Lecture 8: Introduction to Convex Optimization

Reading: *Convex optimization* by Boyd and Vandenberghe.

GU4241/GR5241 Statistical Machine Learning

Linxi Liu

February 9, 2017

Optimization Problems

Terminology

An **optimization problem** for a given function $f : \mathbb{R}^d \to \mathbb{R}$ is a problem of the form

$$\min_{\mathbf{x}} f(\mathbf{x})$$

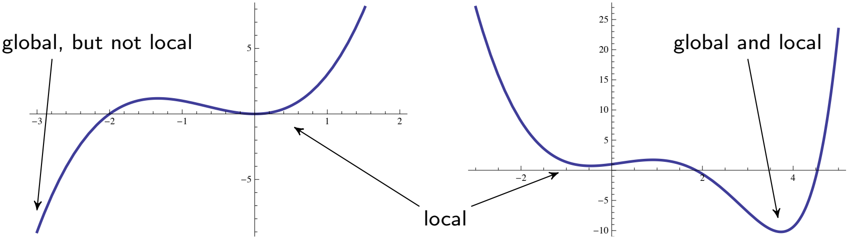
which we read as "find $\mathbf{x}_0 = \arg\min_{\mathbf{x}} f(\mathbf{x})$".
A **constrained optimization problem** adds additional requirements on $\mathbf{x}$,

$$\begin{aligned} &\min_{\mathbf{x}} \ f(\mathbf{x}) \\ \text{subject to} \quad &\mathbf{x} \in G \ , \end{aligned}$$

where $G \subset \mathbb{R}^d$ is called the **feasible set**. The set G is often defined by equations, e.g.

$$\begin{aligned} &\min_{\mathbf{x}} \ f(\mathbf{x}) \\ \text{subject to} \quad &g(\mathbf{x}) \geq 0 \end{aligned}$$

Types of Minima



Local and global minima

A minimum of f at x is called:

- **Global** if f assumes no smaller value on its domain.
- **Local** if there is some open neighborhood U of x such that $f(x)$ is a global minimum of f restricted to U.

Optima

Analytic criteria for local minima

Recall that $\mathbf{x}$ is a local minimum of f if

$$f'(\mathbf{x}) = 0 \qquad \text{and} \qquad f''(\mathbf{x}) > 0 \; .$$

In $\mathbb{R}^d$,

$$\nabla f(\mathbf{x}) = 0 \qquad \text{and} \qquad H_f(\mathbf{x}) = \Big(\frac{\partial f}{\partial x_i \partial x_j}(\mathbf{x}) \Big)_{i,j=1,\ldots,n} \text{ positive definite.}$$

The $d \times d$-matrix $H_f(\mathbf{x})$ is called the **Hessian matrix** of f at $\mathbf{x}$.

Optima

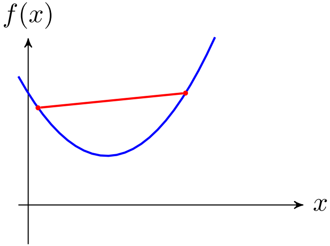
Numerical methods

All numerical minimization methods perform roughly the same steps:

- Start with some point x_0.
- Our goal is to find a sequence $x_0, \ldots, x_m$ such that $f(x_m)$ is a minimum.
- At a given point x_n, compute properties of f (such as $f'(x_n)$ and $f''(x_n)$).
- Based on these values, choose the next point x_{n+1}.

The information $f'(x_n)$, $f''(x_n)$ etc is always *local at* x_n, and we can only decide whether a point is a local minimum, not whether it is global.

Convex Functions



Definition

A function f is **convex** if every line segment between function values lies above the graph of f.

Analytic criterion

A twice differentiable function is convex if $f''(x) \geq 0$ (or $H_f(\mathbf{x})$ positive semidefinite) for all $\mathbf{x}$.

Implications for optimization

If f is convex, then:

- $f'(x) = 0$ is a sufficient criterion for a minimum.
- Local minima are global.
- If f is **strictly convex** ($f'' > 0$ or H_f positive definite), there is only one minimum (which is both gobal and local).

Gradient Descent

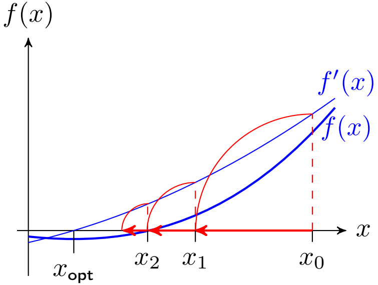
Algorithm

Gradient descent searches for a minimum of f.

1. Start with some point $x \in \mathbb{R}$ and fix a precision $\varepsilon > 0$.
2. Repeat for $n = 1, 2, \ldots$

$$x_{n+1} := x_n - f'(x_n)$$

3. Terminate when $|\, f'(x_n)| < \varepsilon$.



Newton's Method: Roots

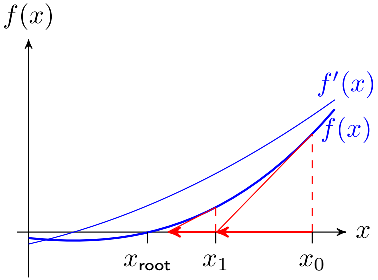
Algorithm

Newton's method searches for a **root** of f, i.e. it solves the equation $f(\mathbf{x}) = 0$.

1. Start with some point $x \in \mathbb{R}$ and fix a precision $\varepsilon > 0$.
2. Repeat for $n = 1, 2, \ldots$

$$x_{n+1} := x_n - f(x_n)/f'(x_n)$$

3. Terminate when $|f(x_n)| < \varepsilon$.



Basic Applications

Function evaluation

Most numerical evaluations of functions ($\sqrt{a}$, $\sin(a)$, $\exp(a)$, etc) are implemented using Newton's method. To evaluate g at a, we have to transform $x = g(a)$ into an equivalent equation of the form

$$f(x, a) = 0 \ .$$

We then fix a and solve for x using Newton's method for roots.

Example: Square root

To eveluate $g(a) = \sqrt{a}$, we can solve

$$f(x, a) = x^2 - a = 0 \ .$$

This is essentially how `sqrt()` is implemented in the standard C library.

Newton's Method: Minima

it is quadratic method

Algorithm

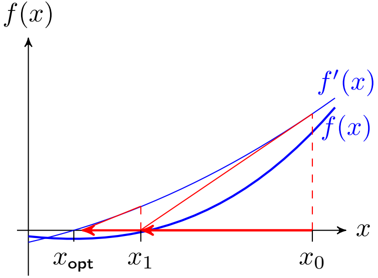
We can use Newton's method for minimization by applying it to solve $f'(\mathbf{x}) = 0$.

1. Start with some point $x \in \mathbb{R}$ and fix a precision $\varepsilon > 0$.
2. Repeat for $n = 1, 2, \ldots$

$$x_{n+1} := x_n - f'(x_n)/f''(x_n)$$

3. Terminate when $|\, f'(x_n)| < \varepsilon$.

| f(xn+1) - f(x*) | < c/n^2



Multiple Dimensions

In $\mathbb{R}^d$ we have to replace the derivatives by their vector space analogues.

Gradient descent

$$\mathbf{x}_{n+1} := \mathbf{x}_n - \nabla f(\mathbf{x}_n)$$

Newton's method for minima

$$\mathbf{x}_{n+1} := \mathbf{x}_n - H_f^{-1}(\mathbf{x}_n) \cdot \nabla f(\mathbf{x}_n)$$

The inverse of $H_f(\mathbf{x})$ exists only if the matrix is positive definite (not if it is only semidefinite), i.e. f has to be strictly convex.

The Hessian measures the curvature of f.

Effect of the Hessian

Multiplication by H_f^{-1} in general changes the direction of $\nabla f(\mathbf{x}_n)$. The correction takes into account how $\nabla f(\mathbf{x})$ changes away from $\mathbf{x}_n$, as estimated using the Hessian at $\mathbf{x}_n$.

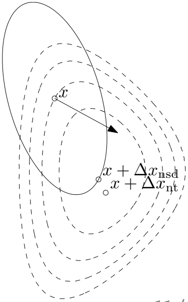


Figure: Arrow is ∇f, $x + \Delta x_{\mathsf{nt}}$ is Newton step.

Newton: Properties

Convergence

- The algorithm always converges if $f'' > 0$ (or H_f positive definite).
- The speed of convergence separates into two phases:
  - In a (possibly small) region around the minimum, f can always be approximated by a quadratic function.
  - Once the algorithm reaches that region, the error decreases at quadratic rate. Roughly speaking, the number of correct digits in the solution doubles in each step.
  - Before it reaches that region, the convergence rate is linear.

High dimensions

computational cost is high, used in high dimension data

- The required number of steps hardly depends on the dimension of $\mathbb{R}^d$. Even in $\mathbb{R}^{10000}$, you can usually expect the algorithm to reach high precision in half a dozen steps.
- Caveat: The individual steps can become very expensive, since we have to invert H_f in each step, which is of size $d \times d$.

Next: Constrained Optimization

So far

- If f is differentiable, we can search for local minima using gradient descent.
- If f is sufficiently nice (convex and twice differentiable), we know how to speed up the search process using Newton's method.

Constrained problems

- The numerical minimizers use the criterion $\nabla f(x) = 0$ for the minimum.
- In a constrained problem, the minimum is *not* identified by this criterion.

Next steps

We will figure out how the constrained minimum can be identified. We have to distinguish two cases:

- Problems involving only equalities as constraints (easy).
- Problems also involving inequalities (a bit more complex).

Optimization Under Constraints

Objective

$$\min f(\mathbf{x})$$
$$\text{subject to } g(\mathbf{x}) = 0$$

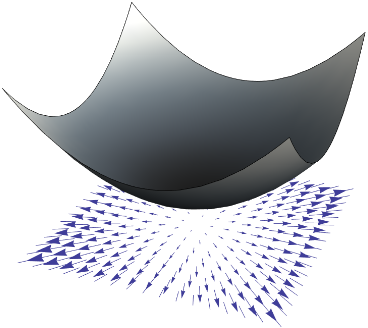
Idea

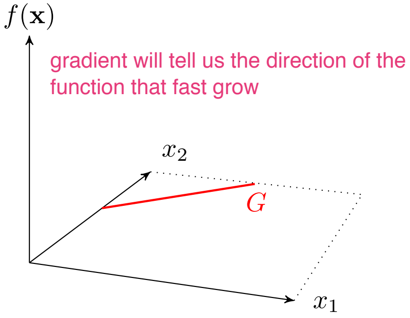
- The feasible set is the set of points $\mathbf{x}$ which satisfy $g(\mathbf{x}) = 0$,

  $$G := \{\mathbf{x} \,|\, g(\mathbf{x}) = 0\} \;.$$

  If g is reasonably smooth, G is a smooth surface in $\mathbb{R}^d$.
- We restrict the function f to this surface and call the restricted function f_g.
- The constrained optimization problem says that we are looking for the minimum of f_g.

Lagrange Optimization





Constraint g.

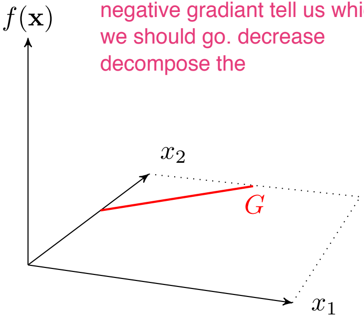
$$f(\mathbf{x}) = x_1^2 + x_2^2$$

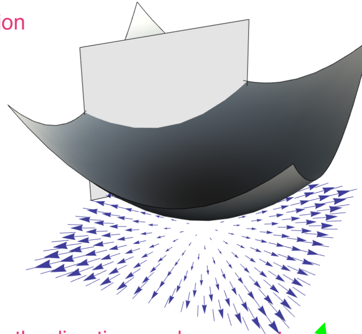
The blue arrows are the gradients $\nabla f(\mathbf{x})$ at various values of $\mathbf{x}$.

Here, g is linear, so the graph of g is a (sloped) affine plane. The intersection of the plane with the x_1-x_2-plane is the set G of all points $\mathbf{x}$ with $g(\mathbf{x}) = 0$.

Lagrange Optimization

negative gradiant tell us which direction
we should go. decrease
decompose the

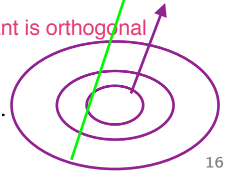




the direction can be opposet

- We can make the function f_g given by the constraint $g(\mathbf{x}) = 0$ visible by placing a plane vertically through G. The graph of f_g is the intersection of the graph of f with the plane.

gradiant is orthogonal



- Here, f_g has parabolic shape.
- The gradient of f at the miniumum of f_g is *not* 0.

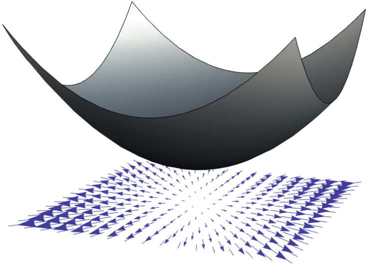
Gradients and Contours

Fact

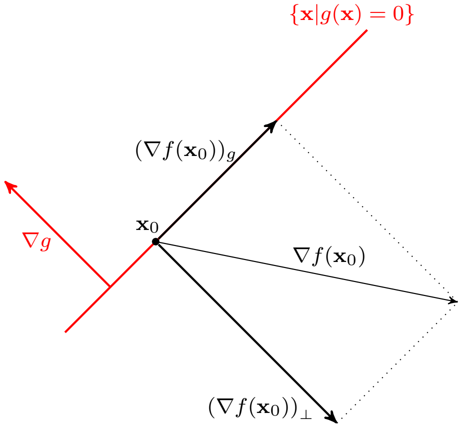
Gradients are orthogonal to contour lines.

Intuition

- The gradient points in the direction in which f grows most rapidly.
- Contour lines are sets along which f does not change.



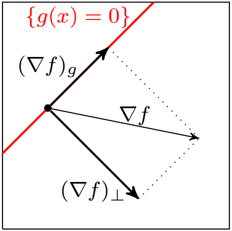
The Crucial Bit



Again, in detail.

Idea

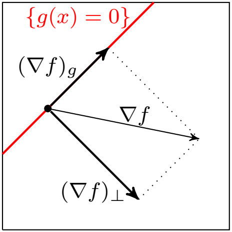
- Decompose ∇f into a component $(\nabla f)_g$ in the set $\{\mathbf{x} \mid g(\mathbf{x}) = 0\}$ and a remainder $(\nabla f)_\perp$.
- The two components are orthogonal.
- If f_g is minimal within $\{\mathbf{x} \mid g(\mathbf{x}) = 0\}$, the component within the set vanishes.
- The remainder need not vanish.



Again, in detail.

Idea

- Decompose ∇f into a component $(\nabla f)_g$ in the set $\{\mathbf{x} \,|\, g(\mathbf{x}) = 0\}$ and a remainder $(\nabla f)_\perp$.
- The two components are orthogonal.
- If f_g is minimal within $\{\mathbf{x} \,|\, g(\mathbf{x}) = 0\}$, the component within the set vanishes.
- The remainder need not vanish.



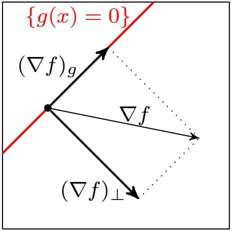
Consequence

- We need a criterion for $(\nabla f)_g = 0$.

Again, in detail.

Idea

- Decompose ∇f into a component $(\nabla f)_g$ in the set $\{\mathbf{x} \,|\, g(\mathbf{x}) = 0\}$ and a remainder $(\nabla f)_\perp$.
- The two components are orthogonal.
- If f_g is minimal within $\{\mathbf{x} \,|\, g(\mathbf{x}) = 0\}$, the component within the set vanishes.
- The remainder need not vanish.



Solution

- If $(\nabla f)_g = 0$, then ∇f is orthogonal to the set $g(\mathbf{x}) = 0$.
- Since gradients are orthogonal to contours, and the set is a contour of g, ∇g is also orthogonal to the set.
- Hence: At a minimum of f_g, the two gradients point in the same direction: $\nabla f + \lambda \nabla g = 0$ for some scalar $\lambda \neq 0$.

Solution: Constrained Optimization

Solution

The constrained optimization problem

$$\min_{\mathbf{x}} \quad f(\mathbf{x})$$
$$\text{s.t.} \quad g(\mathbf{x}) = 0$$

is solved by solving the equation system

$$\begin{aligned} \nabla f(\mathbf{x}) + \lambda \nabla g(\mathbf{x}) &= 0 \\ g(\mathbf{x}) &= 0 \end{aligned}$$

Text

The vectors ∇f and ∇g are D-dimensional, so the system contains $D+1$ equations for the $D+1$ variables $x_1, \ldots, x_D, \lambda$.

first case: X* E d(G): d(f) = -λd(g), λ≦0
second case: X* E int G: d(f) = 0; g(x) < 0
combine: λg(x) = 0, λ≧ 0
d(f) = -λd(g)
λ ≧ 0 KKT CONDITION

Inequality Constraints

Objective

For a function f and a convex function g, solve

g(x) = 0

d(f) int G

$$\min f(\mathbf{x})$$
$$\text{subject to } g(\mathbf{x}) \leq 0$$

i.e. we replace $g(\mathbf{x}) = 0$ as previously by $g(\mathbf{x}) \leq 0$. This problem is called an optimization problem with **inequality constraint**.

Text

Feasible set

We again write G for the set of all points which satisfy the constraint,

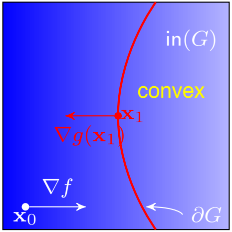
$$G := \{\mathbf{x} \,|\, g(\mathbf{x}) \leq 0\} \ .$$

G is often called the **feasible set** (the same name is used for equality constraints).

Two Cases

Case distinction

1. The location $\mathbf{x}$ of the minimum can be in the *interior* of G
2. $\mathbf{x}$ may be on the *boundary* of G.



lighter shade of blue = larger value of f

Decomposition of G

$$G = \text{in}(G) \cup \partial G = \text{ interior } \cup \text{ boundary}$$

Note: The interior is given by $g(\mathbf{x}) < 0$, the boundary by $g(\mathbf{x}) = 0$.

Criteria for minimum

1. **In interior:** $f_g = f$ and hence $\nabla f_g = \nabla f$. We have to solve a standard optimization problem with criterion $\nabla f = 0$.
2. **On boundary:** Here, $\nabla f_g \neq \nabla f$. Since $g(\mathbf{x}) = 0$, the geometry of the problem is the same as we have discussed for equality constraints, with criterion $\nabla f = \lambda \nabla g$. λ has to greater than 0
   However: In this case, the sign of λ matters.

On the Boundary

Observation

- An extremum on the boundary is a minimum only if ∇f points *into* G.
- Otherwise, it is a maximum instead.

Criterion for minimum on boundary

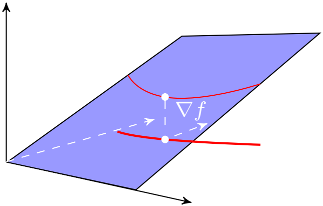
Since ∇g points *away* from G (since g increases away from G), ∇f and ∇g have to point in opposite directions:

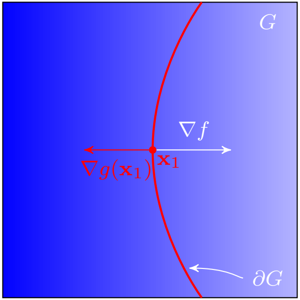
$$\nabla f = \lambda \nabla g \qquad \text{with } \lambda < 0$$

Convention

To make the sign of λ explicit, we constrain λ to positive values and instead write:

$$\nabla f = -\lambda \nabla g$$
$$\text{s.t. } \lambda > 0$$





Combining the Cases

Combined problem

$$\begin{aligned} \nabla f &= -\lambda \nabla g \\ \text{s.t.} \quad g(\mathbf{x}) &\leq 0 \\ \lambda &= 0 \text{ if } \mathbf{x} \in \text{in}(G) \\ \lambda &> 0 \text{ if } \mathbf{x} \in \partial G \end{aligned}$$

Text

Can we get rid of the "if $\mathbf{x} \in \cdot$" distinction?

Yes: Note that $g(\mathbf{x}) < 0$ if $\mathbf{x}$ in interior and $g(\mathbf{x}) = 0$ on boundary. Hence, we always have either $\lambda = 0$ or $g(\mathbf{x}) = 0$ (and never both).

That means we can substitute

$$\begin{aligned} \lambda &= 0 \text{ if } \mathbf{x} \in \text{in}(G) \\ \lambda &> 0 \text{ if } \mathbf{x} \in \partial G \end{aligned}$$

by

$$\lambda \cdot g(\mathbf{x}) = 0 \qquad \text{and} \qquad \lambda \geq 0\ .$$

Solution: Inequality Constraints

Combined solution

The optimization problem with inequality constraints

$$\min f(\mathbf{x})$$
$$\text{subject to } g(\mathbf{x}) \leq 0$$

can be solved by solving

$$\text{s.t.} \qquad \left.\begin{aligned} \nabla f(\mathbf{x}) &= -\lambda \nabla g(\mathbf{x}) \\ \lambda g(\mathbf{x}) &= 0 \end{aligned}\right\} \longleftarrow \text{system of } d+1 \text{ equations for } d+1 \text{ variables } x_1, \ldots, x_D, \lambda$$
$$g(\mathbf{x}) \leq 0$$
$$\lambda \geq 0$$

These conditions are known as the **Karush-Kuhn-Tucker** (or **KKT**) conditions.

Remarks

Haven't we made the problem more difficult?

- To simplify the minimization of f for $g(\mathbf{x}) \leq 0$, we have made f more complicated and added a variable and two constraints. Well done.
- However: In the original problem, we *do not know how to minimize* f, since the usual criterion $\nabla f = 0$ does not work.
- By adding λ and additional constraints, we have reduced the problem to solving a system of equations.

Summary: Conditions

Condition	Ensures that...	Purpose
$\nabla f(\mathbf{x}) = -\lambda \nabla g(\mathbf{x})$	If $\lambda = 0$: ∇f is 0	Opt. criterion inside G
	If $\lambda > 0$: ∇f is anti-parallel to ∇g	Opt. criterion on boundary
$\lambda g(\mathbf{x}) = 0$	$\lambda = 0$ in interior of G	Distinguish cases in(G) and ∂G
$\lambda \geq 0$	∇f cannot flip to orientation of ∇g	Optimum on ∂G is minimum

Why Should g be Convex?

More precisely

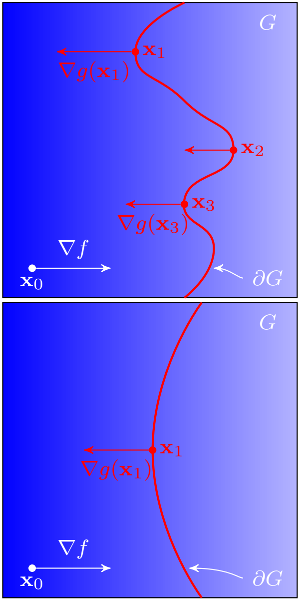
If g is a convex function, then $G = \{\mathbf{x} \,|\, g(\mathbf{x}) \leq 0\}$ is a convex set. Why do we require convexity of G?

Problem

If G is not convex, the KKT conditions do not guarantee that $\mathbf{x}$ is a minimum. (The conditions still hold, i.e. if G is not convex, they are necessary conditions, but not sufficient.)

Example (Figure)

- f is a linear function (lighter color = larger value)
- ∇f is identical everywhere
- If G is not convex, there can be several points ($\mathbf{x}_1$, $\mathbf{x}_2$, $\mathbf{x}_3$) which satisfy the KKT conditions. Only $\mathbf{x}_1$ minimizes f on G.
- G is convex, such problems cannot occur.



Interior Point Methods

Numerical methods for constrained problems

Once we have transformed our problem using Lagrange multipliers, we still have to solve a problem of the form

$$\begin{aligned} & \nabla f(\mathbf{x}) = -\lambda \nabla g(\mathbf{x}) \\ \text{s.t.} \quad & \lambda g(\mathbf{x}) = 0 \quad \text{and} \quad g(\mathbf{x}) \leq 0 \quad \text{and} \quad \lambda \geq 0 \end{aligned}$$

numerically.

Barrier functions

Idea

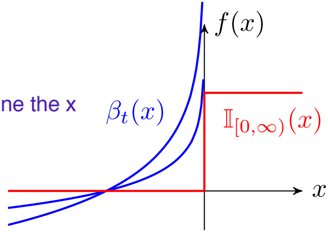
A constraint in the problem

$$\min f(x) \qquad \text{s.t.} \quad g(x) < 0$$

min: f(x) +βt(g(x)), use barrier function to confine the x

can be expressed as an indicator function:

$$\min f(x) + const. \cdot \mathbb{I}_{[0,\infty)}(g(x))$$



The constant must be chosen large enough to enforce the constraint.

as t increase, the β(x) would close to the original indicator function

Problem: The indicator function is piece-wise constant and not differentiable at 0. Newton or gradient descent are not applicable.

Barrier function

A **barrier function** approximates $\mathbb{I}_{[0,\infty)}$ by a smooth function, e.g.

$$\beta_t(x) := -\frac{1}{t}\log(-x) \ .$$

Newton for Constrained Problems

Interior point methods

We can (approximately) solve

$$\min f(x) \text{ s.t. } \quad g_i(x) < 0 \qquad \text{for } i = 1, \dots, m$$

by solving

$$\min f(x) + \sum_{i=1}^{m} \beta_{i,t}(x) \; .$$

with one barrier function $\beta_{i,t}$ for each constraint g_i.
We do not have to adjust a multiplicative constant since $\beta_t(x) \to \infty$ as $x \nearrow 0$.

Constrained problems: General solution strategy

1. Convert constraints into solvable problem using Lagrange multipliers.
2. Convert constraints of transformed problem into barrier functions.
3. Apply numerical optimization (usually Newton's method).

Recall: SVM

Original optimization problem

$$\min_{\mathbf{v}_{\mathsf{H}},c} \|\mathbf{v}_{\mathsf{H}}\|_2 \qquad \text{s.t.} \quad y_i(\langle \mathbf{v}_{\mathsf{H}}, \tilde{\mathbf{x}}_i \rangle - c) \geq 1 \quad \text{for } i = 1, \ldots, n$$

Problem with inequality constraints $g_i(\mathbf{v}_{\mathsf{H}}) \leq 0$ for $g_i(\mathbf{v}_{\mathsf{H}}) := 1 - y_i(\langle \mathbf{v}_{\mathsf{H}}, \tilde{\mathbf{x}}_i \rangle - c)$.

Transformed problem

If we transform the problem using Lagrange multipliers $\alpha_1, \ldots, \alpha_n$, we obtain:

$$\begin{aligned} \max_{\boldsymbol{\alpha} \in \mathbb{R}^n} \qquad & W(\boldsymbol{\alpha}) := \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_i \alpha_j \tilde{y}_i \tilde{y}_j \langle \tilde{\mathbf{x}}_i, \tilde{\mathbf{x}}_j \rangle \\ \text{s.t.} \qquad & \sum_{i=1}^{n} \tilde{y}_i \alpha_i = 0 \\ & \alpha_i \geq 0 \qquad \text{for } i = 1, \ldots, n \end{aligned}$$

This is precisely the "dual problem" we obtained before using geometric arguments. We can find the max-margin hyperplane using an interior point method.

Relevance in Statistics

Minimization problems

Most methods that we encounter in this class can be phrased as minimization problem. For example:

Problem	Objective function
ML estimation	negative log-likelihood
Classification	empirical risk bayes classifier
Regression	fitting or prediction error rss
Unsupervised learning	suitable cost function (later)

More generally

The lion's share of algorithms in statistics or machine learning fall into either of two classes:

1. Optimization methods.
2. Simulation methods (e.g. Markov chain Monte Carlo algorithms).