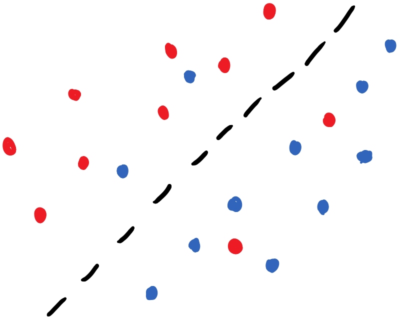
COMS 4771 Lecture 9

1. Soft-margin SVMs and surrogate losses
2. Convex optimization

Soft-margin SVMs and surrogate losses

Non-separable cases

Non-separable cases:
No linear classifier has zero training error on S.



But if non-separability is only due to a handful of points,
can we still find a good linear classifier?

no need to achieve
0 training error rate

Soft-margin SVMs (Cortes and Vapnik, 1995)

When $S = ((\boldsymbol{x}^{(1)}, y^{(1)}), \ldots, (\boldsymbol{x}^{(n)}, y^{(n)}))$ is not linearly separable, the (primal) SVM optimization problem

$$\begin{aligned} \min_{\boldsymbol{w} \in \mathbb{R}^d, \theta \in \mathbb{R}} \quad & \frac{1}{2}\|\boldsymbol{w}\|_2^2 \\ \text{s.t.} \quad & y^{(i)}\Big(\langle \boldsymbol{w}, \boldsymbol{x}^{(i)} \rangle - \theta\Big) \geq 1 \qquad \text{for } i = 1, 2, \ldots, n \end{aligned}$$

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has no solution.

Introduce **slack variables** $\xi_1, \xi_2, \ldots, \xi_n \geq 0$, and a trade-off parameter $C > 0$:

$$\begin{aligned} \min_{\boldsymbol{w} \in \mathbb{R}^d, \theta \in \mathbb{R}, \boldsymbol{\xi} \in \mathbb{R}^n} \quad & \frac{1}{2}\|\boldsymbol{w}\|_2^2 + C \sum_{i=1}^{n} \xi_i \\ \text{s.t.} \quad & y^{(i)}\Big(\langle \boldsymbol{w}, \boldsymbol{x}^{(i)} \rangle - \theta\Big) \geq 1 - \xi_i \qquad \text{for } i = 1, 2, \ldots, n \\ & \xi_i \geq 0 \qquad \text{for } i = 1, 2, \ldots, n \end{aligned}$$

Text

which is **always feasible**—"soft margin" SVM.

Soft-margin SVMs (Cortes and Vapnik, 1995)

Winner of 2008 ACM Paris Kanellakis Award:

For "their revolutionary development of a highly effective algorithm known as Support Vector Machines (SVM), a set of related supervised learning methods used for data classification and regression", which is "one of the most frequently used algorithms in machine learning, and is used in medical diagnosis, weather forecasting, and intrusion detection among many other practical applications".

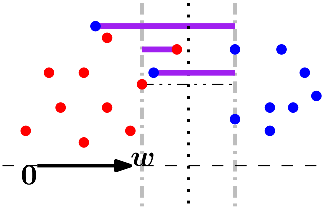
Other winners include: public key cryptography, Lempel-Ziv compression, Splay Trees, interior point method for linear programming, ...
and AdaBoost (discussed later in the course).

Slack interpretation

$$\min_{\boldsymbol{w}\in\mathbb{R}^d,\theta\in\mathbb{R},\boldsymbol{\xi}\in\mathbb{R}^n} \quad \frac{1}{2}\|\boldsymbol{w}\|_2^2 + C\sum_{i=1}^{n}\xi_i$$

$$\text{s.t.} \quad y^{(i)}\left(\langle \boldsymbol{w}, \boldsymbol{x}^{(i)}\rangle - \theta\right) \geq 1 - \xi_i \qquad \text{for } i = 1, 2, \ldots, n$$

$$\xi_i \geq 0 \qquad \text{for } i = 1, 2, \ldots, n$$



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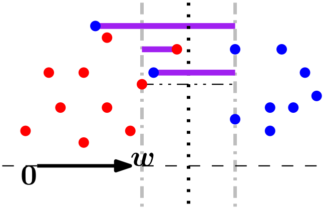

- For a given $(\boldsymbol{w}, \theta)$, $\xi_i / \|\boldsymbol{w}\|_2$ measures distance that $\boldsymbol{x}^{(i)}$ must be moved so that $y^{(i)}\langle \boldsymbol{w}, \boldsymbol{x}^{(i)} - \theta\rangle \geq 1$.

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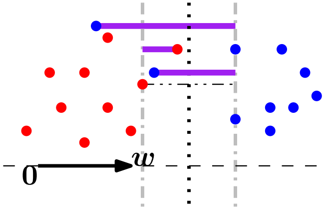

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- C controls trade-off between slack penalties and size of margin (which is $1/\|\boldsymbol{w}\|_2$).

Constraints with non-negative slack variables: (using $\lambda = 1/(nC)$)

$$\min_{\boldsymbol{w}\in\mathbb{R}^d, \theta\in\mathbb{R}, \boldsymbol{\xi}\in\mathbb{R}^n} \quad \frac{\lambda}{2}\|\boldsymbol{w}\|_2^2 + \frac{1}{n}\sum_{i=1}^{n}\xi_i$$

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A different interpretation of slack

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Equivalent unconstrained form:

$$\min_{\boldsymbol{w}\in\mathbb{R}^d,\theta\in\mathbb{R}} \quad \frac{\lambda}{2}\|\boldsymbol{w}\|_2^2 + \frac{1}{n}\sum_{i=1}^{n}\Big[1 - y^{(i)}\Big(\langle \boldsymbol{w}, \boldsymbol{x}^{(i)}\rangle - \theta\Big)\Big]_+$$

Notation: $[a]_+ := \max\{0, a\}$.

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$$\mathrm{HL}(\boldsymbol{w}, \theta; \boldsymbol{x}, y) := \Big[1 - y(\langle \boldsymbol{w}, \boldsymbol{x}\rangle - \theta)\Big]_+.$$

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trade off : larger margin ? lower hinge

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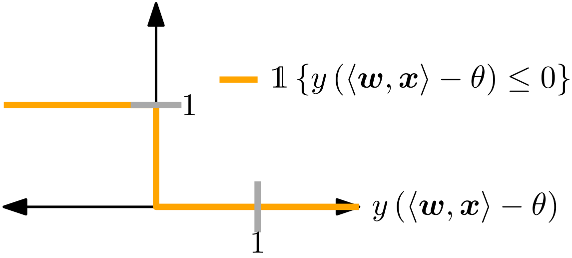
Zero-one loss vs. hinge loss



Zero-one loss: count if $f_{\boldsymbol{w},\theta}(\boldsymbol{x}) \neq y$.

$$\mathbb{1}\{y(\langle \boldsymbol{w}, \boldsymbol{x}\rangle - \theta) \le 0\} \;\le\; \Big[1 - y(\langle \boldsymbol{w}, \boldsymbol{x}\rangle - \theta)\Big]_+ \;=\; \mathrm{HL}(\boldsymbol{w}, \theta; \boldsymbol{x}, y).$$

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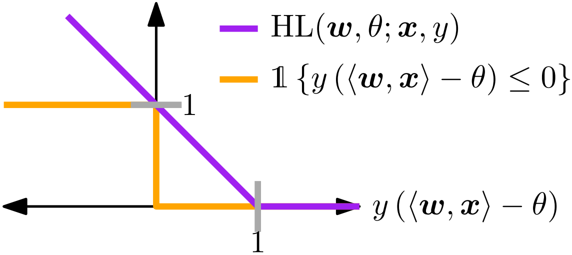

Hinge loss: an upper-bound on zero-one loss.

$$\boxed{\mathbb{1}\{y(\langle \boldsymbol{w}, \boldsymbol{x}\rangle - \theta) \le 0\}} \le \left[1 - \boxed{y(\langle \boldsymbol{w}, \boldsymbol{x}\rangle - \theta)}\right]_+ = \mathrm{HL}(\boldsymbol{w}, \theta; \boldsymbol{x}, y).$$

wrong predication!

When this smaller than one, a penalty would be incured!

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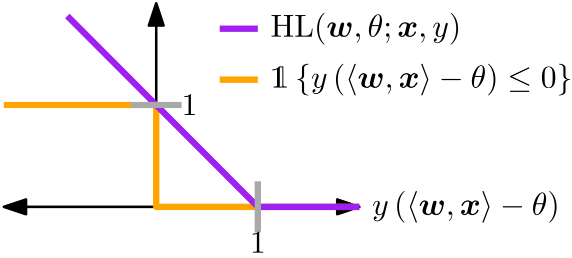

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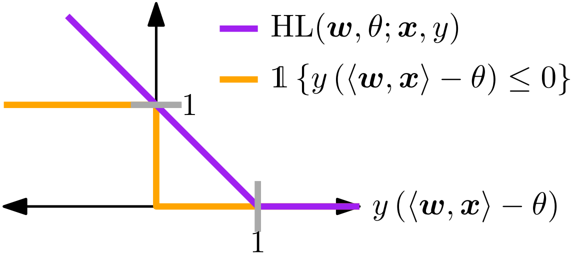

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This is **computationally tractable** (unlike minimizing training error) because the hinge loss is a **convex function** of $(\boldsymbol{w}, \theta)$, and so is $\frac{\lambda}{2}\|\boldsymbol{w}\|_2^2$.

General form

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

$$\min_{\boldsymbol{w} \in \mathbb{R}^d, \theta \in \mathbb{R}} \qquad \frac{1}{n} \sum_{i=1}^{n} \mathbb{1}\left\{ y^{(i)} \Big(\langle \boldsymbol{w}, \boldsymbol{x}^{(i)} \rangle - \theta \Big) \leq 0 \right\}$$

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Generic learning objective:

$$\min_{\boldsymbol{w} \in \mathbb{R}^d} \qquad R(\boldsymbol{w}) + \frac{1}{n} \sum_{i=1}^{n} \ell(\boldsymbol{w}; \boldsymbol{x}^{(i)}, y^{(i)})$$

- **Regularization**: encodes "learning bias" (e.g., preference for large margins), sometimes promotes stability.
- **Data fitting/empirical loss**: how poorly does the classifier "fit" the data.

Similarity to maximum likelihood

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Text

Maximum likelihood estimation for a parameteric family $\{p(\cdot; \boldsymbol{\theta}) : \boldsymbol{\theta} \in \mathcal{T}\}$ (assuming data $\boldsymbol{z}^{(1)}, \ldots, \boldsymbol{z}^{(n)}$ are iid):

$$\min_{\boldsymbol{\theta} \in \mathbb{R}^d} \qquad -\frac{1}{n} \sum_{i=1}^{n} \log p(\boldsymbol{z}^{(i)}; \boldsymbol{\theta})$$

(i.e., minimize $1/n$ times negative log-likelihood of parameter $\boldsymbol{\theta}$).

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Sometimes generic learning objective is called "generalized (and penalized, because of $R(\boldsymbol{w})$) maximum likelihood estimation".

Learning via optimization

- Many different choices for regularization and loss.
  - $R(\boldsymbol{w}) \propto \|\boldsymbol{w}\|_2^2$: encourage large margins
  - $R(\boldsymbol{w}) \propto \|\boldsymbol{w}\|_1$: encourage $\boldsymbol{w}$ to be sparse
  - $R(\boldsymbol{w}) \propto \sum_{i=1}^{n} w_i \ln w_i$: "maximum entropy" interpretation
  - $\ell(\boldsymbol{w}, \theta; \boldsymbol{x}, y) = [\langle \boldsymbol{w}, \boldsymbol{x} \rangle - \theta - y]_+^2$
  - $\ell(\boldsymbol{w}, \theta; \boldsymbol{x}, y) = \ln(1 + \exp(-y(\langle \boldsymbol{w}, \boldsymbol{x} \rangle - \theta)))$ ("logistic regression")
  - ...
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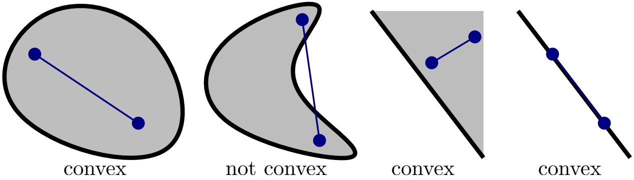
- **Next**: techniques for analyzing and solving these optimization problems.

Introduction to convexity

Convex sets

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



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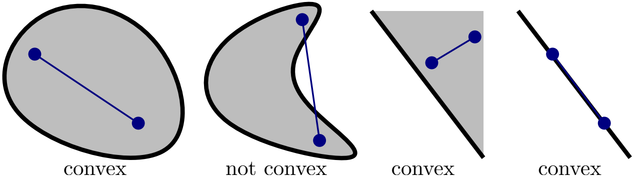


Examples:

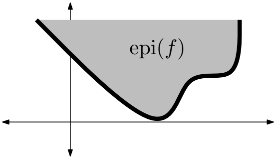
- All of $\mathbb{R}^d$.
- Empty set.
- Affine hyperplanes.
- Half-spaces: $\{\boldsymbol{a} \in \mathbb{R}^d : \langle \boldsymbol{a}, \boldsymbol{x} \rangle - b \leq 0\}$.
- Intersections of convex sets.
- Convex hulls of points.

Convex functions

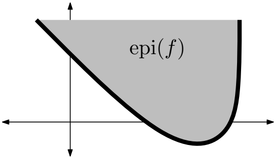
For any function $f\colon \mathbb{R}^d \to \mathbb{R}$, the **epigraph** of f, denoted $\operatorname{epi}(f)$, is the set

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

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



f is not convex



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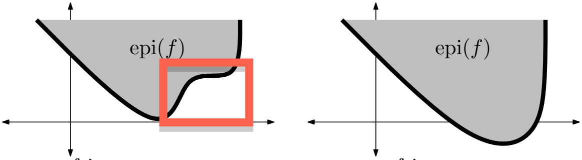

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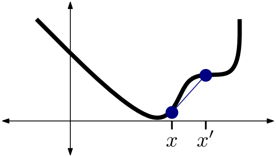
Examples:

- $f(x) = c^x$ for any $c > 0$ (on $\mathbb{R}$)
- $f(x) = |x|^c$ for any $c \geq 1$ (on $\mathbb{R}$)
- $f(\boldsymbol{x}) = c$ for any constant $c \in \mathbb{R}$.
- $f(\boldsymbol{x}) = \langle \boldsymbol{a}, \boldsymbol{x} \rangle$ for any $\boldsymbol{a} \in \mathbb{R}^d$.
- $f(\boldsymbol{x}) = \|\boldsymbol{x}\|_p$ for any $1 \leq p \leq \infty$.
- $f(\boldsymbol{x}) = \langle \boldsymbol{x}, \boldsymbol{A}\boldsymbol{x} \rangle$ for symmetric positive semidefinite $\boldsymbol{A}$.

Equivalent definition of convex functions

A function $f\colon \mathbb{R}^d \to \mathbb{R}$ is convex if and only if, for any $\boldsymbol{x}, \boldsymbol{x}' \in \mathbb{R}^d$ and $\alpha \in [0,1]$,

$$f\big((1-\alpha)\boldsymbol{x} + \alpha\boldsymbol{x}'\big) \ \le \ (1-\alpha)\cdot f(\boldsymbol{x}) + \alpha \cdot f(\boldsymbol{x}').$$



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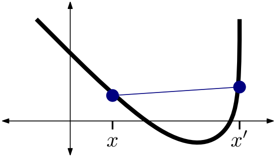
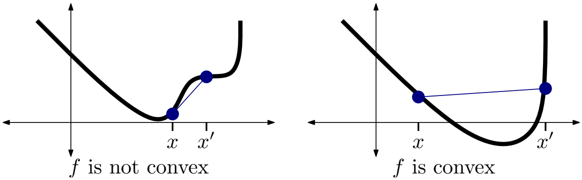


f is convex

Equivalent definition of convex functions

A function $f\colon \mathbb{R}^d \to \mathbb{R}$ is convex if and only if, for any $\boldsymbol{x}, \boldsymbol{x}' \in \mathbb{R}^d$ and $\alpha \in [0,1]$,

$$f\big((1-\alpha)\boldsymbol{x} + \alpha\boldsymbol{x}'\big) \;\le\; (1-\alpha)\cdot f(\boldsymbol{x}) + \alpha \cdot f(\boldsymbol{x}').$$



Covex points

Jensen's inequality

If $f\colon \mathbb{R}^d \to \mathbb{R}$ is convex, then for any $\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_n \in \mathbb{R}^d$ and $\alpha_1, \alpha_2, \ldots, \alpha_n \in [0,1]$ such that $\sum_{i=1}^n \alpha_i = 1$,

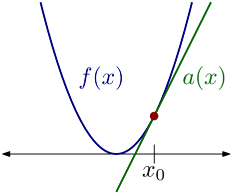
$$f\left(\sum_{i=1}^n \alpha_i \boldsymbol{x}_i\right) \le \sum_{i=1}^n \alpha_i \cdot f(\boldsymbol{x}_i).$$

Differentiable functions

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

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

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



$$a(x) = f(x_0) + f'(x_0)(x - x_0)$$

Text

Convexity of differentiable functions

Differentiable functions

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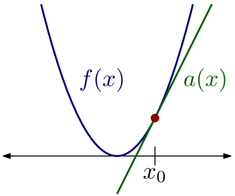

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Twice-differentiable functions

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

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

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

Building new convex functions from old ones

- $f(\boldsymbol{x}) = c \cdot h(\boldsymbol{x}) + g(\boldsymbol{x})$ for convex functions h, g and scalar $c \geq 0$.

  Example: $f(\boldsymbol{x}) = -2\langle \boldsymbol{a}, \boldsymbol{x} \rangle + 1$.

- $f(\boldsymbol{x}) = \max\{h(\boldsymbol{x}),\ g(\boldsymbol{x})\}$ for convex functions h, g.

  Example: $f(\boldsymbol{x}) = \max\{0,\ 1 - \langle \boldsymbol{a}, \boldsymbol{x} \rangle\}$.

- $f(\boldsymbol{x}) = g(\boldsymbol{A}\boldsymbol{x} + \boldsymbol{b})$ for any $\boldsymbol{A} \in \mathbb{R}^{m \times d}$ and $\boldsymbol{b} \in \mathbb{R}^m$ and convex function $g \colon \mathbb{R}^m \to \mathbb{R}$.

  Examples: $f(\boldsymbol{x}) = \exp(\langle \boldsymbol{a}, \boldsymbol{x} \rangle)$, $f(\boldsymbol{x}) = \langle \boldsymbol{a}, \boldsymbol{x} \rangle^2$.

- $f(\boldsymbol{x}) = g(h_1(\boldsymbol{x}), \dots, h_m(\boldsymbol{x}))$ for any convex $h_1, \dots, h_m$ and convex $g \colon \mathbb{R}^m \to \mathbb{R}$ such that g is non-decreasing in each argument.

  Example: $f(\boldsymbol{x}) = \exp(\langle \boldsymbol{a}, \boldsymbol{x} \rangle^2)$ (but not $\exp(-\langle \boldsymbol{a}, \boldsymbol{x} \rangle^2)$).

- Many other composition rules.

How to test for convexity

- First principles (via definitions).
- First- or second-derivative tests (assuming derivatives exist).
- Valid transformation of existing convex functions.

Convex optimization problems

Optimization problems

A typical optimization problem is written as

$$\begin{aligned} \min_{\boldsymbol{x} \in \mathbb{R}^d} \quad & f_0(\boldsymbol{x}) \\ \text{s.t.} \quad & f_i(\boldsymbol{x}) \leq 0 \quad i = 1, 2, \ldots, n \end{aligned}$$

where $f_0 \colon \mathbb{R}^d \to \mathbb{R}$ is the **objective function** and $f_1, f_2, \ldots, f_n \colon \mathbb{R}^d \to \mathbb{R}$ are the **constraint functions**.

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A point $\boldsymbol{x} \in A$ achieving the optimal value is a **(global) minimizer** of the problem.

Convex optimization problems

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

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

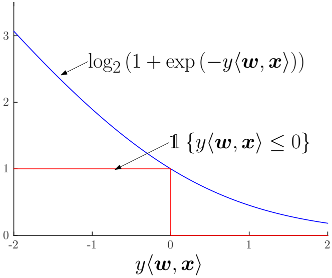
Fact: the feasible set $A := \{\boldsymbol{x} \in \mathbb{R}^d : f_i(\boldsymbol{x}) \leq 0 \text{ for all } i = 1, 2, \dots, n\}$ is a convex set.

Example: non-negative logistic regression

Training data $S := ((\boldsymbol{x}^{(1)}, y^{(1)}), \ldots, (\boldsymbol{x}^{(n)}, y^{(n)}))$ with $(\boldsymbol{x}^{(i)}, y^{(i)}) \in \mathbb{R}^d \times \{\pm 1\}$.

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

$$\text{s.t.} \quad w_i \geq 0 \quad \text{for } i = 1, 2, \ldots, d.$$



Like SVM, but using a different surrogate loss, no regularization term, and only want non-negative weights.

Example: non-negative logistic regression

Objective function:

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Second-derivative test of convexity: Is $\nabla^2 f_0(\boldsymbol{w})$ positive semidefinite?

$$\nabla^2 f_0(\boldsymbol{w}) = \frac{1}{n} \sum_{i=1}^{n} \frac{1}{1 + e^{\langle \boldsymbol{w}, \boldsymbol{x}^{(i)} \rangle}} \cdot \frac{e^{\langle \boldsymbol{w}, \boldsymbol{x}^{(i)} \rangle}}{1 + e^{\langle \boldsymbol{w}, \boldsymbol{x}^{(i)} \rangle}} \boldsymbol{x}^{(i)} (\boldsymbol{x}^{(i)})^\top.$$

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Yes: for any $\boldsymbol{v} \in \mathbb{R}^d$,

$$\langle \nabla^2 f_0(\boldsymbol{w})\boldsymbol{v}, \boldsymbol{v}\rangle = \frac{1}{n}\sum_{i=1}^{n} \frac{1}{1+e^{\langle \boldsymbol{w}, \boldsymbol{x}^{(i)}\rangle}} \cdot \frac{e^{\langle \boldsymbol{w}, \boldsymbol{x}^{(i)}\rangle}}{1+e^{\langle \boldsymbol{w}, \boldsymbol{x}^{(i)}\rangle}} \langle \boldsymbol{v}, \boldsymbol{x}^{(i)}\rangle^2 \geq 0.$$

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Conclusion: objective function $f_0(\boldsymbol{w})$ is convex.

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Overall problem is a convex optimization problem. $\square$

Local minimizers

Consider an optimization problem (not necessarily convex):

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

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

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

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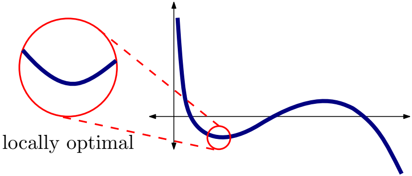
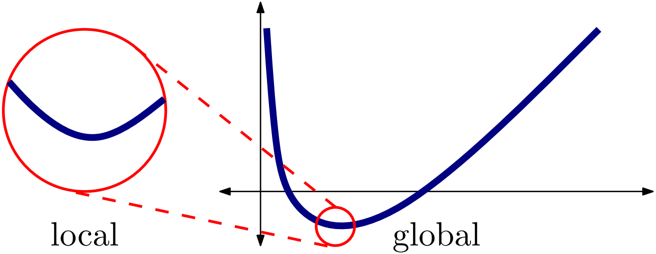
Nothing looks better than $\tilde{\boldsymbol{x}}$ in the immediate vicinity of $\tilde{\boldsymbol{x}}$.



LOCAL-TO-GLOBAL PHENOMENON

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



Solving convex optimization problems

Unconstrained convex optimization problems

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

(f is the convex objective function).

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Optimality condition for differentiable convex objectives

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

guarantee convex

Local optimization for convex objectives

Local optimization

Main idea: locally change $\boldsymbol{x} \to \boldsymbol{x} + \boldsymbol{\delta}$ to improve its objective value $f(\boldsymbol{x}) \to f(\boldsymbol{x} + \boldsymbol{\delta})$.

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Moral: to be useful, the change $\boldsymbol{\delta}$ must satisfy

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

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

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

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

Gradient descent for differentiable objectives

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

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

  - Update:

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Here, $\eta_1, \eta_2, \ldots > 0$ 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 $\boldsymbol{x} \in \mathbb{R}^d$ and $\boldsymbol{\lambda} = \nabla f(\boldsymbol{x}) \in \mathbb{R}^d$, find $\eta > 0$ so that $f(\boldsymbol{x} - \eta\boldsymbol{\lambda}) < f(\boldsymbol{x})$ by a reasonable amount.

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

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

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

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

Backtracking line search

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

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

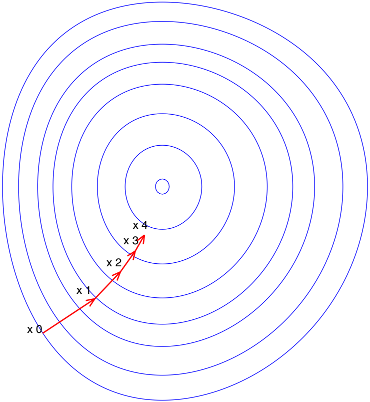
Main idea: $f(\boldsymbol{x} - \eta\boldsymbol{\lambda}) \approx f(\boldsymbol{x}) - \eta\|\boldsymbol{\lambda}\|_2^2$, so optimistically hope to decrease value by about $\eta\|\boldsymbol{\lambda}\|_2^2$ when η is small enough.

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

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

Many other line search methods are possible.

Illustration of gradient descent

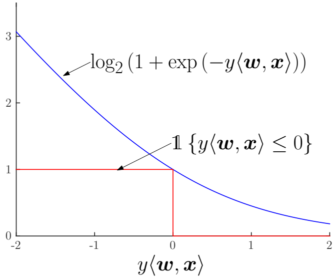


If f is convex (and satisfies some other smoothness and curvature conditions), then $f(\boldsymbol{x}^{(t)})$ converges to the optimal value at a geometric rate.

Example: (unconstrained) logistic regression

Training data $S := ((\boldsymbol{x}^{(1)}, y^{(1)}), \ldots, (\boldsymbol{x}^{(n)}, y^{(n)}))$ with $(\boldsymbol{x}^{(i)}, y^{(i)}) \in \mathbb{R}^d \times \{\pm 1\}$.

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



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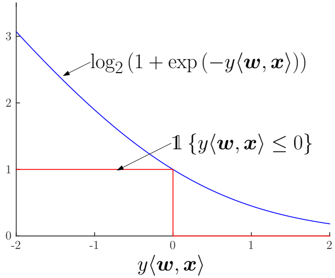

We've already established that objective $f(\boldsymbol{w})$ is convex.

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

Example: (unconstrained) logistic regression

Gradient of f at $\boldsymbol{w}$:

$$\nabla f(\boldsymbol{w}) = -\frac{1}{n}\sum_{i=1}^{n}\frac{1}{1+e^{y^{(i)}\langle \boldsymbol{w},\boldsymbol{x}^{(i)}\rangle}}y^{(i)}\boldsymbol{x}^{(i)}$$

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Gradient descent algorithm:

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

$$\begin{aligned}
\boldsymbol{w}^{(t+1)} &:= \boldsymbol{w}^{(t)} - \eta_t \nabla f(\boldsymbol{w}^{(t)}) \\
&= \boldsymbol{w}^{(t)} + \eta_t \frac{1}{n} \sum_{i=1}^{n} \frac{1}{1 + e^{y^{(i)} \langle \boldsymbol{w}, \boldsymbol{x}^{(i)} \rangle}} y^{(i)} \boldsymbol{x}^{(i)}.
\end{aligned}$$

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 ($\|\nabla f(\boldsymbol{x})\|_2 \le \epsilon$ for some small parameter $\epsilon > 0$).

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

  We really just care about true error.

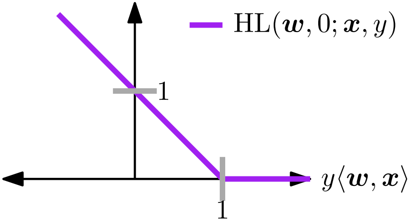
- Running gradient descent to convergence not strictly necessary: **may be beneficial to stop early (e.g., based on hold-out error).**

Non-differentiable convex objectives

Some convex functions f are not differentiable everywhere;
gradient descent not even well-specified for these problems.

Example: hinge loss

$$f(\boldsymbol{w}) = \mathrm{HL}(\boldsymbol{w}, 0; \boldsymbol{x}, y) = \Big[1 - y\langle \boldsymbol{w}, \boldsymbol{x}\rangle\Big]_+ .$$



Not differentiable at $\boldsymbol{w} \in \mathbb{R}^d$ where $y\langle \boldsymbol{w}, \boldsymbol{x}\rangle = 1$.

Subgradients

Although not every function f is differentiable everywhere,
every **convex function** f has **subgradients** *everywhere*†.

We say $\boldsymbol{\lambda} \in \mathbb{R}^d$ is a **subgradient** of a function $f\colon \mathbb{R}^d \to \mathbb{R}$ at $\boldsymbol{x}_0 \in \mathbb{R}^d$ if

$$f(\boldsymbol{x}) \geq f(\boldsymbol{x}_0) + \langle \boldsymbol{\lambda}, \boldsymbol{x} - \boldsymbol{x}_0 \rangle \quad \forall \boldsymbol{x} \in \mathbb{R}^d.$$

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There might be many subgradients at a given point x_0—i.e., many affine lower bounds: call the entire set the **subdifferential of f at x_0**, $\partial f(\boldsymbol{x}_0)$.

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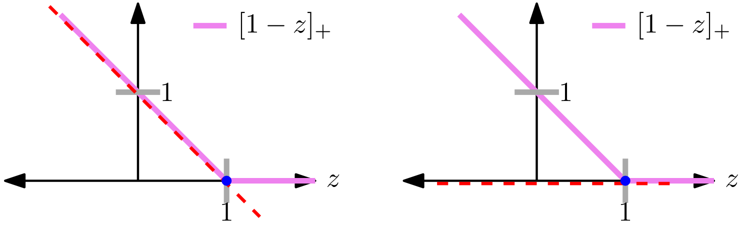
Example: subgradient of hinge loss

Consider one-dimensional function $f(z) := [1 - z]_+ = \max\{0, 1 - z\}$.



Two subgradients of f at $z = 1$: -1 and 0.

$$f(z) \;\geq\; f(1) + (-1) \cdot (z - 1) \;=\; 1 - z\;;$$
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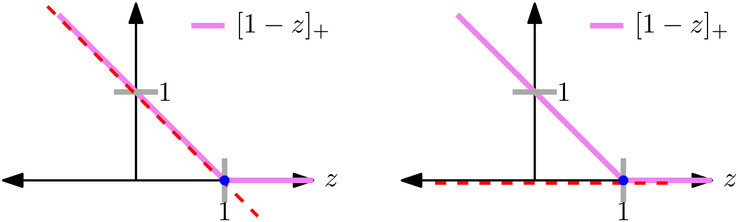

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Actually, **infinitely-many subgradients**: $\boxed{\text{all } \lambda \in [-1, 0] \text{ satisfy}}$

$$f(z) \;\geq\; f(1) + \lambda\cdot(z-1).$$

Subgradient calculus

Suppose $g, g_1, g_2, \ldots, g_n$ are convex functions.
Below, sufficient conditions under which f is convex, and corresponding subdifferential:

- **Addition**: If $f(\boldsymbol{x}) = g_1(\boldsymbol{x}) + g_2(\boldsymbol{x})$, then $\partial f(\boldsymbol{x}) = \partial g_1(\boldsymbol{x}) + \partial g_2(\boldsymbol{x})$.
- **Positive scaling**: If $f(\boldsymbol{x}) = \alpha \cdot g(\boldsymbol{x})$ for some $\alpha > 0$, then $\partial f(\boldsymbol{x}) = \alpha \cdot \partial g(\boldsymbol{x})$.
- **Affine composition**: If $f(\boldsymbol{x}) = g(\boldsymbol{A}\boldsymbol{x} + \boldsymbol{b})$, then $\partial f(\boldsymbol{x}) = \boldsymbol{A}^\top \partial g(\boldsymbol{A}\boldsymbol{x} + \boldsymbol{b})$.
- **Finite pointwise maximum**: If $f(\boldsymbol{x}) = \max_{i \in [n]} g_i(\boldsymbol{x})$, then

$$\partial f(\boldsymbol{x}) = \operatorname{conv}\left(\bigcup_{i \in [n] : g_i(\boldsymbol{x}) = f(\boldsymbol{x})} \partial g_i(\boldsymbol{x}) \right).$$

- **More general composition**: If $h \colon \mathbb{R}^n \to \mathbb{R}$ is convex and non-decreasing in each argument, and $f(\boldsymbol{x}) := h(g_1(\boldsymbol{x}), g_2(\boldsymbol{x}), \ldots, g_n(\boldsymbol{x}))$, then

$$\partial f(\boldsymbol{x}) = \bigcup_{(\lambda_1, \lambda_2, \ldots, \lambda_n) \in \partial h(g_1(\boldsymbol{x}), g_2(\boldsymbol{x}), \ldots, g_n(\boldsymbol{x}))} \partial\left(\sum_{i=1}^n \lambda_i g_i(\boldsymbol{x}) \right).$$

Subgradient descent for general convex objectives

- Start with some initial $\boldsymbol{x}^{(1)} \in \mathbb{R}^d$.
- For $t = 1, 2, \ldots$ until some stopping condition is satisfied.
  - Compute *any* subgradient $\boldsymbol{\lambda}^{(t)}$ of f at $\boldsymbol{x}^{(t)}$.
  - Update:

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