of diameter D and containing the unit ball satisfies*

$$\phi_s \gtrsim \frac{s}{nD}.$$

This proof is similar to that of Theorem 10.12, with one important extension. Rather than applying the argument to a partition of the original convex body K , we restrict the argument to K_δ , the points in K that have high local conductance. Since this subset takes up most of K , and is convex, we will be able to use its isoperimetry to lower bound the conductance.

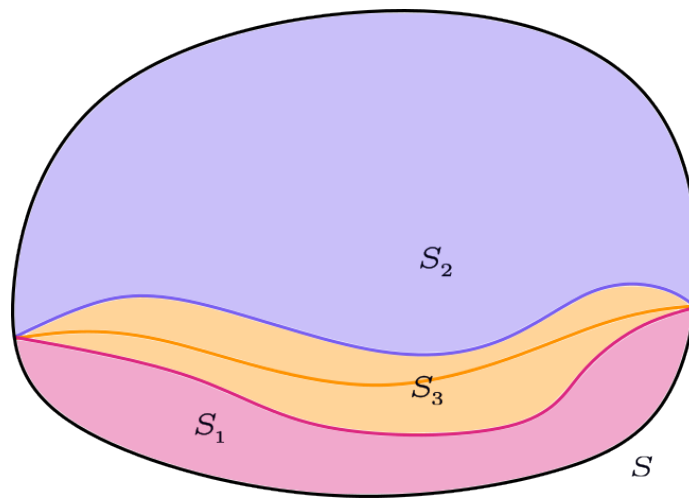
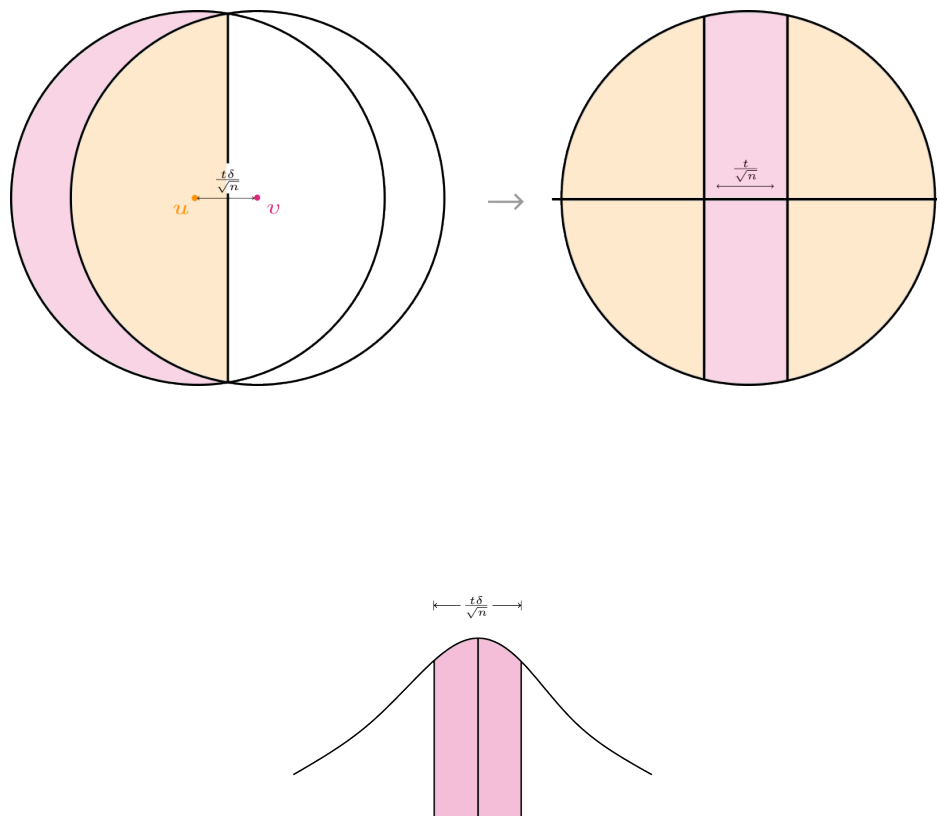


Figure 10.3: Partitions of convex body



Proof. As before, we consider the following partition of K . Let $K = S_1 \cup S_2$ be a partition into measurable sets. We will prove that

$$\int_{S_1} P_x(S_2) dx \geq \frac{\delta}{C\sqrt{n}D} \min\{\text{vol}(S_1) - \frac{s}{2}, \text{vol}(S_2) - \frac{s}{2}\} \quad (10.2)$$

Since the uniform distribution is stationary,

$$\int_{S_1} P_x(S_2) dx = \int_{S_2} P_x(S_1) dx.$$

Consider the points that are “deep” inside these sets:

$$S'_1 = \left\{x \in S_1 : P_x(S_2) < \frac{1}{8}\right\} \text{ and } S'_2 = \left\{x \in S_2 : P_x(S_1) < \frac{1}{8}\right\}.$$

Let S'_3 be the rest i.e., $S'_3 = K \setminus S'_1 \setminus S'_2$. Recall that

$$K_\delta = \left\{x \in K : \ell(x) \geq \frac{3}{4}\right\}$$

and define $S''_i = S'_i \cap K_\delta$. Note that by Lemma 10.15, for $\delta \leq s/(4\sqrt{n})$,

$$\text{vol}(S''_i) \geq \text{vol}(S'_i) - s.$$

Suppose $\text{vol}(S''_1) < \text{vol}(S_1 \cap K_\delta)/2$. Then

$$\int_{S_1} P_x(S_2) dx \geq \frac{1}{8} \text{vol}(S_1 \cap K_\delta \setminus S''_1) \geq \frac{1}{16} \text{vol}(S_1 \cap K_\delta) \geq \frac{1}{16} \left(\text{vol}(S_1) - \frac{s}{2}\right)$$

which proves (10.2).

So we can assume that $\text{vol}(S''_1) \geq \text{vol}(S_1 \cap K_\delta)/2$ and similarly $\text{vol}(S''_2) \geq \text{vol}(S_2 \cap K_\delta)/2$. Now, for any $u \in S''_1$ and $v \in S''_2$,

$$d_{TV}(P_u, P_v) \geq 1 - P_u(S_2) - P_v(S_1) > 1 - \frac{1}{4}.$$

Applying Lemma 10.10 with $t = 3/8$, we get that

$$|u - v| \geq \frac{3\delta}{8\sqrt{n}}.$$

Thus $d(S''_1, S''_2) \geq 3\delta/(8\sqrt{n})$. Applying Theorem 10.11 to the partition S''_1, S''_2, S''_3 of K_δ , we have

$$\begin{aligned} \text{vol}(S''_3) &\geq \frac{3\delta}{4\sqrt{n}D} \min\{\text{vol}(S''_1), \text{vol}(S''_2)\} \\ &\geq \frac{3\delta}{8\sqrt{n}D} \min\{\text{vol}(S_1) - \frac{s}{2}, \text{vol}(S_2) - \frac{s}{2}\}. \end{aligned}$$

We can now prove (10.2) as follows:

$$\begin{aligned} \int_{S_1} P_x(S_2) dx &= \frac{1}{2} \int_{S_1} P_x(S_2) dx + \frac{1}{2} \int_{S_2} P_x(S_1) dx \\ &\geq \frac{1}{2} \text{vol}(S''_3) \cdot \frac{1}{8} \\ &\geq \frac{3\delta}{128\sqrt{n}D} \min\{\text{vol}(S_1), \text{vol}(S_2)\} \end{aligned}$$

which implies that the conductance is at least $3s/(512nD)$. □

The mixing rate then follows by applying Theorem 10.6 and Corollary 10.7.

Tightness of the bound

The mixing rate of $O(n^2 D^2)$ for the ball walk is in fact the best possible even from a warm start (with the assumption of a unit ball inside the convex body and diameter D). To see this, consider a cylinder whose cross-section is a unit ball and axis is $[0, D]$ along e_1 . Suppose the starting distribution is uniform in the part of the cylinder in $[0, D/3]$. Then we claim that to reach the opposite third of the cylinder needs $\Omega(n^2 D^2)$ steps with high probability. Each step has length at most δ in a random direction, and this is about δ/\sqrt{n} along e_1 . Viewing this as an unbiased random walk along e_1 , the effective diameter is $D/(\delta/\sqrt{n})$ and hence the number of steps to cross an interval of length $D/3$ is $\Omega(n D^2 / \delta^2) = \Omega(n^2 D^2)$.

Exercise 10.19. Prove the above claim rigorously.

Speedy walk

In the above analysis of the ball walk, the dependence on the error parameter ε , the distance to the target distribution, is polynomial in $1/\varepsilon$ rather than its logarithm. The speedy walk is a way to improve the analysis. In the speedy walk, at a point x , we sample the next step uniformly from the intersection of $(x + \delta B^n) \cap K$. The resulting Markov chain is the subsequence of *proper* steps of the ball walk.

Exercise 10.20. Show that the stationary density of the speedy walk in a convex body is proportional to the local conductance.

Theorem 10.21. *The conductance of the speedy walk is $\Omega(1/nD)$.*

To analyze the ball walk, we then need to show that the number of “wasted” steps is not too many. This follows from the assumption of a warm start and Lemma 10.15.

■ 10.3 Generating a warm start

To get the mixing rate of $O(n^2 D^2)$, we need a warm start, i.e., a distribution whose density at any point is within $O(1)$ of the target density.

Algorithm 28: Warm Start

```

Input: membership oracle for  $K$  s.t.  $B^n \subseteq K \subseteq DB^n$ .
Let  $x$  be a random point in  $B^n$ . Define  $K_i = 2^{i/n} B^n \cap K$ .
for  $i = 1, \dots, n \log D$  do
    | 1. Use ball walk from  $x$  to generate random point  $y$  in  $K_i$ .
    | 2. Set  $x = y$ .
end
return  $x$ .

```

Since $K_{i+1} \subseteq 2^{1/n} K_i$, we have $\text{vol}(K_{i+1}) \leq 2 \text{vol}(K_i)$ and hence a 2-warm start is maintained. Once we have a random point from K , subsequent random points can be generated by simply continuing the ball walk; thus the cost of the warm start is only for the first sample.

■ 10.4 Isotropic Transformation

The complexity of sampling with the ball walk is polynomial in n, D and $\log(1/\varepsilon)$ to get within ε of the target density. This is not a polynomial algorithm since the dependence is on D and not $\log D$. To get a polynomial algorithm, we need one more ingredient.

We say that a distribution Q is *isotropic* if $\mathbf{E}_Q(x) = 0$ and $\mathbf{E}_Q(xx^T) = I$, i.e., the mean is zero and the covariance matrix (exists and) is the identity. We say that the distribution is C -isotropic if the eigenvalues of its covariance matrix are in $[\frac{1}{C}, C]$. An affine transformation is said to be an *isotropic transformation* if the resulting distribution is isotropic.

Any distribution with bounded second moments has an isotropic transformation. It is clear that satisfying the first condition is merely a translation, so assume the mean is zero. For the second, suppose the covariance matrix is $\mathbf{E}_Q(xx^T) = A$. Then consider $y = A^{-1/2}x$. It is easy to see that

$$\mathbf{E}(yy^T) = A^{-1/2}\mathbf{E}(xx^T)A^{-1/2} = I.$$

For convex bodies, isotropic position comes with a strong guarantee.

Theorem 10.22. *For a convex body in isotropic position (i.e., the uniform distribution over the body is isotropic), we have*

$$\sqrt{\frac{n+2}{n}}B^n \subseteq K \subseteq \sqrt{n(n+2)}B^n.$$

Thus the effective diameter is $O(n)$. If we could place a convex body in isotropic position before sampling, we would have a $\text{poly}(n)$ algorithm. In fact, it is even better than this as most points are within distance $O(\sqrt{n})$ of the center of gravity. We quote a theorem due to Paouris.

Theorem 10.23. *For an isotropic logconcave density p in \mathbb{R}^n and any $t \geq 1$,*

$$\Pr_p(\|x\| \geq ct\sqrt{n}) \leq e^{-t\sqrt{n}}.$$

How to compute an isotropic transformation? This is easy, from the definition, all we need is to estimate its covariance matrix, which can be done from random samples. Thus, if we could sample K , we can compute an isotropic transformation for it. This appears cyclic – we need isotropy for efficient sampling and efficient sampling for isotropy. The solution is simply to bootstrap them.

Algorithm 29: IsotropicTransform

Input: membership oracle for K s.t. $B^n \subseteq K \subseteq DB^n$.

Let x be a random point in B^n , $A = I$ and $K_i = 2^{i/n}B^n \cap K$.

for $i = 1, \dots, n \log D$ **do**

1. Use the ball walk from x to generate N random points $x_1 \dots x_N$ in AK_i .
2. Compute $C = \frac{1}{N} \sum_{i=1}^N x_i x_i^T$ and set $A = C^{-1/2}A$.
3. Set $x = x_N$.

end

return x .

We will choose N large enough so that after the transformation K_i is 2-isotropic and therefore K_{i+1} is 6-isotropic. We can bound N as follows.

Exercise 10.24. Show that if K is isotropic, then with $N = O(n^2)$, the matrix $A = \frac{1}{N} \sum_{i=1}^N x_i x_i^T$ for N random samples from K satisfies $\|A - I\|_{\text{op}} \leq 0.5$.

A tight bound on the sample complexity was established by [1] (see also [11, 63, 68]).

Theorem 10.25. *For an isotropic logconcave distribution Q in \mathbb{R}^n , the covariance $N = O(n)$ random samples satisfies $\|A - I\|_{\text{op}} \leq 0.5$.*

Thus the overall algorithm needs $O(n \log D)$ phases, with $O(n)$ samples in each phase from a near-isotropic distribution, and thus $\text{poly}(n)$ steps per sample.

■ 10.5 Isoperimetry via localization

Theorem 10.11 was refined by KLS [32] as follows (we state it here for logconcave densities).

Theorem 10.26. *For any partition S_1, S_2, S_3 of \mathbb{R}^n , and any logconcave measure μ in \mathbb{R}^n ,*

$$\mu(S_3) \geq \frac{\ln 2}{\mathbf{E}_\mu(\|x - \bar{x}\|)} \min\{\mu(S_1), \mu(S_2)\}.$$

Thus, for a (near-)isotropic distribution, the diameter can be replaced by $O(\sqrt{n})$ and this gives a bound of $O(n^3)$ from a warm start. One way to summarize the analysis so far is that the complexity of sampling a convex body (and in fact a logconcave density) from a warm start is $O^*(n^2/\psi^2)$ where ψ is the isoperimetric ratio of the convex body. In other words, the expansion of the Markov chain reduces to the expansion of the target logconcave density. It then becomes a natural question to find the best possible estimate for the isoperimetric ratio. KLS also provided a conjecture for this.

Conjecture 10.27. *The isoperimetric ratio of any isotropic logconcave density in \mathbb{R}^n is $\Omega(1)$.*

The bound of the conjecture holds for all halfspace induced subsets. So the conjecture says that the worst isoperimetry is achieved up to a constant factor by a halfspace (this version does not need isotropic position). Here we discuss a powerful technique for proving such inequalities.

Classical proofs of isoperimetry for special distributions are based on different types of symmetrization that effectively identify the extremal subsets. Bounding the Cheeger constant for general convex bodies and logconcave densities is more complicated since the extremal sets can be nonlinear and hard to describe precisely, due to the trade-off between minimizing the boundary measure of a subset and utilizing as much of the “external” boundary as possible. The main technique to prove bounds in the general setting has been *localization*, a method to reduce inequalities in high dimension to inequalities in one dimension. We now describe this technique with a few applications.

■ 10.5.1 Localization

We will sketch a proof of the following theorem to illustrate the use of localization. This theorem was also proved by Karzanov and Khachiyan [35] using a different, more direct approach.

Theorem 10.28 ([22, 49, 35]). *Let f be a logconcave function whose support has diameter D and let π_f be the induced measure. Then for any partition of \mathbb{R}^n into measurable sets S_1, S_2, S_3 ,*

$$\pi_f(S_3) \geq \frac{2d(S_1, S_2)}{D} \min\{\pi_f(S_1), \pi_f(S_2)\}.$$

Before discussing the proof, we note that there is a variant of this result in the Riemannian setting.

Theorem 10.29 ([46]). *If $K \subset (M, g)$ is a locally convex bounded domain with smooth boundary, diameter D and $\text{Ric}_g \geq 0$, then the Poincaré constant is at least $\frac{\pi^2}{4D^2}$, i.e., for any g with $\int g = 0$, we have that*

$$\int |\nabla g(x)|^2 dx \geq \frac{\pi^2}{4D^2} \int g(x)^2 dx.$$

For the case of convex bodies in \mathbb{R}^n , this result is equivalent to Theorem 10.28 up to a constant. One benefit of localization is that it does not require a carefully crafted potential. Localization has recently been generalized to Riemannian setting [39]. The origins of this method were in a paper by Payne and Weinberger [61].

We begin the proof of Theorem 10.28. For a proof by contradiction, let us assume the converse of its conclusion, i.e., for some partition S_1, S_2, S_3 of \mathbb{R}^n and logconcave density f , assume that

$$\int_{S_3} f(x) dx < C \int_{S_1} f(x) dx \quad \text{and} \quad \int_{S_3} f(x) dx < C \int_{S_2} f(x) dx$$

where $C = 2d(S_1, S_2)/D$. This can be reformulated as

$$\int_{\mathbb{R}^n} g(x) dx > 0 \quad \text{and} \quad \int_{\mathbb{R}^n} h(x) dx > 0 \tag{10.3}$$

where

$$g(x) = \begin{cases} Cf(x) & \text{if } x \in S_1, \\ 0 & \text{if } x \in S_2, \\ -f(x) & \text{if } x \in S_3. \end{cases} \quad \text{and} \quad h(x) = \begin{cases} 0 & \text{if } x \in S_1, \\ Cf(x) & \text{if } x \in S_2, \\ -f(x) & \text{if } x \in S_3. \end{cases}$$

These inequalities are for functions in \mathbb{R}^n . The next lemma will help us analyze them.

Lemma 10.30 (Localization Lemma [32]). *Let $g, h : \mathbb{R}^n \rightarrow \mathbb{R}$ be lower semi-continuous integrable functions such that*

$$\int_{\mathbb{R}^n} g(x) dx > 0 \quad \text{and} \quad \int_{\mathbb{R}^n} h(x) dx > 0.$$

Then there exist two points $a, b \in \mathbb{R}^n$ and an affine function $\ell : [0, 1] \rightarrow \mathbb{R}_+$ such that

$$\int_0^1 \ell(t)^{n-1} g((1-t)a + tb) dt > 0 \quad \text{and} \quad \int_0^1 \ell(t)^{n-1} h((1-t)a + tb) dt > 0.$$

The points a, b represent an interval and one may think of $\ell(t)^{n-1}$ as proportional to the cross-sectional area of an infinitesimal cone. The lemma says that over this cone truncated at a and b , the integrals of g and h are positive. Also, without loss of generality, we can assume that a, b are in the union of the supports of g and h .

Proof outline. The main idea is the following. Let H be any halfspace such that

$$\int_H g(x) dx = \frac{1}{2} \int_{\mathbb{R}^n} g(x) dx.$$

Let us call this a bisecting halfspace. Now either

$$\int_H h(x) dx > 0 \quad \text{or} \quad \int_{\mathbb{R}^n \setminus H} h(x) dx > 0.$$

Thus, either H or its complementary halfspace will have positive integrals for both g and h , reducing the domain of the integrals from \mathbb{R}^n to a halfspace. If we could repeat this, we might hope to reduce the dimensionality of the domain. For any $(n-2)$ -dimensional affine subspace L , there is a bisecting halfspace containing L in its bounding hyperplane. To see this, let H be a halfspace containing L in its boundary. Rotating H about L we get a family of halfspaces with the same property. This family includes H' , the complementary halfspace of H . The function $\int_H g - \int_{\mathbb{R}^n \setminus H} g$ switches sign from H to H' . Since this is a continuous family, there must be a halfspace for which the function is zero.

If we take all $(n-2)$ -dimensional affine subspaces defined by $\{x \in \mathbb{R}^n : x_i = r_1, x_j = r_2\}$ where r_1, r_2 are rational, then the intersection of all the corresponding bisecting halfspaces is a line or a point (by choosing only rational values for x_i , we are considering a countable intersection). To see why it is a line or a point, assume we are left with a two or higher dimensional set. Since the intersection is convex, there is a point in its interior with at least two coordinates that are rational, say $x_1 = r_1$ and $x_2 = r_2$. But then there is a bisecting halfspace H that contains the affine subspace given by $x_1 = r_1, x_2 = r_2$ in its boundary, and so it properly partitions the current set.

Thus the limit of this bisection process is a function supported on an interval (which could be a single point), and since the function itself is a limit of convex sets (intersections of halfspaces) containing this interval, it is a limit of a sequence of concave functions and is itself concave, with positive integrals. Simplifying further from concave to linear takes quite a bit of work. For the full proof, we refer the reader to [50]. \square

Going back to the proof sketch of Theorem 10.28, we can apply the localization lemma to get an interval $[a, b]$ and an affine function ℓ such that

$$\int_0^1 \ell(t)^{n-1} g((1-t)a + tb) dt > 0 \quad \text{and} \quad \int_0^1 \ell(t)^{n-1} h((1-t)a + tb) dt > 0. \quad (10.4)$$

The functions g, h as we have defined them are not lower semi-continuous. However, this can be addressed by expanding S_1 and S_2 slightly so as to make them open sets, and making the support of f an open set. Since we are proving strict inequalities, these modifications do not affect the conclusion.

Let us partition $[0, 1]$ into Z_1, Z_2, Z_3 as follows:

$$Z_i = \{t \in [0, 1] : (1-t)a + tb \in S_i\}.$$

Note that for any pair of points $u \in Z_1, v \in Z_2$, $|u - v| \geq d(S_1, S_2)/D$. We can rewrite (10.4) as

$$\int_{Z_3} \ell(t)^{n-1} f((1-t)a + tb) dt < C \int_{Z_1} \ell(t)^{n-1} f((1-t)a + tb) dt$$

and

$$\int_{Z_3} \ell(t)^{n-1} f((1-t)a + tb) dt < C \int_{Z_2} \ell(t)^{n-1} f((1-t)a + tb) dt.$$

The functions f and $\ell(\cdot)^{n-1}$ are both logconcave, so $F(t) = \ell(t)^{n-1} f((1-t)a + tb)$ is also logconcave. We get,

$$\int_{Z_3} F(t) dt < C \min \left\{ \int_{Z_1} F(t) dt, \int_{Z_2} F(t) dt \right\}. \quad (10.5)$$

Now consider what Theorem 10.28 asserts for the function $F(t)$ over the interval $[0, 1]$ and the partition Z_1, Z_2, Z_3 :

$$\int_{Z_3} F(t) dt \geq 2d(Z_1, Z_2) \min \left\{ \int_{Z_1} F(t) dt, \int_{Z_2} F(t) dt \right\}. \quad (10.6)$$

We have substituted 1 for the diameter of the interval $[0, 1]$. Also, $2d(Z_1, Z_2) \geq 2d(S_1, S_2)/D = C$. Thus, Theorem 10.28 applied to the function $F(t)$ contradicts (10.5) and to prove the theorem in general, and it suffices to prove it in the one-dimensional case. A combinatorial argument reduces this to the case when each Z_i is a single interval. Proving the resulting inequality up to a factor of 2 is a simple exercise and uses only the unimodality of F . The improvement to the tight bound requires one-dimensional logconcavity. This completes the proof of Theorem 10.28.

The localization lemma has been used to prove a variety of isoperimetric inequalities. The next theorem is a refinement of Theorem 10.28, replacing the diameter by the square-root of the expected squared distance of a random point from the mean. For an isotropic distribution this is an improvement from n to \sqrt{n} . This theorem was proved by Kannan-Lovász-Simonovits in the same paper in which they proposed the KLS conjecture.

Theorem 10.31 ([32]). *For any logconcave density p in \mathbb{R}^n with covariance matrix A , the KLS constant satisfies*

$$\psi_p \gtrsim \frac{1}{\sqrt{\text{tr}(A)}}.$$

The next theorem shows that the KLS conjecture is true for an important family of distributions. The proof is again by localization [19], and the one-dimensional inequality obtained is a Brascamp-Lieb Theorem. We note that the same theorem can be obtained by other means [41, ?].

Theorem 10.32. *Let $h(x) = f(x)e^{-\frac{1}{2}x^\top Bx} / \int f(y)e^{-\frac{1}{2}y^\top By} dy$ where $f : \mathbb{R}^n \rightarrow \mathbb{R}_+$ is an integrable logconcave function and B is positive definite. Then h is logconcave and for any measurable subset S of \mathbb{R}^n ,*

$$\frac{h(\partial S)}{\min \{h(S), h(\mathbb{R}^n \setminus S)\}} \gtrsim \frac{1}{\|B^{-1}\|_{\text{op}}^{\frac{1}{2}}}.$$

In other words, the expansion of h is $\Omega(\|B^{-1}\|_{\text{op}}^{-\frac{1}{2}})$.

The analysis of the Gaussian Cooling algorithm for volume computation [20] uses localization.

Next we mention an application to the anti-concentration of polynomials. This is a corollary of a more general result by Carbery and Wright.

Theorem 10.33 ([14]). *Let q be a degree d polynomial in \mathbb{R}^n . Then for a convex body $K \subset \mathbb{R}^n$ of volume 1, any $\epsilon > 0$, and x drawn uniformly from K ,*

$$\Pr_{x \sim K} \left(|q(x)| \leq \epsilon \max_K |q(x)| \right) \lesssim \epsilon^{\frac{1}{d}} d$$

We conclude this section with a nice interpretation of the localization lemma by Fradelizi and Guedon. They also give a version that extends localization to multiple inequalities.

Theorem 10.34 (Reformulated Localization Lemma [27]). *Let K be a compact convex set in \mathbb{R}^n and f be an upper semi-continuous function. Let P_f be the set of logconcave distributions μ supported by K satisfying $\int f d\mu \geq 0$. The set of extreme points of $\text{conv} P_f$ is exactly:*

1. *the Dirac measure at points x such that $f(x) \geq 0$, or*
2. *the distributions v satisfies*
 - (a) *density function is of the form e^ℓ with linear ℓ ,*
 - (b) *support equals to a segment $[a, b] \subset K$,*
 - (c) *$\int f dv = 0$,*
 - (d) *$\int_a^x f dv > 0$ for $x \in (a, b)$ or $\int_x^b f dv > 0$ for $x \in (a, b)$.*

Since we know the maximizer of any convex function is at extreme points, this shows that one can optimize $\max_{\mu \in P_f} \Phi(\mu)$ for any convex Φ by checking Dirac measures and log-affine functions.

■ 10.6 Hit-and-Run

The ball walk does not mix rapidly from all starting points. While this hurdle can be overcome by starting with a deep point and carefully maintaining a warm start, it is natural to ask if there is a simple process that does truly mix rapidly from any starting point. Hit-and-Run satisfies this requirement.

Algorithm 30: Hit – and – Run

Input: starting point x_0 in a convex body K .
Repeat T times: at current point x ,
1. Pick a uniform random direction ℓ through x .
2. Go to uniform random point y on the chord of K induced by ℓ .
return x .

Since hit-and-run is a symmetric Markov chain, the uniform distribution on K is stationary for it. To sample from a general density proportional to $f(x)$, in Step 2, we sample y according to the density proportional to f restricted to the random line ℓ .

Next we give a formula for the next step distribution from a point u .

Lemma 10.35. *The next step distribution of Hit-and-Run from a point u is given by*

$$P_u(A) = \frac{2}{\text{vol}(S^{n-1})} \int_A \frac{dx}{\|x - u\|^{n-1} \ell(u, x)}$$

where A is any measurable subset of K and $\ell(u, x)$ is the length of the chord in K through u and x .

Exercise 10.36. Prove Lemma 10.35.

The main theorem of this section is the following [51].

Theorem 10.37. [51] *The conductance of Hit-and-Run in a convex body K containing the unit ball and of diameter D is $\Omega(1/nD)$.*

This implies a mixing time of $O(n^2 D^2 \log(M/\varepsilon))$ to get to within distance ε of the target density starting from an M -warm initial density. By taking one step from the initial point, we can bound M by $(D/d)^n$ where d is the minimum distance of the starting point from the boundary. Hence this gives a bound of $\tilde{O}(n^3 D^2)$ from any interior starting point.

The proof of the theorem follows the same high-level outline as that of the ball walk, needing two major ingredients, namely, one-step coupling and isoperimetry. Notably, the isoperimetry is for a non-Euclidean notion of distance. We begin with some suitable definitions.

Define the “median” step-size function F as the $F(x)$ such that

$$\Pr(\|x - y\| \leq F(x)) = \frac{1}{8}$$

where y is a random step from x .

We also need a non-Euclidean notion of distance, namely the classical cross-ratio distance. For points u, v in K , inducing a chord $[p, q]$ with these points in the order p, u, v, q , the cross-ratio distance is

$$d_K(u, v) = \frac{\|u - v\| \|p - q\|}{\|p - u\| \|v - q\|}.$$

It is related to the Hilbert distance (which is a true distance) as follows:

$$d_H(u, v) = \ln(1 + d_K(u, v)).$$

The first ingredient shows that if two points are close geometrically, then their next-step distributions have significant overlap.

Lemma 10.38. *For two points $u, v \in K$ with*

$$d_K(u, v) < \frac{1}{8} \text{ and } \|u - v\| \leq \frac{2}{\sqrt{n}} \max\{F(u), F(v)\}$$

we have $d_{TV}(P_u, P_v) < 1 - \frac{1}{500}$.

The second ingredient is an isoperimetric inequality (independent of any algorithm). The cross-ratio distance has a nice isoperimetry inequality.

Theorem 10.39. *For any partition S_1, S_2, S_3 of a convex body K ,*

$$\text{vol}(S_3) \geq d_K(S_1, S_2) \frac{\text{vol}(S_1)\text{vol}(S_2)}{\text{vol}(K)}.$$

However, this will not suffice to prove a bound on the conductance of all subsets. The reason is that we cannot guarantee a good lower bound on the *minimum* distance between subsets S_1, S_2 . Instead, we will need a weighted isoperimetric inequality, which uses an average distance.

Theorem 10.40. *Let S_1, S_2, S_3 be a partition of a convex body K . Let $h : K \rightarrow \mathbb{R}_+$ be a function s.t. for any $u \in S_1, v \in S_2$, and any x on the chord through u and v , we have*

$$h(x) \leq \frac{1}{3} \min\{1, d_K(u, v)\}.$$

Then,

$$\text{vol}(S_3) \geq \mathbf{E}_K(h(x)) \min\{\text{vol}(S_1), \text{vol}(S_2)\}.$$

For bounding the conductance, we will use a specific function h . To introduce it, we first define a step-size function $s(x)$:

$$s(x) = \sup \left\{ t : \frac{\text{vol}(x + tB^n \cap K)}{\text{vol}(tB^n)} \geq \gamma \right\}$$

for some fixed $\gamma \in (0, 1]$.

Exercise 10.41. Show that the step-size function is concave over any convex body.

We will need the following relationship between the step-size function and the median step function.

Lemma 10.42. *We have*

$$\mathbf{E}_K(s(x)) \geq \frac{1 - \gamma}{\sqrt{n}}.$$

Moreover, for $\gamma \geq 63/64$, we have $F(x) \geq s(x)/32$.

In the proof of Theorem 10.37, we will set $h(x) = \frac{s(x)}{48\sqrt{n}D}$. We are now ready for that proof.

Proof of Thm. 10.37. Let $K = S_1 \cup S_2$ be a partition of K into measurable sets. We will prove that

$$\int_{S_1} P_x(S_2) dx \geq \frac{c}{nD} \min\{\text{vol}(S_1), \text{vol}(S_2)\} \quad (10.7)$$

Note that since the uniform distribution is stationary,

$$\int_{S_1} P_x(S_2) dx = \int_{S_2} P_x(S_1) dx.$$

Consider the points that are “deep” inside these sets, i.e., unlikely to jump out of the set:

$$S'_1 = \left\{ x \in S_1 : P_x(S_2) < \frac{1}{1000} \right\} \text{ and } S'_2 = \left\{ x \in S_2 : P_x(S_1) < \frac{1}{1000} \right\}.$$

Let S'_3 be the rest i.e., $S'_3 = K \setminus S'_1 \setminus S'_2$.

Suppose $\text{vol}(S'_1) < \text{vol}(S_1)/2$. Then

$$\int_{S_1} P_x(S_2) dx \geq \frac{1}{1000} \text{vol}(S_1 \setminus S'_1) \geq \frac{1}{2000} \text{vol}(S_1)$$

which proves (10.7).

So we can assume that $\text{vol}(S'_1) \geq \text{vol}(S_1)/2$ and similarly $\text{vol}(S'_2) \geq \text{vol}(S_2)/2$. Now, for any $u \in S'_1$ and $v \in S'_2$,

$$d_{TV}(P_u, P_v) \geq 1 - P_u(S_2) - P_v(S_1) > 1 - \frac{1}{500}.$$

Applying Lemma 10.38, we get that that one of the following holds:

$$d_K(u, v) \geq \frac{1}{8} \text{ or } \|u - v\| \geq \frac{2}{\sqrt{n}} \max\{F(u), F(v)\}$$

We will now prove that Thm. 10.40 using $h(x) = \frac{s(x)}{48\sqrt{nD}}$ where $s(x)$ is defined with $\gamma = 63/64$. To see that this is a valid choice, first note that if $d_K(u, v) \geq \frac{1}{8}$, then we have $h(x) \leq d_K(u, v)/3$, as needed. So we can assume the second condition above holds. Next, noting that x is some point on the chord through u, v , let the endpoints of the chord be p, q . Suppose WLOG that $x \in [u, q]$. Then, by the concavity of $s(x)$, and using the second part of Lemma 10.42, we have,

$$\begin{aligned} s(x) &\leq \frac{|x - p|}{|u - p|} s(u) \\ &\leq 32 \frac{|x - p|}{|u - p|} F(u) \\ &\leq 16\sqrt{n} \frac{|x - p|}{|u - p|} |u - v| \\ &\leq 16d_K(u, v) \sqrt{nD} \end{aligned}$$

which again implies the desired condition on h .

Now, applying Theorem 10.40 to the partition S'_1, S'_2, S'_3 , and using the first part of Lemma 10.42, we have

$$\begin{aligned} \text{vol}(S'_3) &\geq \mathbf{E}_K(h(x)) \min\{\text{vol}(S'_1), \text{vol}(S'_2)\} \\ &\geq \frac{1}{4000nD} \min\{\text{vol}(S_1), \text{vol}(S_2)\}. \end{aligned}$$

We can now prove (10.7) as follows:

$$\begin{aligned}
\int_{S_1} P_x(S_2) dx &= \frac{1}{2} \int_{S_1} P_x(S_2) dx + \frac{1}{2} \int_{S_2} P_x(S_1) dx \\
&\geq \frac{1}{2} \text{vol}(S'_3) \frac{1}{1000} \\
&\geq \frac{1}{2^{23} n D} \min\{\text{vol}(S'_1), \text{vol}(S'_2)\} \\
&\geq \frac{1}{2^{24} n D} \min\{\text{vol}(S_1), \text{vol}(S_2)\}.
\end{aligned}$$

□

■ 10.7 Dikin walk

Both the ball walk and hit-and-run have a dependence on the “roundness” of the target distribution, e.g., via its diameter or average distance to the center of gravity. Reducing this dependence to logarithmic by rounding is polynomial time but expensive. The current best rounding algorithm (which achieves near-isotropic position) has complexity $O^*(n^3)$. Here we describe a different approach, which is affine-invariant, but requires more knowledge of the convex body. In particular, we will focus on the special case of sampling an explicit polytope $P = \{x : Ax \geq b\}$.

The general Dikin walk is defined as follows. For a convex set K with a positive definite matrix $\mathbf{H}(u)$ for each point $u \in K$, let

$$E_u(r) = \{x : (x - u)^\top \mathbf{H}(u)(x - u) \leq r\}.$$

Algorithm 31: DikinWalk

Input: starting point x_0 in a polytope $P = \{x : \mathbf{A}x \geq b\}$.

Set $r = \frac{1}{8}$.

Repeat T times: at current point x ,

1. Pick y from $E_x(r)$.

2. Go to y with probability $\min\left\{1, \frac{\text{vol}(E_x(r))}{\text{vol}(E_y(r))}\right\}$.

return x .

■ 10.7.1 Strong Self-Concordance

We require a family of matrices to have the following properties. Usually but not necessarily, these matrices come from the Hessian of some convex function.

Definition 10.43 (Symmetric self-concordance). For any convex set $K \subset \mathbb{R}^n$, we call a matrix function $\mathbf{H} : K \rightarrow \mathbb{R}^{n \times n}$ is self-concordant if for any $u \in K$, we have

$$-2\|h\|_{\mathbf{H}(u)} \mathbf{H}(u) \preceq \frac{d}{dt} \mathbf{H}(u + th) \preceq 2\|h\|_{\mathbf{H}(u)} \mathbf{H}(u).$$

We call \mathbf{H} is a symmetric $\bar{\nu}$ -self-concordant barrier if \mathbf{H} is self-concordant and for any $u \in K$,

$$E_u(1) \subseteq K \cap (2u - K) \subseteq E_u(\sqrt{\bar{\nu}}).$$

The following lemma shows that self-concordant matrix functions also enjoy a similar regularity as the usual self-concordant functions.

Lemma 10.44. *Given any self-concordant matrix function \mathbf{H} on $K \subset \mathbb{R}^n$, we define $\|v\|_x^2 = v^\top \mathbf{H}(x)v$. Then, for any $x, y \in K$ with $\|x - y\|_x < 1$, we have*

$$(1 - \|x - y\|_x)^2 \mathbf{H}(x) \preceq \mathbf{H}(y) \preceq \frac{1}{(1 - \|x - y\|_x)^2} \mathbf{H}(x).$$

Proof. Let $h = y - x$, $x_t = x + th$ and $\phi(t) = h^\top \mathbf{H}(x_t)h$. Then,

$$|\phi'(t)| = \left| h^\top \frac{d}{dt} \mathbf{H}(x_t) h \right| \leq 2 \|h\|_{x_t}^3 = 2\phi(t)^{3/2}.$$

Hence, we have $\left| \frac{d}{dt} \frac{1}{\sqrt{\phi(t)}} \right| \leq 1$. Therefore, we have $\frac{1}{\sqrt{\phi(t)}} \geq \frac{1}{\sqrt{\phi(0)}} - t$ and hence,

$$\phi(t) \leq \frac{\phi(0)}{(1 - t\sqrt{\phi(0)})^2}. \quad (10.8)$$

Now we fix any v and define $\psi(t) = v^\top \mathbf{H}(x_t)v$. Then,

$$|\psi'(t)| = \left| v^\top \frac{d}{dt} \mathbf{H}(x_t) v \right| \leq 2 \|h\|_{x_t} \|v\|_{x_t}^2 = 2\phi(t)\psi(t).$$

Using (10.8) at the end, we have

$$\left| \frac{d}{dt} \ln \psi(t) \right| \leq \frac{2\sqrt{\phi(0)}}{(1 - t\sqrt{\phi(0)})}.$$

Integrating both sides from 0 to 1,

$$\left| \ln \frac{\psi(1)}{\psi(0)} \right| \leq \int_0^1 \frac{2\sqrt{\phi(0)}}{(1 - t\sqrt{\phi(0)})} dt = 2 \ln \left(\frac{1}{1 - \sqrt{\phi(0)}} \right).$$

The result follows from this, $\psi(1) = v^\top \mathbf{H}(y)v$, $\psi(0) = v^\top \mathbf{H}(x)v$, and $\phi(0) = \|x - y\|_x^2$. \square

Many natural barriers, including the logarithmic barrier and the LS-barrier, satisfy a much stronger condition than self-concordant. However, this is not always true, as one can construct counterexamples even in one-dimension.

Definition 10.45. For any convex set $K \subset \mathbb{R}^n$, we say a matrix function $\mathbf{H} : K \rightarrow \mathbb{R}^{n \times n}$ is strongly self-concordant if for any $u \in K$, we have

$$\left\| \mathbf{H}(x)^{-1/2} D\mathbf{H}(x)[h] \mathbf{H}(x)^{-1/2} \right\|_F \leq 2 \|h\|_x$$

where $D\mathbf{H}(x)[h]$ is the directional derivative of \mathbf{H} at x in the direction h .

Similar to Lemma 10.44, we have a global version of Lemma 10.44.

Lemma 10.46. Given any strongly self-concordant matrix function \mathbf{H} on $K \subset \mathbb{R}^n$. For any $x, y \in K$ with $\|x - y\|_x < 1$, we have

$$\|\mathbf{H}(x)^{-\frac{1}{2}}(\mathbf{H}(y) - \mathbf{H}(x))\mathbf{H}(x)^{-\frac{1}{2}}\|_F \leq \frac{\|x - y\|_x}{(1 - \|x - y\|_x)^2}.$$

Proof. Let $x_t = (1 - t)x + ty$. Then, we have

$$\|\mathbf{H}(x)^{-\frac{1}{2}}(\mathbf{H}(y) - \mathbf{H}(x))\mathbf{H}(x)^{-\frac{1}{2}}\|_F = \int_0^1 \|\mathbf{H}(x)^{-\frac{1}{2}} \frac{d}{dt} \mathbf{H}(x_t) \mathbf{H}(x)^{-\frac{1}{2}}\|_F dt.$$

We note that \mathbf{H} is self-concordant. Hence, Lemma 10.44 shows that

$$\begin{aligned} \|\mathbf{H}(x)^{-\frac{1}{2}} \frac{d}{dt} \mathbf{H}(x_t) \mathbf{H}(x)^{-\frac{1}{2}}\|_F^2 &= \text{tr} \mathbf{H}(x)^{-1} \left(\frac{d}{dt} \mathbf{H}(x_t) \right) \mathbf{H}(x)^{-1} \left(\frac{d}{dt} \mathbf{H}(x_t) \right) \\ &\leq \frac{1}{(1 - \|x - x_t\|_x)^4} \text{tr} \mathbf{H}(x_t)^{-1} \left(\frac{d}{dt} \mathbf{H}(x_t) \right) \mathbf{H}(x_t)^{-1} \left(\frac{d}{dt} \mathbf{H}(x_t) \right) \\ &\leq \frac{4}{(1 - \|x - x_t\|_x)^4} \|x - x_t\|_{x_t}^2 \\ &\leq \frac{4}{(1 - \|x - x_t\|_x)^6} \|x - x_t\|_x^2 \end{aligned}$$

where we used the assumption in the second inequality and Lemma 10.44 again for the last inequality. Hence,

$$\begin{aligned} \|\mathbf{H}(x)^{-\frac{1}{2}}(\mathbf{H}(y) - \mathbf{H}(x))\mathbf{H}(x)^{-\frac{1}{2}}\|_F &\leq \int_0^1 \frac{2\|x - x_t\|_x}{(1 - \|x - x_t\|_x)^3} dt \\ &= \int_0^1 \frac{2t\|x - y\|_x}{(1 - t\|x - y\|_x)^3} dt \\ &= \frac{\|x - y\|_x}{(1 - \|x - y\|_x)^2}. \end{aligned}$$

□

We note that strong self-concordance is stronger than self-concordance since the Frobenius norm is always larger or equal to the spectral norm. As an example, we will verify that the conditions hold for the standard log barrier (Lemma ??).

The Dikin walk has the following guarantee.

Theorem 10.47. *The mixing rate of the Dikin walk for a symmetric, strongly self-concordant matrix function with convex log determinant is $O(n\bar{\nu})$.*

Each step of the standard Dikin walk is fast, and does not need matrix multiplication.

Theorem 10.48. *The Dikin walk with the logarithmic barrier for a polytope $\{\mathbf{A}x \geq b\}$ can be implemented in time $O(\text{nnz}(\mathbf{A}) + n^2)$ per step while maintaining the mixing rate of $O(mn)$.*

The next lemma results from studying strong self-concordance for classical barriers. The KLS constant below is conjectured to be $O(1)$ and known to be $O(\sqrt{\log n})$.

Lemma 10.49. *Let ψ_n be the KLS constant of isotropic logconcave densities in \mathbb{R}^n , namely, for any isotropic logconcave density p and any set $S \subset \mathbb{R}^n$, we have*

$$\int_{\partial S} p(x) dx \geq \frac{1}{\psi_n} \min \left\{ \int_S p(x) dx, \int_{\mathbb{R}^n \setminus S} p(x) dx \right\}.$$

Let $\mathbf{H}(x)$ be the Hessian of the universal or entropic barriers. Then, we have

$$\left\| \mathbf{H}(x)^{-1/2} D\mathbf{H}(x)[h] \mathbf{H}(x)^{-1/2} \right\|_F = O(\psi_n) \|h\|_x.$$

In short, the universal and entropic barriers in \mathbb{R}^n are strongly self-concordant up to a scaling factor depending on ψ_n .

In fact, the proof shows that up to a logarithmic factor the strong self-concordance of these barriers is equivalent to the KLS conjecture.

■ 10.8 Mixing with Strong Self-Concordance

A key ingredient of the proof of Theorem 10.47 is the following lemma.

Lemma 10.50. *For two points $x, y \in P$, with $\|x - y\|_x \leq \frac{1}{8\sqrt{n}}$, we have $d_{TV}(P_x, P_y) \leq \frac{3}{4}$.*

Proof. We have to prove two things: first, the rejection probability is small, second the ellipsoids used by the Dikin walk at x, y have large overlap. More precisely, we have

$$\begin{aligned} d_{TV}(P_x, P_y) &\leq \frac{1}{2}\text{rej}_x + \frac{1}{2}\text{rej}_y + \frac{1}{2} \frac{\text{vol}(P_x \setminus P_y)}{\text{vol}(P_x)} + \frac{1}{2} \frac{\text{vol}(P_y \setminus P_x)}{\text{vol}(P_y)} \\ &= \frac{1}{2}\text{rej}_x + \frac{1}{2}\text{rej}_y + 1 - \frac{1}{2} \frac{\text{vol}(P_x \cap P_y)}{\text{vol}(P_x)} - \frac{1}{2} \frac{\text{vol}(P_x \cap P_y)}{\text{vol}(P_y)} \end{aligned} \quad (10.9)$$

where rej_x and rej_y are the rejection probabilities at x and y .

For the rejection probability at x , we consider the algorithm pick z from $E_x(r)$. Let $f(z) = \ln \det \mathbf{H}(z)$. The acceptance probability of the sample z is

$$\min \left\{ 1, \frac{\text{vol}(E_x(r))}{\text{vol}(E_z(r))} \right\} = \min \left\{ 1, \sqrt{\frac{\det(\mathbf{H}(z))}{\det(\mathbf{H}(x))}} \right\}. \quad (10.10)$$

By the assumption that f is a convex function, we have that

$$\ln \frac{\det(\mathbf{H}(z))}{\det(\mathbf{H}(x))} = f(z) - f(x) \geq \langle \nabla f(x), z - x \rangle. \quad (10.11)$$

To simplify the notation, we assume $\mathbf{H}(x) = \mathbf{I}$. Since z is sampled from unit ball of radius r centered at x , we know that

$$\mathbf{P}(v^\top(z - x) \geq -\epsilon r \|v\|_2) \geq 1 - e^{-n\epsilon^2/2}.$$

In particular, with probability at least 0.99 in z , we have

$$\langle \nabla f(x), z - x \rangle \geq -\frac{4r}{\sqrt{n}} \|\nabla f(x)\|_2. \quad (10.12)$$

To compute $\|\nabla f(x)\|_2^2$, it is easier to compute directional derivative of ∇f . Note that

$$\begin{aligned} \|\nabla f(x)\|_2 &= \max_{\|v\|_2=1} \nabla f(x)^\top v \\ &= \max_{\|v\|_2=1} \text{tr}(\mathbf{H}(x)^{-1} D\mathbf{H}(x)[v]) \\ &= \max_{\|v\|_2=1} \text{tr} \left(\mathbf{H}(x)^{-\frac{1}{2}} D\mathbf{H}(x)[v] \mathbf{H}(x)^{-\frac{1}{2}} \right) \\ &\leq \max_{\|v\|_2=1} \sqrt{n} \|\mathbf{H}(x)^{-\frac{1}{2}} D\mathbf{H}(x)[v] \mathbf{H}(x)^{-\frac{1}{2}}\|_F \\ &\leq \sqrt{n} \end{aligned} \quad (10.13)$$

where the first inequality follows from $|\sum_{i=1}^n \lambda_i| \leq \sqrt{n} \sqrt{\sum_{i=1}^n \lambda_i^2}$ and the second inequality follows from the definition of strong self-concordance.

Combining (10.10), (10.11), (10.12) and (10.13), we see that with probability at least 0.99 in z , acceptance probability of the sample z is

$$\min \left\{ 1, \frac{\text{vol}(E_x(r))}{\text{vol}(E_z(r))} \right\} \geq e^{-2r} \geq 0.77 \quad (10.14)$$

where we used that $r = \frac{1}{8}$. Hence, the overall rejection probability rej_x (and similarly rej_y) satisfies

$$\text{rej}_x \leq 0.24 \quad \text{and} \quad \text{rej}_y \leq 0.24. \quad (10.15)$$

Now, we bound the fraction of volume in the intersection of the ellipsoids at x, y . Again, we can assume that $\mathbf{H}(x) = \mathbf{I}$. Then, the strongly self-concordance and Lemma 10.46 shows that

$$\|\mathbf{H}(y) - \mathbf{I}\|_F \leq 2\|x - y\|_x \leq \frac{1}{4\sqrt{n}}. \quad (10.16)$$

In particular, we have that

$$\frac{1}{2}\mathbf{I} \preceq \mathbf{H}(y) \preceq \frac{3}{2}\mathbf{I}. \quad (10.17)$$

We partition the eigenvalues λ_i of $\mathbf{H}(y)$ into those of value at least 1 and the rest. Then consider the ellipsoid E whose eigenvalues are $\min\{1, \lambda_i\}$. This is contained in both $E_x(1)$ and $E_y(1)$. We will see that $\text{vol}(E)$ is a constant fraction of the volume of both $E_x(1)$ and $E_y(1)$. First, we compare E and $E_x(1)$

$$\frac{\text{vol}(E)}{\text{vol}(E_x(1))} = \prod_{i:\lambda_i < 1} \lambda_i = \prod_{i:\lambda_i < 1} (1 - (1 - \lambda_i)) \geq \exp \left(-2 \sum_{i:\lambda_i < 1} (1 - \lambda_i) \right) \quad (10.18)$$

where we used that $1 - x \geq \exp(-2x)$ for $0 \leq x \leq \frac{1}{2}$ and $\lambda_i \geq \frac{1}{2}$ (10.17). From the inequality (10.16), it follows that

$$\sqrt{\sum_i (\lambda_i - 1)^2} \leq \frac{1}{4\sqrt{n}}.$$

Therefore, $\sum_{i:\lambda_i < 1} |\lambda_i - 1| \leq \frac{1}{4}$. Putting it into (10.18), we have

$$\frac{\text{vol}(P_x \cap P_y)}{\text{vol}(P_x)} = \frac{\text{vol}(E)}{\text{vol}(E_x(1))} \geq e^{-\frac{1}{2}}. \quad (10.19)$$

Similarly, we have

$$\frac{\text{vol}(P_x \cap P_y)}{\text{vol}(P_y)} = \frac{\prod_{i:\lambda_i < 1} \lambda_i}{\prod_{i:\lambda_i > 1} \lambda_i} = \frac{1}{\prod_{i:\lambda_i > 1} \lambda_i} \geq \frac{1}{\exp(\sum_{i:\lambda_i > 1} (\lambda_i - 1))} \geq e^{-\frac{1}{4}}. \quad (10.20)$$

Putting (10.15), (10.19) and (10.20) into (10.9), we have

$$d_{\text{TV}}(P_x, P_y) \leq \frac{0.24}{2} + \frac{0.24}{2} + 1 - \frac{e^{-\frac{1}{2}}}{2} + \frac{e^{-\frac{1}{4}}}{2} \leq \frac{3}{4}$$

□

The next lemma establishes isoperimetry. This only needs the symmetric containment assumption. The isoperimetry is for the cross-ratio distance. For a convex body K , and any two points $u, v \in K$, suppose that p, q are the endpoints of the chord through u, v in K , so that these points occur in the order p, u, v, q . Then, the *cross-ratio* distance between u and v is defined as

$$d_K(u, v) = \frac{\|u - v\|_2 \|p - q\|_2}{\|p - u\|_2 \|v - q\|_2}.$$

This distance enjoys the following isoperimetric inequality.

Theorem 10.51 ([48]). *For any convex body K , and disjoint subsets S_1, S_2 of it, and $S_3 = K \setminus S_1 \setminus S_2$, we have*

$$\text{vol}(S_3) \geq d_K(S_1, S_2) \frac{\text{vol}(S_1)\text{vol}(S_2)}{\text{vol}(K)}.$$

We now relate the cross-ratio distance to the ellipsoidal norm.

Lemma 10.52. *For $u, v \in K$, $d_K(u, v) \geq \frac{\|u - v\|_u}{\sqrt{v}}$.*

Proof. Consider the ellipsoid at u . For the chord $[p, q]$ induced by u, v with these points in the order p, u, v, q , suppose that $\|p - u\|_2 \leq \|v - q\|_2$. Then by Lemma 10.47, $p \in K \cap (2u - K)$. And hence $\|p - u\|_u \leq \sqrt{v}$. Therefore,

$$d_K(u, v) = \frac{\|u - v\|_2 \|p - q\|_2}{\|p - u\|_2 \|v - q\|_2} \geq \frac{\|u - v\|_2}{\|p - u\|_2} = \frac{\|u - v\|_u}{\|p - u\|_u} \geq \frac{\|u - v\|_u}{\sqrt{v}}.$$

We can now prove the main conductance bound.

*

We follow the standard high-level outline [75]. Consider any measurable subset $S_1 \subseteq K$ and let $S_2 = K \setminus S_1$ be its complement. Define the points with low escape probability for these subsets as

$$S'_i = \left\{ x \in S_i : P_x(K \setminus S_i) < \frac{1}{8} \right\}$$

and $S'_3 = K \setminus S'_1 \setminus S'_2$. Then, for any $u \in S'_1, v \in S'_2$, we have $d_{\text{TV}}(P_u, P_v) > 1 - \frac{1}{4}$. Hence, by Lemma 10.50, we have $\|u - v\|_u \geq \frac{1}{8\sqrt{n}}$. Therefore, by Lemma 10.52,

$$d_K(u, v) \geq \frac{1}{8\sqrt{n} \cdot \sqrt{v}}.$$

We can now bound the conductance of S_1 . We may assume that $\text{vol}(S'_i) \geq \text{vol}(S_i)/2$; otherwise, it immediately follows that the conductance of S_1 is $\Omega(1)$. Assuming this, we have

$$\begin{aligned} \int_{S_1} P_x(S_2) dx &\geq \int_{S'_3} \frac{1}{8} dx \geq \frac{1}{8} \text{vol}(S'_3) \\ \text{using isoperimetry (Theorem 10.51)} &\geq \frac{1}{8} d_K(S'_1, S'_2) \frac{\text{vol}(S'_1) \text{vol}(S'_2)}{\text{vol}(P)} \\ &\geq \frac{1}{512\sqrt{n\nu}} \min \{ \text{vol}(S_1), \text{vol}(S_2) \}. \end{aligned}$$

□

■ 10.9 Hamiltonian Monte Carlo

Hamiltonian dynamics is an alternative way to formulate Newtonian mechanics. The Hamiltonian H captures both the potential and kinetic energy of a particle as a function of its position and velocity. The dynamics can be described by the following differential equations.

$$\begin{aligned} \frac{dx}{dt} &= \frac{\partial H(x, v)}{\partial v}, \\ \frac{dv}{dt} &= -\frac{\partial H(x, v)}{\partial x}. \end{aligned}$$

These equations preserve the Hamiltonian function H . In the simplest Euclidean setting, it can be defined as follows.

$$H(x, v) = f(x) + \frac{1}{2} \|v\|^2$$

so that

$$\frac{dx}{dt} = v, \quad \frac{dv}{dt} = -\nabla f(x)$$

or

$$\frac{d^2x}{dt^2} = -\nabla f(x).$$

More generally, the Hamiltonian can depend on a function that defines a local metric:

$$H(x, v) = f(x) + \frac{1}{2} \log((2\pi)^n \det g(x)) + \frac{1}{2} v^T g(x)^{-1} v$$

where $g(x)$ is a matrix, and when it is PSD, it defines a local norm at x . In this sense, we can view the dynamics as evolving on a manifold with local metric $g(x)$. Here in this chapter, we will focus on the case when $g(x) = I$, the standard Euclidean metric.

(Riemannian) Hamiltonian Monte Carlo (or RHMC) [?, ?][?, ?] is a Markov Chain Monte Carlo method for sampling from a desired distribution. Each step of the method consists of the following: At a current point x ,

1. Pick a random velocity y according to a local distribution defined by x (in the simplest setting, this is the standard Gaussian distribution for every x).
2. Move along the Hamiltonian curve defined by Hamiltonian dynamics at (x, y) for time (distance) δ .

For the choice of H above, the marginal distribution of the current point x approaches the target distribution with density proportional to e^{-f} . Note that HMC does not require a Metropolis filter! Thus, unlike the walks we have seen so far, its step sizes are not limited by this consideration even in high dimension. Hamiltonian Monte Carlo can be used for sampling from a general distribution $e^{-H(x, y)}$.

Definition 10.53. Given a continuous, twice-differentiable function $H : \mathcal{M} \times \mathbb{R}^n \subset \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R}$ (Hamiltonian) where \mathcal{M} is the x domain of H , we say $(x(t), y(t))$ follows a *Hamiltonian curve* if it satisfies the *Hamiltonian equations*

$$\begin{aligned}\frac{dx}{dt} &= \frac{\partial H(x, y)}{\partial y}, \\ \frac{dy}{dt} &= -\frac{\partial H(x, y)}{\partial x}.\end{aligned}\tag{10.21}$$

We define the map $T_\delta(x, y) \stackrel{\text{def}}{=} (x(\delta), y(\delta))$ where the $(x(t), y(t))$ follows the Hamiltonian curve with the initial condition $(x(0), y(0)) = (x, y)$.

Hamiltonian Monte Carlo is a Markov chain generated by a sequence of randomly Hamiltonian curves.

Algorithm 32: Hamiltonian Monte Carlo

Input: some initial point $x^{(1)} \in \mathcal{M}$.
for $i = 1, 2, \dots, T$ **do**
 Sample y according to $e^{-H(x^{(k)}, y)} / \pi(x^{(k)})$ where $\pi(x) = \int_{\mathbb{R}^n} e^{-H(x, y)} dy$.
 With probability $\frac{1}{2}$, set $(x^{(k+1)}, y^{(k+1)}) = T_\delta(x^{(k)}, y)$.
 Otherwise, $(x^{(k+1)}, y^{(k+1)}) = T_{-\delta}(x^{(k)}, y)$.
end
Output: $(x^{(T+1)}, y^{(T+1)})$.

Time-reversibility

Lemma 10.54 (Energy Conservation). *For any Hamiltonian curve $(x(t), y(t))$, we have that*

$$\frac{d}{dt} H(x(t), y(t)) = 0.$$

Proof. Note that

$$\frac{d}{dt} H(x(t), y(t)) = \frac{\partial H}{\partial x} \frac{dx}{dt} + \frac{\partial H}{\partial y} \frac{dy}{dt} = \frac{\partial H}{\partial x} \frac{\partial H}{\partial y} - \frac{\partial H}{\partial y} \frac{\partial H}{\partial x} = 0.$$

□

Lemma 10.55 (Measure Preservation). *For any $t \geq 0$, we have that*

$$\det(DT_t(x, y)) = 1$$

where $DT_t(x, y)$ is the Jacobian of the map T_t at the point (x, y) .

Proof. Let $(x(t, s), y(t, s))$ be a family of Hamiltonian curves given by $T_t(x + sd_x, y + sd_y)$. We write

$$u(t) = \frac{\partial}{\partial s} x(t, s)|_{s=0}, \quad v(t) = \frac{\partial}{\partial s} y(t, s)|_{s=0}.$$

By differentiating the Hamiltonian equations (10.21) w.r.t. s , we have that

$$\begin{aligned}\frac{du}{dt} &= \frac{\partial^2 H(x, y)}{\partial y \partial x} u + \frac{\partial^2 H(x, y)}{\partial y \partial y} v, \\ \frac{dv}{dt} &= -\frac{\partial^2 H(x, y)}{\partial x \partial x} u - \frac{\partial^2 H(x, y)}{\partial x \partial y} v, \\ (u(0), v(0)) &= (d_x, d_y).\end{aligned}$$

This can be captured by the following matrix ODE

$$\begin{aligned}\frac{d\Phi}{dt} &= \begin{pmatrix} \frac{\partial^2 H(x(t), y(t))}{\partial y \partial x} & \frac{\partial^2 H(x(t), y(t))}{\partial y \partial y} \\ -\frac{\partial^2 H(x(t), y(t))}{\partial x \partial x} & -\frac{\partial^2 H(x(t), y(t))}{\partial x \partial y} \end{pmatrix} \Phi(t) \\ \Phi(0) &= I\end{aligned}$$

using the equation

$$DT_t(x, y) \begin{pmatrix} d_x \\ d_y \end{pmatrix} = \begin{pmatrix} u(t) \\ v(t) \end{pmatrix} = \Phi(t) \begin{pmatrix} d_x \\ d_y \end{pmatrix}.$$

Therefore, $DT_t(x, y) = \Phi(t)$. Next, we observe that

$$\frac{d}{dt} \log \det \Phi(t) = \text{tr} \left(\Phi(t)^{-1} \frac{d}{dt} \Phi(t) \right) = \text{tr} \begin{pmatrix} \frac{\partial^2 H(x(t), y(t))}{\partial y \partial x} & \frac{\partial^2 H(x(t), y(t))}{\partial y \partial y} \\ -\frac{\partial^2 H(x(t), y(t))}{\partial x \partial x} & -\frac{\partial^2 H(x(t), y(t))}{\partial x \partial y} \end{pmatrix} = 0.$$

Hence,

$$\det \Phi(t) = \det \Phi(0) = 1.$$

□

Using the previous two lemmas, we can see that Hamiltonian Monte Carlo indeed converges to the desired distribution.

Lemma 10.56 (Time reversibility). **Let $p_x(x')$ denote the probability density of one step of the Hamiltonian Monte Carlo starting at x . We have that*

$$\pi(x)p_x(x') = \pi(x')p_{x'}(x)$$

for almost everywhere in x and x' where $\pi(x) = \int_{\mathbb{R}^n} e^{-H(x, y)} dy$.

Proof. Fix x and x' . Let $F_\delta^x(y)$ be the x component of $T_\delta(x, y)$. Let $V_+ = \{y : F_\delta^x(y) = x'\}$ and $V_- = \{y : F_{-\delta}^x(y) = x'\}$. Then,

$$\pi(x)p_x(x') = \frac{1}{2} \int_{y \in V_+} \frac{e^{-H(x, y)}}{|\det(DF_\delta^x(y))|} + \frac{1}{2} \int_{y \in V_-} \frac{e^{-H(x, y)}}{|\det(DF_{-\delta}^x(y))|}.$$

We note that this formula assumed that DF_δ^x is invertible. Sard's theorem showed that $F_\delta^x(N)$ is measure 0 where $N \stackrel{\text{def}}{=} \{y : DF_\delta^x(y) \text{ is not invertible}\}$. Therefore, the formula is correct except for a measure zero subset.

By reversing time for the Hamiltonian curve, we have that for the same V_\pm ,

$$\pi(x')p_{x'}(x) = \frac{1}{2} \int_{y \in V_+} \frac{e^{-H(x', y')}}{|\det(DF_{-\delta}^{x'}(y'))|} + \frac{1}{2} \int_{y \in V_-} \frac{e^{-H(x', y')}}{|\det(DF_\delta^{x'}(y'))|} \quad (10.22)$$

where y' denotes the y component of $T_\delta(x, y)$ and $T_{-\delta}(x, y)$ in the first and second sum respectively.

We compare the first terms in both equations. Let $DT_\delta(x, y) = \begin{pmatrix} A & B \\ C & D \end{pmatrix}$. Since $T_\delta \circ T_{-\delta} = I$ and $T_\delta(x, y) = (x', y')$, the inverse function theorem shows that $DT_{-\delta}(x', y')$ is the inverse map of $DT_\delta(x, y)$. Hence, we have that

$$DT_{-\delta}(x', y') = \begin{pmatrix} A & B \\ C & D \end{pmatrix}^{-1} = \begin{pmatrix} \cdots & -A^{-1}B(D - CA^{-1}B)^{-1} \\ \cdots & \cdots \end{pmatrix}.$$

Therefore, we have that $F_\delta^x(y) = B$ and $F_{-\delta}^{x'}(y') = -A^{-1}B(D - CA^{-1}B)^{-1}$. Hence, we have that

$$\left| \det(DF_{-\delta}^{x'}(y')) \right| = \left| \det A^{-1} \det B \det(D - CA^{-1}B)^{-1} \right| = \frac{|\det B|}{\left| \det \begin{pmatrix} A & B \\ C & D \end{pmatrix} \right|}.$$

Using that $\det(DT_t(x, y)) = \det \begin{pmatrix} A & B \\ C & D \end{pmatrix} = 1$ (Lemma 10.55), we have that

$$\left| \det(DF_{-\delta}^{x'}(y')) \right| = |\det(DF_\delta^x(y))|.$$

Hence, we have that

$$\begin{aligned} \frac{1}{2} \int_{y \in V_+} \frac{e^{-H(x,y)}}{|\det(DF_\delta^x(y))|} &= \frac{1}{2} \int_{y \in V_+} \frac{e^{-H(x,y)}}{|\det(DF_{-\delta}^{x'}(y'))|} \\ &= \frac{1}{2} \int_{y \in V_+} \frac{e^{-H(x',y')}}{|\det(DF_{-\delta}^{x'}(y'))|} \end{aligned}$$

where we used that $e^{-H(x,y)} = e^{-H(x',y')}$ (Lemma 10.54) at the end.

For the second term in (10.22), by the same calculation, we have that

$$\frac{1}{2} \int_{y \in V_-} \frac{e^{-H(x,y)}}{|\det(DF_\delta^x(y))|} = \frac{1}{2} \int_{y \in V_+} \frac{e^{-H(x',y')}}{|\det(DF_\delta^{x'}(y'))|}$$

□

Convergence

First we consider the convergence in the case when $H(x, v) = f(x) + \frac{1}{2} \|v\|^2$ for a strongly convex function f . So the marginal of the stationary distribution along x is proportional to e^{-f} . The idea here is coupling (as we did for Langevin dynamics). We consider two separate processes x and y , with their next step directions chosen to be identical. The key lemma is that with this setting the squared distance decreases up to a certain time that depends on the condition number.

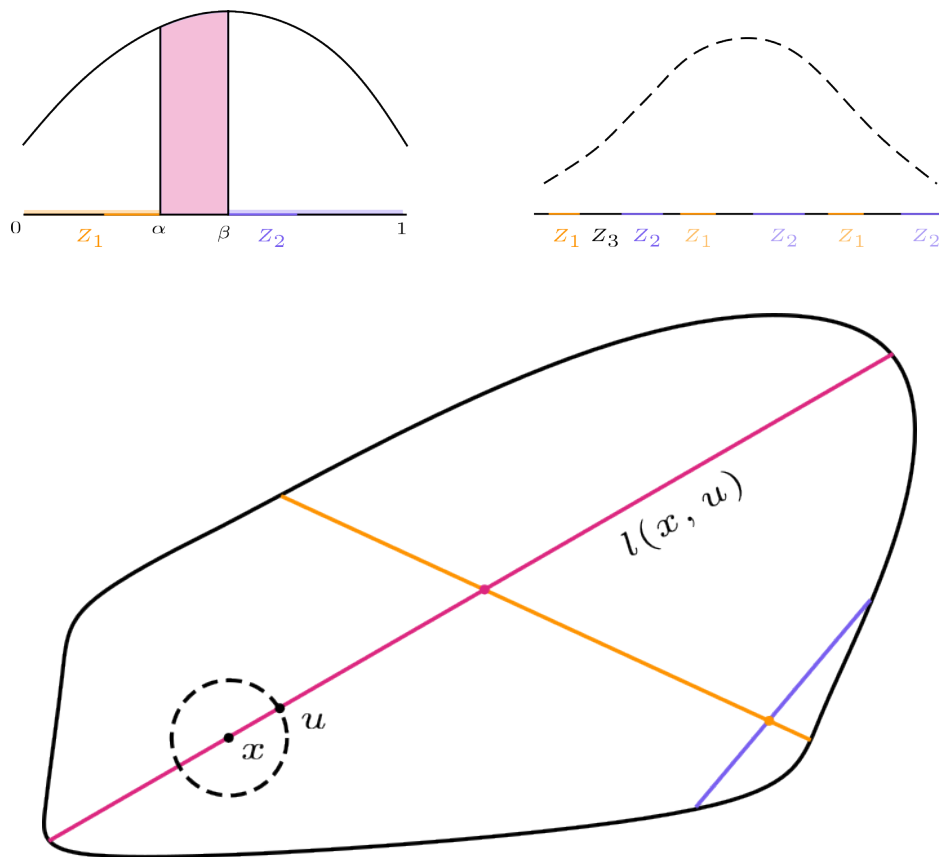
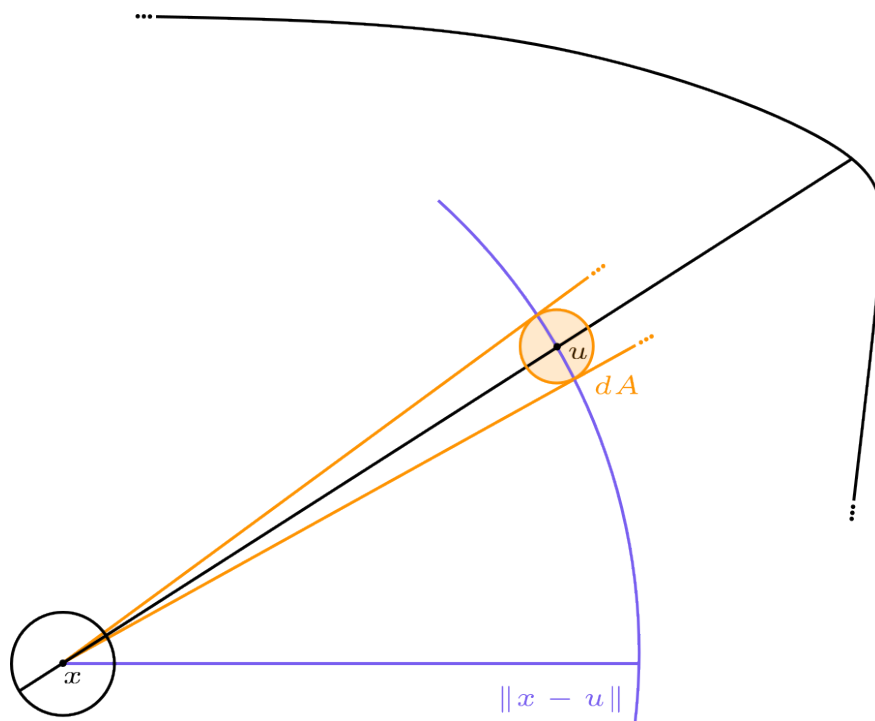


Figure 10.4: Hit-and-Run Algorithm



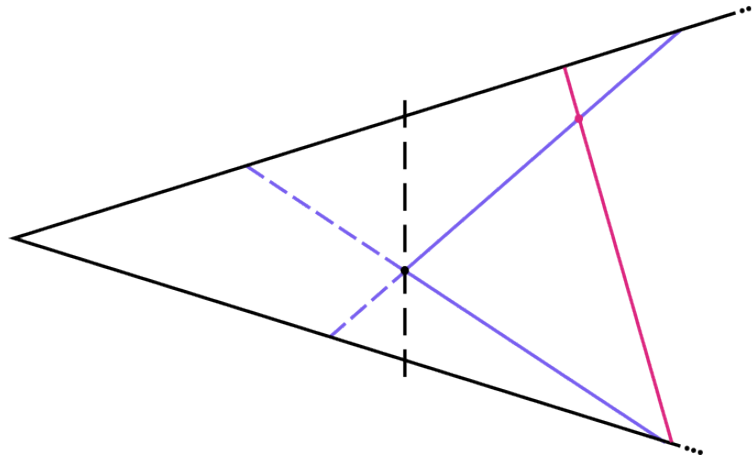


Figure 10.5: Hit-and-Run from a corner

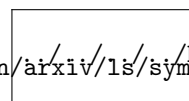
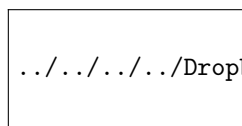
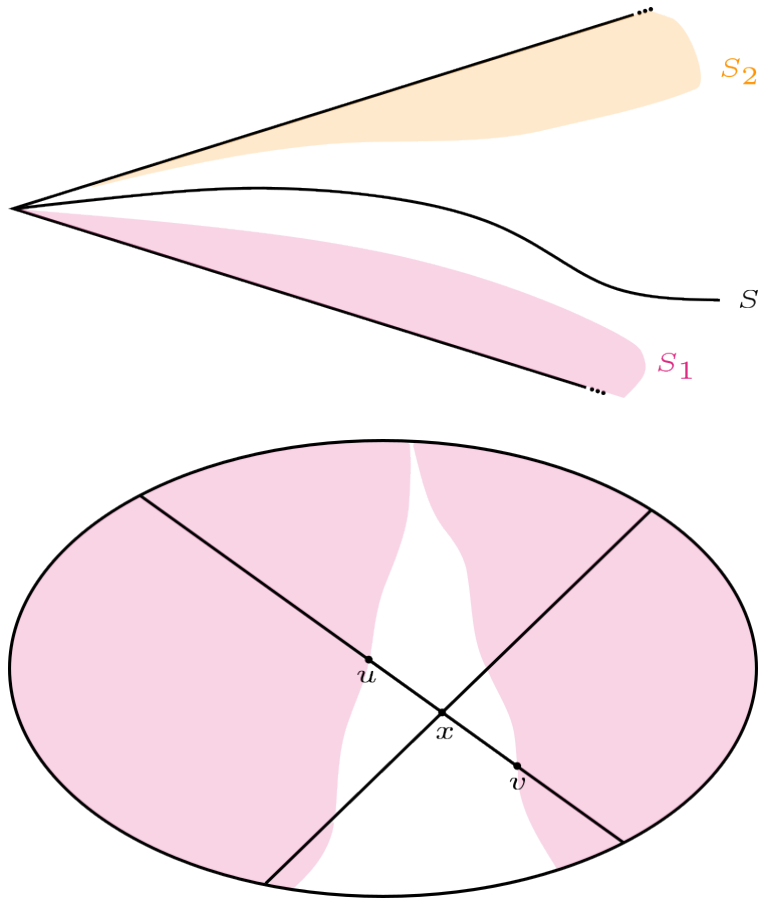


Figure 10.6: (a) $E_u(1) \subseteq K \cap (2u - K) \subseteq E_u(\sqrt{\nu})$. (b) Strong self-concordance measures the rate of change of Hessian of a barrier in the Frobenius norm

■ 11.1 Simulated Annealing

In this chapter we study a sampling-based approach for optimization and integration in high dimension. The main idea is to sample a sequence of logconcave distributions, starting with one that is easy to integrate and ending with the function whose integral is desired. This process is known as *simulated annealing*. The same high-level algorithm can be used for optimization, volume computation/integration or rounding. For integration, the desired integral can be expressed as the following telescoping product:

$$\int_{\mathbb{R}^n} f = \int f_0 \frac{\int f_1}{\int f_0} \frac{\int f_2}{\int f_1} \cdots \frac{\int f_m}{\int f_{m-1}}$$

where $f_m = f$. Each ratio $\int f_{i+1} / \int f_i$ is the expectation of the estimator $Y = \frac{f_{i+1}(X)}{f_i(X)}$ for X drawn from the density proportional to f_i . What sequence of functions should we use?

Algorithm 33: SimulatedAnnealing

1. For $i = 0, \dots, m$, define

$$a_i = b \left(1 + \frac{1}{\sqrt{n}} \right)^i \text{ and } f_i(x) = f(x)^{a_i}.$$

2. Let X_0^1, \dots, X_0^k be independent random points with density proportional to f_0 .
3. For $i = 0, \dots, m-1$: starting with X_i^1, \dots, X_i^k , generate random points $X_{i+1} = \{X_{i+1}^1, \dots, X_{i+1}^k\}$; update a running estimate g based on these samples; update the isotropy transformation using the samples.
4. Output the final estimate of g .

return x .

For optimization, the function f_m is set to be a sufficiently high power of f , the function to be maximized while g is simply the maximum objective value so far. For integration and rounding, $f_m = f$, the target function to be integrated or rounded. For integration, the function g starts out as the integral of f_0 and is multiplied by the ratio $\int f_{i+1} / \int f_i$ in each step. For rounding, g is simply the estimate of the isotropic transformation for the current function.

For sampling and optimization, it is natural to ask why one uses a sequence of functions rather than jumping straight to the target function f_m . For optimizing a linear function $c^T x$ over a convex set K , all we need to do is sample according to the density proportional to $e^{-a(c^T x)}$ for a sufficiently large coefficient a (recall Theorem 9.6). The reason for using a sequence is that the function f_m and corresponding density p_m can be very far from the starting function or distribution, and hence the mixing time can be high. The sequence ensures that samples from the current function provide a good (warm) start for sampling from the next function. This is captured in the next lemma.

Theorem 11.1. *Let $p_i(x) = f_i(x) / \int f_i$ with f_i defined as in the annealing algorithm for some logconcave function $f : \mathbb{R}^n \rightarrow \mathbb{R}_+$. Then a random sample $X \sim p_i$ satisfies*

$$\mathbf{E}_{p_i} \left(\frac{p_i(x)}{p_{i+1}(x)} \right) = O(1).$$

The underlying mathematical property behind this lemma is the following.

Lemma 11.2. *Let f be a logconcave function in \mathbb{R}^n . Then $Z(a) = a^n \int_{\mathbb{R}^n} f(x)^a$ is logconcave for $a \geq 0$. If f has support K , then $Z(a) = a^n \int_K f(ax)$ is logconcave for $a > 0$.*

■ 11.2 Volume Computation

For volume computation, we can apply annealing as follows. We assume that the input convex body K contains a unit ball, has diameter bounded by D and is given by a membership oracle. The polynomial-time algorithm of Dyer, Frieze and Kannan [23] uses a sequence of uniform distributions on convex bodies, starting with the ball contained inside the input body K . Each body in the sequence is a ball intersected with the given convex body K : $K_i = 2^{\frac{i}{n}} r B \cap K$ and $f_i(x)$ is the indicator of K_i . The length the sequence is $m = O(n \log D)$ so that the final body is just K . A variance computation shows that $O(m/\epsilon^2)$ samples per distribution suffice to get an overall $1 + \epsilon$ multiplicative error approximation with high probability. The total number of samples is $O^*(m^2) = O^*(n^2)$ and the complexity of the resulting algorithm is $O^*(n^5)$ as shown in [33]. Table 11.1 below summarizes progress on the volume problem over the past three decades. Besides improving the complexity of volume computation, each step has typically resulted in new techniques. For more details, we refer the reader to surveys on the topic [66, 73].

Year/Authors	New ingredients	Steps
1989/Dyer-Frieze-Kannan [23]	Everything	n^{23}
1990/Lovász-Simonovits [49]	Better isoperimetry	n^{16}
1990/Lovász [47]	Ball walk	n^{10}
1991/Applegate-Kannan [5]	Logconcave sampling	n^{10}
1990/Dyer-Frieze [22]	Better error analysis	n^8
1993/Lovász-Simonovits [50]	Localization lemma	n^7
1997/Kannan-Lovász-Simonovits [33]	Speedy walk, isotropy	n^5
2003/Lovász-Vempala [53]	Annealing, hit-and-run	n^4
2015/Cousins-Vempala [20] (well-rounded)	Gaussian Cooling	n^3
2017/Lee-Vempala (polytopes)	Hamiltonian Walk	$mn^{\frac{2}{3}}$

Table 11.1: The complexity of volume estimation, each step uses $\tilde{O}(n)$ bit of randomness. The last algorithm needs $\tilde{O}(mn^{\omega-1})$ steps per iteration while the rest need $O(n^2)$ per oracle query.

In [53] this was improved by sampling from a sequence of nonuniform distributions. Then we consider the following estimator:

$$Y = \frac{f_{i+1}(X)}{f_i(X)}.$$

We see that

$$\mathbf{E}_{f_i}(Y) = \frac{\int f_{i+1}}{\int f_i}.$$

In the algorithm of DFK and KLS, this ratio is bounded by a constant in each phase, giving a total of $O^*(n)$ phases since the ratio of final to initial integrals is exponential. Instead of uniform densities, we consider

$$f_i(x) \propto \exp(-a_i \|x\|) \chi_K(x) \text{ or } f_i(x) \propto \exp(-a_i \|x\|^2) \chi_K(x).$$

The coefficient a_i (inverse “temperature”) will be changed by a factor of $(1 + \frac{1}{\sqrt{n}})$ in each phase, which implies that $m = \tilde{O}(\sqrt{n})$ phases suffice to reach the target distribution. This is perhaps surprising since the ratio of the initial integral to the final is typically $n^{\Omega(n)}$. Yet the algorithm uses only $\tilde{O}(\sqrt{n})$ phases, and hence estimates a ratio of $n^{\tilde{\Omega}(\sqrt{n})}$ in one or more phases. The key insight is that even though the expected ratio might be large, its variance is not.

Lemma 11.3. *For $X \sim f_i$ with $f_i(x) = e^{-a_i\|x\|} \chi_K(x)$ for a convex body K , or $f_i(x) = f(x)^{a_i}$ for a logconcave function f , we have that the estimator $Y = \frac{f_{i+1}(X)}{f_i(X)}$ satisfies*

$$\frac{\mathbf{E}(Y^2)}{\mathbf{E}(Y)^2} \leq \left(\frac{a_{i+1}^2}{(2a_{i+1} - a_i)a_i} \right)^n$$

which is bounded by a constant for $a_i = a_{i+1} \left(1 + \frac{1}{\sqrt{n}}\right)$.

Theorem 11.4 ([53]). *The volume of a convex body in \mathbb{R}^n (given by a membership oracle) can be computed to relative error ε using $\tilde{O}(n^4/\varepsilon^2)$ oracle queries and $\tilde{O}(n^2)$ arithmetic operations per query.*

The LV algorithm has two parts. In the first it finds a transformation that puts the body in near-isotropic position. The complexity of this part is $\tilde{O}(n^4)$. In the second part, it runs the annealing schedule, while maintaining that the distribution being sampled is *well-rounded*, a weaker condition than isotropy. Well-roundedness requires that a level set of measure $\frac{1}{8}$ contains a constant-radius ball and the trace of the covariance (expected squared distance of a random point from the mean) to be bounded by $O(n)$, so that R/r is effectively $O(\sqrt{n})$. To achieve the complexity guarantee for the second phase, it suffices to use the KLS bound of $\psi_p \gtrsim n^{-\frac{1}{2}}$. Connecting improvements in the Cheeger constant directly to the complexity of volume computation was an open question for a couple of decades. To apply improvements in the Cheeger constant, one would need to replace well-roundedness with (near-)isotropy and maintain that. However, maintaining isotropy appears to be much harder — possibly requiring a sequence of $\Omega(n)$ distributions and $\Omega(n)$ samples from each, providing no gain over the current complexity of $O^*(n^4)$ even if the KLS conjecture turns out to be true.

A faster algorithm is known for well-rounded convex bodies (any isotropic logconcave density satisfies $\frac{R}{r} = O(\sqrt{n})$ and is well-rounded). This variant of simulated annealing, called Gaussian cooling utilizes the fact that the KLS conjecture holds for a Gaussian density restricted by any convex body, and completely avoids computing an isotropic transformation.

Theorem 11.5 ([20]). *The volume of a well-rounded convex body, i.e., with $R/r = O^*(\sqrt{n})$, can be computed using $O^*(n^3)$ oracle calls.*

In 2021, it was shown that the complexity of rounding a convex body can be bounded as $O^*(n^3\psi_n^2)$ where ψ_n is the KLS constant bound for any isotropic logconcave density in \mathbb{R}^n . Together with the next theorem, it follows that the volume of a convex body can be computed in the same complexity. The current bound on the KLS constant implies that this is in fact $O^*(n^3)$.

Theorem 11.6. *A near-isotropic transformation for any convex body in \mathbb{R}^n can be computed using $\tilde{O}(n^3)$ oracle calls and the volume of any convex body in \mathbb{R}^n can be computed using $O^*(n^3)$ oracle calls.*

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■ A.1 Divergence and Integration by Parts

The divergence (operator) of a function $\phi : \mathbb{R}^n \rightarrow \mathbb{R}$ is given by

$$\nabla \cdot f = \sum_{i=1}^n \frac{\partial f}{\partial x_i}.$$

For a vector field $v : \mathbb{R}^n \rightarrow \mathbb{R}^n$, we have

$$\nabla \cdot (fv) = \nabla f \cdot v + f(\nabla \cdot v).$$

From this, over a domain Ω , we have

$$\int_{\Omega} \nabla f \cdot v = \int_{\Omega} \nabla \cdot (fv) - \int_{\omega} f(\nabla \cdot v).$$

And using the divergence theorem, namely, $\int_{\Omega} \nabla f = \int_{\partial\Omega} f \vec{n}$, where \vec{n} is the normal vector at a point in $\partial\Omega$, we have:

$$\int_{\Omega} \nabla f \cdot v = \int_{\partial\Omega} fv \cdot \vec{n} - \int_{\omega} f(\nabla \cdot v).$$

The first term on the RHS become zero if the vector field v goes to 0 at the boundary of the domain (e.g., if the domain is \mathbb{R}^n , then if it decays at infinity).

■ A.2 Tips for Computing Gradients

In this section, we give some tips on how to do calculus.

■ A.2.1 Computing gradients via directional derivatives

Usually, computing gradients coordinate-by-coordinate is not the best way and we should avoid using summation notation as much as possible as it creates too many subscripts and is prone to mistakes. Instead, it is usually better to compute the gradient via directional derivatives. Here, we give a few examples for this. We define $Df(x)[h]$ be the directional derivative of f at x along the direction h . Namely,

$$Df(x)[h] \stackrel{\text{def}}{=} \left. \frac{d}{dt} \right|_{t=0} f(x + th).$$

Similarly, we use $D^k f(x)[h_1, h_2, \dots, h_k]$ to denote the directional k -th derivative of f at x along directions h_1, \dots, h_k .

Lemma A.1. *Given $A \in \mathbb{R}^{n \times d}$. Let $\Phi(x) = \sum_{i=1}^n f(a_i^\top x)$ where a_i is the i -th row of A . Then, we have $\nabla \Phi(x) = A^\top f'(Ax)$ and $\nabla^2 \Phi(x) = A^\top \text{diag}(f''(Ax))A$ where $f'(Ax)$ is the vector defined by $(f'(Ax))_i = f'(a_i^\top x)$.*

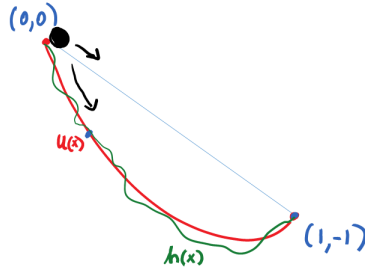


Figure A.1: The “fastest” curve

Proof. Note that

$$D\Phi(x)[h] = \sum_{i=1}^n f'(a_i^\top x) a_i^\top h,$$

$$D^2\Phi(x)[h, h] = \sum_{i=1}^n f''(a_i^\top x) (a_i^\top h)^2.$$

To write it in the traditional form, we note that

$$\nabla\Phi(x)^\top h = D\Phi(x)[h] = f'(Ax)^\top Ah = (A^\top f'(Ax))^\top h.$$

Since both side are the same for all h , we have $\nabla\Phi(x) = A^\top f'(Ax)$.

Similarly, we have

$$h^\top \nabla^2\Phi(x)h = D^2\Phi(x)[h, h]$$

$$= \sum_{i=1}^n (f''(Ax))_i (Ah)_i^2$$

$$= h^\top A^\top \text{diag}(f''(Ax)) Ah.$$

Since $\nabla^2\Phi(x) - A^\top \text{diag}(f''(Ax))A$ is symmetric and both side are the same for all h , we have $\nabla^2\Phi(x) = A^\top \text{diag}(f''(Ax))A$. \square

Exercise A.2. Use the above method to compute the gradient and Hessian of $f(X) = \log \det A^\top X A$.

Here is a more complicated example.

Lemma A.3 (Brachistochrone Problem). *Let $(x, u(x))$ be the curve from $(0, 0)$ to $(1, -1)$ where the first coordinate is the x axis and the second coordinate is the y axis. Suppose that this is the curve that takes the shortest time for a bead to slide along the curve frictionlessly from $(0, 0)$ to $(1, -1)$ under uniform gravity. Then, we have that*

$$2uu'' + (u')^2 + 1 = 0.$$

Remark. Take a look at Wikipedia for the Brachistochrone curve. It is counterintuitive!

Proof. Given a curve $u = u(x)$, the total travel time is

$$T(u) = \int_0^1 \frac{ds(x)}{v(x)} = \int_0^1 \frac{\sqrt{1 + (u'(x))^2}}{v(x)} dx$$

where ds is the arc length element and $v(x)$ is the velocity at x . By conservation of energy, i.e., the gained kinetic energy must equal the lost potential energy for every point along the curve, we know that

$$\frac{1}{2}mv(x)^2 = -mgu(x).$$

Hence, we have $v(x) = \sqrt{-2gu(x)}$ and so

$$T(u) = \int_0^1 \sqrt{\frac{1 + (u'(x))^2}{-2gu(x)}} dx.$$

Since u is a *shortest* curve, any local change in u cannot reduce the time, i.e.,

$$DT(u)[h] = 0$$

for any change h of the curve u . We next compute the directional derivative of $T(u)$, i.e., $\frac{d}{dt}|_{t=0}T(u+th)$:

$$\begin{aligned} DT(u)[h] &= \int_0^1 -\frac{1}{2} \frac{\sqrt{1 + (u'(x))^2}}{\sqrt{-2gu(x)}^{3/2}} \frac{d}{dt} u(x) dx + \int_0^1 \frac{1}{2} \frac{2u'(x)}{\sqrt{-2gu(x)}\sqrt{1 + (u'(x))^2}} \frac{d}{dt} u'(x) dx. \\ &= \int_0^1 -\frac{1}{2} \frac{\sqrt{1 + (u'(x))^2}}{\sqrt{-2gu(x)}u(x)} h(x) dx + \int_0^1 \frac{u'(x)h'(x)}{\sqrt{-2gu(x)}\sqrt{1 + (u'(x))^2}} dx. \end{aligned}$$

Note that the second term involves $h'(x)$. To change the term $h'(x)$ to $h(x)$, we use the integration by parts (with respect to x , not t !):

$$\int_0^1 \frac{u'(x)h'(x)}{\sqrt{-2gu(x)}\sqrt{1 + (u'(x))^2}} dx = \left[\frac{u'(x)h(x)}{\sqrt{-2gu(x)}\sqrt{1 + (u'(x))^2}} \right]_0^1 - \int_0^1 \frac{d}{dx} \left(\frac{u'(x)}{\sqrt{-2gu(x)}\sqrt{1 + (u'(x))^2}} \right) h(x) dx.$$

Since the endpoints of the curve are fixed, we have $h(1) = h(0) = 0$. Hence, the first term on the right hand side is 0. Continuing,

$$\begin{aligned} DT(u)[h] &= \int_0^1 -\frac{1}{2} \frac{\sqrt{1 + (u'(x))^2}}{\sqrt{-2gu(x)}u(x)} h(x) dx - \int_0^1 \frac{d}{dx} \left(\frac{u'(x)}{\sqrt{-2gu(x)}\sqrt{1 + (u'(x))^2}} \right) h(x) dx \\ &= \int_0^1 -\frac{1}{2} \frac{\sqrt{1 + (u'(x))^2}}{\sqrt{-2gu(x)}u(x)} h(x) dx - \int_0^1 \frac{u''(x)}{\sqrt{-2gu(x)}\sqrt{1 + (u'(x))^2}} h(x) dx \\ &\quad + \int_0^1 \frac{1}{2} \frac{u'(x)^2}{\sqrt{-2gu(x)}u(x)\sqrt{1 + (u'(x))^2}} h(x) dx \\ &\quad + \int_0^1 \frac{u'(x)u'(x)u''(x)}{\sqrt{-2gu(x)}(1 + (u'(x))^2)^{3/2}} h(x) dx. \end{aligned}$$

Hence, we have $DT(u)[h] = \int_0^1 a(x)h(x)dx$ where

$$\begin{aligned} a(x) &= \frac{-1}{2} \frac{\sqrt{1 + (u'(x))^2}}{\sqrt{-2gu(x)}u(x)} - \frac{u''(x)}{\sqrt{-2gu(x)}\sqrt{1 + (u'(x))^2}} + \frac{1}{2} \frac{u'(x)^2}{\sqrt{-2gu(x)}u(x)\sqrt{1 + (u'(x))^2}} \\ &\quad + \frac{u'(x)u'(x)u''(x)}{\sqrt{-2gu(x)}(1 + (u'(x))^2)^{3/2}}. \end{aligned} \tag{A.1}$$

Note that $a(x)$ is the gradient of T . Since $DT(u)[h] = 0$ for all $h(x)$, we have that $a(x) = 0$ for all x . Multiplying both sides of (A.1) by $2\sqrt{-2gu(x)}(1 + (u'(x))^2)^{3/2}u(x)$, we have

$$\begin{aligned} 0 &= (1 + (u'(x))^2)^2 - 2u(x)u''(x)(1 + (u'(x))^2) + u'(x)^2(1 + (u'(x))^2) + 2u(x)u'(x)^2u''(x) \\ &= -1 - u'(x)^2 - 2u(x)u''(x). \end{aligned}$$

□

■ A.2.2 Taking derivatives on both sides

Suppose we have a function $f(x, y)$ and $g(x)$ such that $f(x, g(x)) = 0$. The implicit function theorem shows that

$$D_x f(x, g(x)) + D_y f(x, g(x)) Dg(x) = 0$$

where $D_x f$ is the Jacobian of f with respect to x variables and $Dg(x)$ is the Jacobian of g . We note that the formula can be obtained from taking derivative on both sides with respect to x . Sometimes, taking derivatives on the both sides can greatly simplify calculations. Here are some examples.

Lemma A.4. Consider $x_t = \operatorname{argmin}_{x \in \mathbb{R}^n} f_t(x)$ where f_t are strictly convex. Then, we have

$$\frac{dx_t}{dt} = (\nabla^2 f_t(x_t))^{-1} \nabla \frac{df_t}{dt}(x_t).$$

Proof. By the optimality condition, we have $\nabla f_t(x_t) = 0$. Taking derivatives on both sides, we have

$$\nabla^2 f_t(x_t) \frac{dx_t}{dt} + \nabla \frac{df_t}{dt}(x_t) = 0.$$

Since f_t are strictly convex, $\nabla^2 f_t(x_t)$ is positive definite and is invertible. Hence, we have that the result. \square

In section 5.5, we used this to compute the derivative of central path.

■ A.3 Solving optimization problems by hand

In this section, we introduce the KKT condition and show how to use it to solve optimization problem by hand.

Theorem A.5 (Karush–Kuhn–Tucker theorem). Consider the following optimization problem

$$\min_{x \in \Omega} f(x) \text{ subject to } h_i(x) \leq 0 \text{ and } \ell_j(x) = 0 \text{ for all } i, j$$

for some open set Ω and continuously differentiable functions f , h_i and ℓ_j . If x is a local minimum, x satisfies the KKT conditions:

- *Stationary:* $\nabla f(x) + \sum_i u_i \nabla h_i(x) + \sum_j v_j \nabla \ell_j(x) = 0$
- *Complementary Slackness:* $u_i h_i(x) = 0$ for all i
- *Primal Feasibility:* $h_i(x) \leq 0$ and $\ell_j(x) = 0$ for all i, j
- *Dual Feasibility:* $u_i \geq 0$ for all i

We prove Holder's inequality as an example:

Fact A.6. For any vector $x, y \in \mathbb{R}^n$, we have $\|xy\|_1 \leq \|x\|_p \|y\|_q$ for any $1 \leq p \leq \infty$ and $1 \leq q \leq \infty$ with $\frac{1}{p} + \frac{1}{q} = 1$.

Proof. By symmetries, it suffices to compute

$$\max_{\|x\|_p \leq 1} \sum_i x_i y_i$$

for non-zero y . Now, we use the KKT theorem with $f(x) = -\sum_i x_i y_i$, $h(x) = \|x\|_p - 1$ and $\Omega = \mathbb{R}^n$. By the KKT conditions, for any maximizer x , we have that

$$\begin{aligned} -\nabla f(x) + u \nabla h(x) &= 0, \\ u h(x) &= 0, \\ h(x) &\leq 0, u \geq 0. \end{aligned}$$

Note that $\nabla f(x) = y$ and $(\nabla h(x))_i = \frac{1}{p} \|x\|_p^{1-p} \cdot p x_i^{p-1} = \|x\|_p^{1-p} \cdot x^{p-1}$. From the stationary condition, we have

$$y = u \|x\|_p^{1-p} \cdot x^{p-1}.$$

To compute u , we note that y is non-zero and hence $u \neq 0$. From the complementary slackness, we have $h(x) = 0$ and hence $\|x\|_p = 1$. Therefore, we have

$$y = u \cdot x^{p-1}.$$

Hence, we have $1 = \sum_i x_i^p = \sum_i (y_i/u)^{\frac{p}{p-1}} = \sum_i (y_i/u)^q$. Hence, we have $u = \|y\|_q$

Now, we can compute $\sum_i x_i y_i$ as follows

$$\sum_i x_i y_i = \sum_i \left(\frac{y_i}{u}\right)^{\frac{1}{p-1}} y_i = \frac{1}{u^{1/(p-1)}} \sum_i y_i^{p/(p-1)} = \|y\|_q.$$

□

Appendix B

Notation

[illegible]