

Convex optimization

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Soft-margin SVMs

Formulated learning as a mathematical optimization problem defined by training data $\{(\mathbf{x}_i, y_i)\}_{i=1}^n$:

$$\min_{\mathbf{w} \in \mathbb{R}^d, t \in \mathbb{R}} \quad \frac{\lambda}{2} \|\mathbf{w}\|_2^2 + \frac{1}{n} \sum_{i=1}^n \ell_{\text{hinge}}(\mathbf{w}, t; \mathbf{x}_i, y_i),$$

where

$$\ell_{\text{hinge}}(\mathbf{w}, t; \mathbf{x}, y) := \left[1 - y(\langle \mathbf{w}, \mathbf{x} \rangle - t) \right]_+.$$

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General form

Empirical risk minimization (i.e., minimize training error rate):

$$\min_{\mathbf{w} \in \mathbb{R}^d, t \in \mathbb{R}} \quad \frac{1}{n} \sum_{i=1}^n \mathbb{1}\{y_i(\langle \mathbf{w}, \mathbf{x}_i \rangle - t) \leq 0\}$$

Soft-margin SVM:

$$\min_{\mathbf{w} \in \mathbb{R}^d, t \in \mathbb{R}} \quad \frac{\lambda}{2} \|\mathbf{w}\|_2^2 + \frac{1}{n} \sum_{i=1}^n \ell_{\text{hinge}}(\mathbf{w}, t; \mathbf{x}_i, y_i)$$

Generic learning objective:

$$\min_{\mathbf{w} \in \mathbb{R}^d} \quad R(\mathbf{w}) + \frac{1}{n} \sum_{i=1}^n \ell(\mathbf{w}; \mathbf{x}_i, y_i)$$

- **Regularization term:** encodes “learning bias” (e.g., prefer large margins).
- **Training loss term:** how poor is the “fit” to the training data.

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Learning via optimization

- Many different choices for regularization and loss.

- $R(\mathbf{w}) = \lambda \|\mathbf{w}\|_2^2 / 2$: encourage large margins
- $R(\mathbf{w}) = \lambda \|\mathbf{w}\|_1$: encourage \mathbf{w} to be sparse
- $R(\mathbf{w}) = \lambda \sum_{i=1}^{d-1} |w_{i+1} - w_i|$: useful for ordered features.
- $\ell(\mathbf{w}; \mathbf{x}, y) = [\langle \mathbf{w}, \mathbf{x} \rangle - y]_+^2$
- $\ell(\mathbf{w}, t; \mathbf{x}, y) = \ln(1 + \exp(-y(\langle \mathbf{w}, \mathbf{x} \rangle - t)))$ (logistic regression)
- ...
- Also used beyond classification (e.g., regression, parameter estimation, clustering)

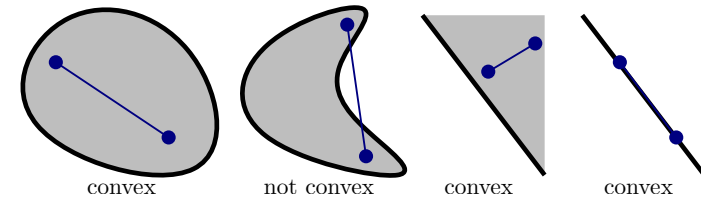
- For classification problems, often want ℓ to be an upper-bound on zero-one loss—i.e., a **surrogate loss**.
- Trade-off parameter $\lambda > 0$: usually determine using cross validation.
- Computationally easier when overall objective function is **convex**: possible to efficiently find global minimizer in polynomial time.

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Introduction to convexity

Convex sets

A set A is **convex** if, for every pair of points $\{x, x'\}$ in A , the line segment between x and x' is also contained in A .



Examples:

- ▶ All of \mathbb{R}^d .
- ▶ Empty set.
- ▶ Affine hyperplanes.
- ▶ Half-spaces: $\{a \in \mathbb{R}^d : \langle a, x \rangle - b \leq 0\}$.
- ▶ Intersections of convex sets.
- ▶ Convex hulls:
 $\text{conv}(S) := \{\sum_{i=1}^k \alpha_i x_i : k \in \mathbb{N}, x_i \in S, \alpha_i \geq 0, \sum_{i=1}^k \alpha_i = 1\}$.

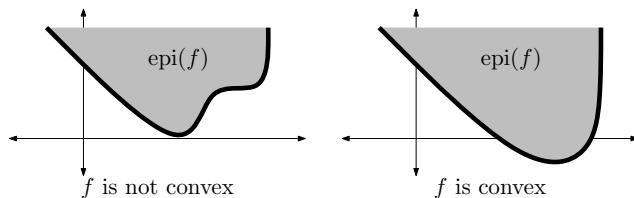
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Convex functions

For any function $f: \mathbb{R}^d \rightarrow \mathbb{R}$, the **epigraph** of f , denoted $\text{epi}(f)$, is the set

$$\text{epi}(f) := \{(x, b) \in \mathbb{R}^{d+1} : f(x) \leq b\}.$$

A function f is **convex** if $\text{epi}(f)$ is a convex set in \mathbb{R}^{d+1} .



Examples:

- ▶ $f(x) = c^x$ for any $c > 0$ (on \mathbb{R})
- ▶ $f(x) = |x|^c$ for any $c \geq 1$ (on \mathbb{R})
- ▶ $f(x) = c$ for any constant $c \in \mathbb{R}$.
- ▶ $f(x) = \langle a, x \rangle$ for any $a \in \mathbb{R}^d$.
- ▶ $f(x) = \|x\|$ for any norm $\|\cdot\|$.
- ▶ $f(x) = \langle x, Ax \rangle$ for symmetric positive semidefinite A .

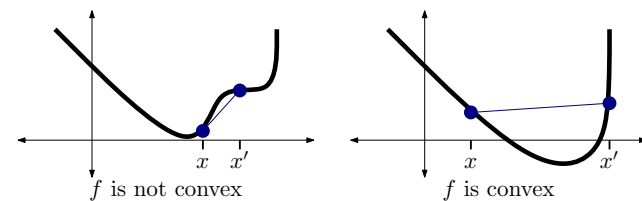
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Jensen's inequality

Equivalent definition of convex functions

A function $f: \mathbb{R}^d \rightarrow \mathbb{R}$ is convex iff for any $x, x' \in \mathbb{R}^d$ and $\alpha \in [0, 1]$,

$$f((1 - \alpha)x + \alpha x') \leq (1 - \alpha) \cdot f(x) + \alpha \cdot f(x').$$



Jensen's inequality

If $f: \mathbb{R}^d \rightarrow \mathbb{R}$ is convex, then for any $x_1, x_2, \dots, x_n \in \mathbb{R}^d$ and $\alpha_1, \alpha_2, \dots, \alpha_n \in [0, 1]$ such that $\sum_{i=1}^n \alpha_i = 1$,

$$f\left(\sum_{i=1}^n \alpha_i x_i\right) \leq \sum_{i=1}^n \alpha_i \cdot f(x_i).$$

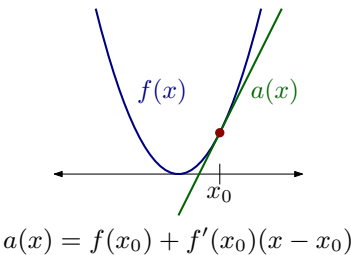
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Differentiable functions

If $f: \mathbb{R}^d \rightarrow \mathbb{R}$ is differentiable, then f is convex if and only if

$$f(\mathbf{x}) \geq f(\mathbf{x}_0) + \langle \nabla f(\mathbf{x}_0), \mathbf{x} - \mathbf{x}_0 \rangle$$

for all $\mathbf{x}, \mathbf{x}_0 \in \mathbb{R}^d$.



Twice-differentiable functions

If $f: \mathbb{R}^d \rightarrow \mathbb{R}$ is twice-differentiable, then f is convex if and only if

$$\nabla^2 f(\mathbf{x}) \succeq \mathbf{0}$$

for all $\mathbf{x} \in \mathbb{R}^d$ (i.e., the Hessian, or matrix of second-derivatives, is positive semidefinite for all \mathbf{x}).

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Convex optimization problems

Optimization problems

A typical optimization problem (in standard form) is written as

$$\begin{array}{ll} \min_{\mathbf{x} \in \mathbb{R}^d} & f_0(\mathbf{x}) \\ \text{s.t.} & f_i(\mathbf{x}) \leq 0 \quad \text{for all } i = 1, 2, \dots, n. \end{array}$$

- ▶ $f_0: \mathbb{R}^d \rightarrow \mathbb{R}$ is the **objective function**;
- ▶ $f_1, f_2, \dots, f_n: \mathbb{R}^d \rightarrow \mathbb{R}$ are the **constraint functions**;
- ▶ inequalities $f_i(\mathbf{x}) \leq 0$ are **constraints**;
- ▶ $A := \{\mathbf{x} \in \mathbb{R}^d : f_i(\mathbf{x}) \leq 0 \text{ for all } i = 1, 2, \dots, n\}$ is the **feasible region**.
- ▶ **The goal**: Find $\mathbf{x} \in A$ so that $f_0(\mathbf{x})$ is as small as possible.
- ▶ **(Optimal) value** of the optimization problem is the smallest such value of $f_0(\mathbf{x})$ achieved by a feasible point $\mathbf{x} \in A$.
- ▶ Point $\mathbf{x} \in A$ achieving the optimal value is a **(global) minimizer** of the problem.

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Convex optimization problems

Standard form of a **convex optimization problem**:

$$\begin{array}{ll} \min_{\mathbf{x} \in \mathbb{R}^d} & f_0(\mathbf{x}) \\ \text{s.t.} & f_i(\mathbf{x}) \leq 0 \quad \text{for all } i = 1, 2, \dots, n \end{array}$$

where $f_0, f_1, \dots, f_n: \mathbb{R}^d \rightarrow \mathbb{R}$ are *convex functions*.

Fact: the feasible set $A := \{\mathbf{x} \in \mathbb{R}^d : f_i(\mathbf{x}) \leq 0 \text{ for all } i = 1, 2, \dots, n\}$ is a convex set.

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Example: Soft-margin SVM

$$\begin{aligned} \min_{\mathbf{w} \in \mathbb{R}^d, t \in \mathbb{R}, \boldsymbol{\xi} \in \mathbb{R}^n} \quad & \frac{\lambda}{2} \|\mathbf{w}\|_2^2 + \frac{1}{n} \sum_{i=1}^n \xi_i \\ \text{s.t.} \quad & y_i (\langle \mathbf{w}, \mathbf{x}_i \rangle - t) \geq 1 - \xi_i \quad \text{for all } i = 1, 2, \dots, n, \\ & \xi_i \geq 0 \quad \text{for all } i = 1, 2, \dots, n. \end{aligned}$$

Bringing to standard form:

$$\begin{aligned} \min_{\mathbf{w} \in \mathbb{R}^d, t \in \mathbb{R}, \boldsymbol{\xi} \in \mathbb{R}^n} \quad & \frac{\lambda}{2} \|\mathbf{w}\|_2^2 + \frac{1}{n} \sum_{i=1}^n \xi_i \quad (\text{sum of two convex functions, also convex}) \\ \text{s.t.} \quad & 1 - \xi_i - y_i (\langle \mathbf{w}, \mathbf{x}_i \rangle - t) \leq 0 \quad \text{for all } i = 1, \dots, n \quad (\text{linear}) \\ & -\xi_i \leq 0 \quad \text{for all } i = 1, \dots, n \quad (\text{linear}) \end{aligned}$$

Local minimizers

Consider an optimization problem (not necessarily convex):

$$\begin{aligned} \min_{\mathbf{x} \in \mathbb{R}^d} \quad & f_0(\mathbf{x}) \\ \text{s.t.} \quad & \mathbf{x} \in A. \end{aligned}$$

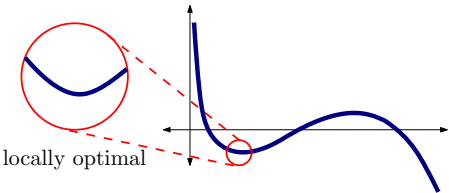
We say $\tilde{\mathbf{x}} \in A$ is a **local minimizer** if there is an open ball

$$U := \left\{ \mathbf{x} \in \mathbb{R}^d : \|\mathbf{x} - \tilde{\mathbf{x}}\|_2 < r \right\}$$

of positive radius $r > 0$ such that $\tilde{\mathbf{x}}$ is a global minimizer for

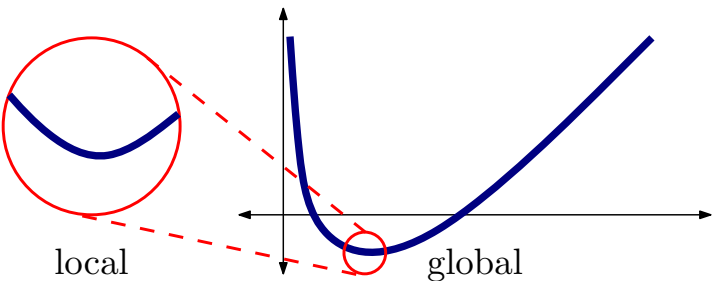
$$\begin{aligned} \min_{\mathbf{x} \in \mathbb{R}^d} \quad & f_0(\mathbf{x}) \\ \text{s.t.} \quad & \mathbf{x} \in A \cap U. \end{aligned}$$

Nothing looks better than $\tilde{\mathbf{x}}$ in the immediate vicinity of $\tilde{\mathbf{x}}$.



Local minimizers of convex opt. problems

If the optimization problem is **convex**, and $\tilde{\mathbf{x}} \in A$ is a **local minimizer**, then it is also a **global minimizer**.



Local optimization algorithms

Unconstrained convex optimization problem

$$\min_{\mathbf{x} \in \mathbb{R}^d} f(\mathbf{x})$$

(f is the convex objective function; feasible region is \mathbb{R}^d).

Optimality condition for differentiable convex objectives

\mathbf{x}^* is a global minimizer if and only if $\nabla f(\mathbf{x}^*) = \mathbf{0}$.

Unfortunately, can't always find closed-form solution to system of equations $\nabla f(\mathbf{x}) = \mathbf{0}$. \rightarrow Resort to iterative methods to find a solution.

Locally change $\mathbf{x} \rightarrow \mathbf{x} + \delta$.
Hopefully improve objective value $f(\mathbf{x}) \rightarrow f(\mathbf{x} + \delta)$.

How to pick δ ?

By convexity of f : $f(\mathbf{x} + \delta) \geq f(\mathbf{x}) + \langle \nabla f(\mathbf{x}), \delta \rangle$.

If $\langle \nabla f(\mathbf{x}), \delta \rangle \geq 0$, then

$$f(\mathbf{x} + \delta) \geq f(\mathbf{x}). \quad \text{Clearly a bad direction.}$$

Moral: to be useful, the change δ must satisfy

$$\langle \nabla f(\mathbf{x}), \delta \rangle < 0.$$

For example, $\delta := -\eta \nabla f(\mathbf{x})$ for some $\eta > 0$:

$$\langle \nabla f(\mathbf{x}), -\eta \nabla f(\mathbf{x}) \rangle = -\eta \|\nabla f(\mathbf{x})\|_2^2 < 0$$

as long as $\nabla f(\mathbf{x}) \neq \mathbf{0}$.

Gradient descent for differentiable objectives

- ▶ Start with some initial $\mathbf{x}^{(1)} \in \mathbb{R}^d$.
- ▶ For $t = 1, 2, \dots$ until some stopping condition is satisfied.
 - ▶ Compute gradient of f at $\mathbf{x}^{(t)}$:

$$\boldsymbol{\lambda}^{(t)} := \nabla f(\mathbf{x}^{(t)}).$$

- ▶ Update:

$$\mathbf{x}^{(t+1)} := \mathbf{x}^{(t)} - \eta_t \boldsymbol{\lambda}^{(t)}.$$

Here, $\eta_1, \eta_2, \dots > 0$ are the **step sizes**. Common choices include:

1. Set $\eta_t := c$ for some constant $c > 0$.
2. Set $\eta_t := c/\sqrt{t}$ for some constant $c > 0$.
3. Set η_t using a line search procedure.

Backtracking line search

Goal: given $\mathbf{x} \in \mathbb{R}^d$ and $\boldsymbol{\lambda} = \nabla f(\mathbf{x}) \in \mathbb{R}^d$, find $\eta > 0$ so that $f(\mathbf{x} - \eta \boldsymbol{\lambda}) < f(\mathbf{x})$ by a reasonable amount.

- ▶ Start with $\eta := 1$.
- ▶ While $f(\mathbf{x} - \eta \boldsymbol{\lambda}) > f(\mathbf{x}) - \frac{1}{2} \eta \|\boldsymbol{\lambda}\|_2^2$: Set $\eta := \frac{1}{2} \eta$.

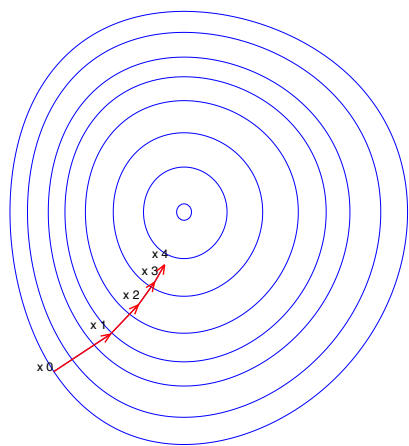
Main idea: $f(\mathbf{x} - \eta \boldsymbol{\lambda}) \approx f(\mathbf{x}) - \eta \|\boldsymbol{\lambda}\|_2^2$ when η is small, so can optimistically hope to decrease value by about $\eta \|\boldsymbol{\lambda}\|_2^2$.

Settle for decreasing by $\frac{1}{2} \eta \|\boldsymbol{\lambda}\|_2^2$: upon termination of while-loop,

$$f(\mathbf{x} - \eta \boldsymbol{\lambda}) \leq f(\mathbf{x}) - \frac{1}{2} \eta \|\boldsymbol{\lambda}\|_2^2.$$

Many other line search methods are possible.

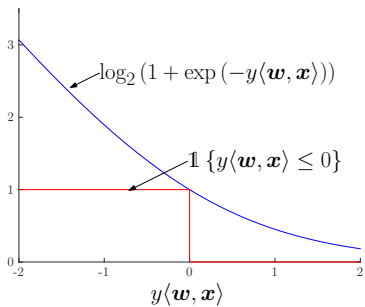
Illustration of gradient descent



If f is convex (and satisfies some other smoothness and curvature conditions), then $f(x^{(t)})$ converges to the optimal value at a geometric rate.

Example: logistic regression ($y \in \{-1, +1\}$)

$$\min_{w \in \mathbb{R}^d} f(w) := \frac{1}{|S|} \sum_{(x,y) \in S} \ln(1 + \exp(-y\langle w, x \rangle))$$



Easy to check that f is convex.

Question: How do we compute its gradient at a given point $w \in \mathbb{R}^d$?

Example: logistic regression ($y \in \{-1, +1\}$)

Gradient of f at w :

$$\begin{aligned} \nabla f(w) &= -\frac{1}{|S|} \sum_{(x,y) \in S} \frac{1}{1 + e^{y\langle w, x \rangle}} yx \\ &= -\frac{1}{|S|} \sum_{(x,y) \in S} (1 - P_w(Y=y \mid X=x)) yx. \end{aligned}$$

Gradient descent algorithm for logistic regression:

- ▶ Start with some initial $w^{(1)} \in \mathbb{R}^d$.
- ▶ For $t = 1, 2, \dots$ until some stopping condition is satisfied.

$$\begin{aligned} w^{(t+1)} &:= w^{(t)} - \eta_t \nabla f(w^{(t)}) \\ &= w^{(t)} + \eta_t \frac{1}{|S|} \sum_{(x,y) \in S} (1 - P_{w^{(t)}}(Y=y \mid X=x)) yx. \end{aligned}$$

Stopping condition

- ▶ In many applications of (convex) optimization, care about solving problems to very high precision.

Example: stop when gradient is close enough to zero ($\|\nabla f(x)\|_2 \leq \epsilon$ for some small parameter $\epsilon > 0$).

- ▶ For machine learning applications: optimization problem based on training data often just a means-to-an-end.

We really just care about true error rate.

- ▶ Running gradient descent to convergence not strictly necessary: **may be beneficial to stop early (e.g., when hold-out error rate starts to increase significantly).**

Key takeaways

1. Formulation of empirical risk minimization (with general loss functions and regularizers) as an optimization problem.
2. Convex sets, convex functions, ways to check convexity of a function.
3. Standard form of convex optimization problems, concept of local and global minimizers.
4. Gradient descent algorithm (for unconstrained problems with differentiable objectives); high-level idea of backtracking line search.
5. Stopping condition for machine learning applications.