Optimization for Machine Learning (in a Nutshell)

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- What is optimization?
  - Examples in machine learning
  - Unconstrained vs constrained
- Convex optimization
  - Convex sets
  - Convex functions
  - Convex optimization

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  - Gradient descent
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  - SVM in primal and dual forms
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What is optimization?

- Finding (one or more) minimizer of a function subject to constraints

$$\arg\min_x f_0(x)$$
$$\text{s.t.} f_i(x) \leq 0, i = \{1, \ldots, k\}$$
$$h_j(x) = 0, j = \{1, \ldots l\}$$

- Most of the machine learning problems are, in the end, optimization problems.

Examples

- (Soft) Linear SVM

$$\arg\min_{w} \sum_{i=1}^{n} ||w||^2 + C \sum_{i=1}^{n} \xi_i$$

$$\text{s.t. } 1 - y_i x_i^T w \leq \xi_i$$

$$\xi_i \geq 0$$

- Maximum Likelihood

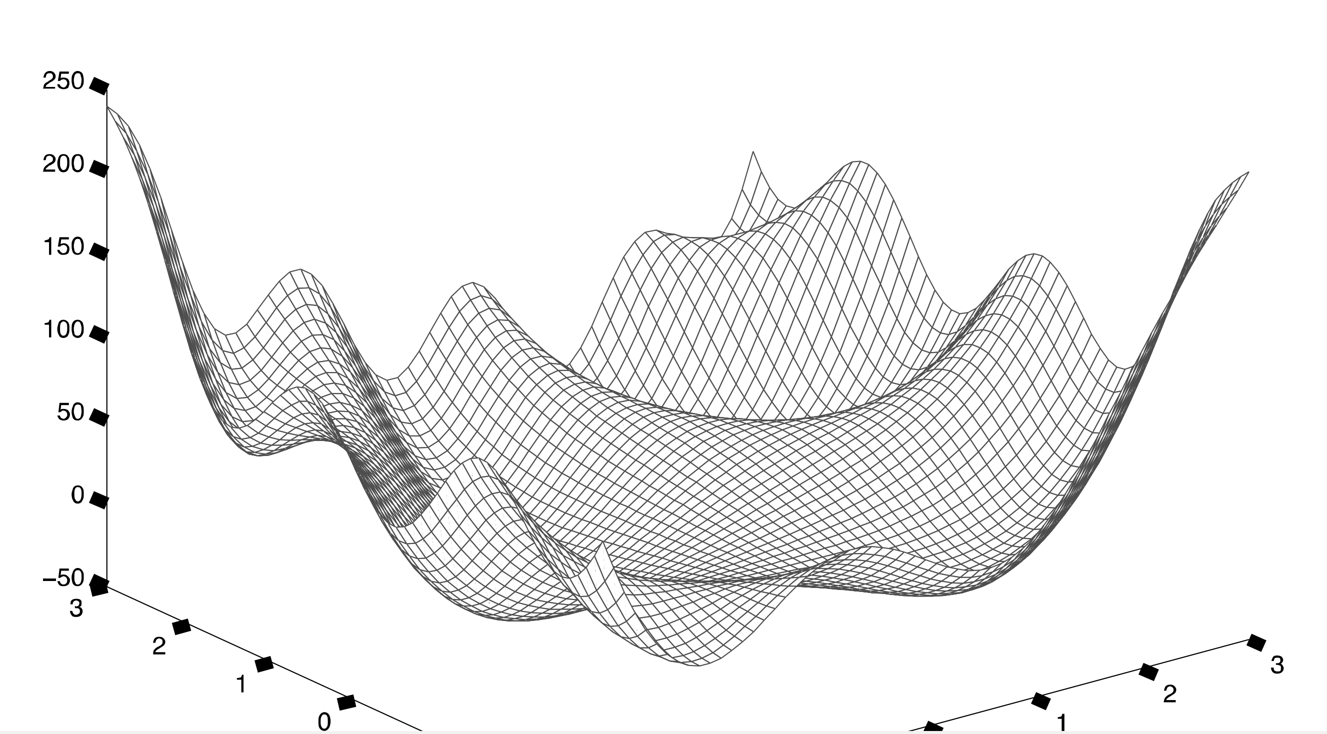
$$\arg\max_{\theta} \sum_{i=1}^{n} \log p_\theta(x_i)$$

- K-means

$$\arg \min_{\mu_1, \mu_2, \ldots, \mu_k} J(\mu) = \sum_{j=1}^{k} \sum_{i \in C_j} ||x_i - \mu_j||^2$$

Optimization is difficult in general

- Minimize f(x)



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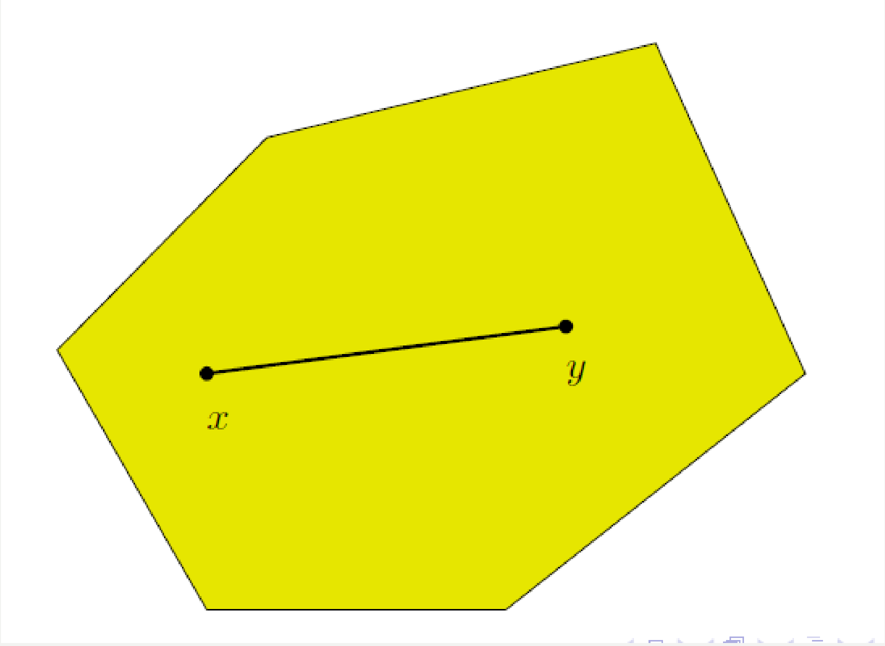
Convex sets

- **Def:** A set $C \subseteq \mathbb{R}^n$ is convex if for $x, y \in C$ and any $a \in [0, 1]$,

$$ax + (1-a)y \in C$$



Examples of convex set

- All of $\mathbb{R}^n$ (obvious)

- Non-negative orthant, $\mathbb{R}^n_+$: let $x \succeq 0$, $y \succeq 0$, clearly $\alpha x + (1-\alpha)y \succeq 0$.
- Affine subspaces: $Ax = b$, $Ay = b$, then

$$A(\alpha x + (1-\alpha)y) = \alpha Ax + (1-\alpha)Ay = \alpha b + (1-\alpha)b = b.$$

- Arbitrary intersections of convex sets: let C_i be convex for $i \in \mathcal{I}$, $C = \bigcap_i C_i$, then

$$x \in C, y \in C \quad \Rightarrow \quad \alpha x + (1-\alpha)y \in C_i \ \forall\, i \in \mathcal{I}$$

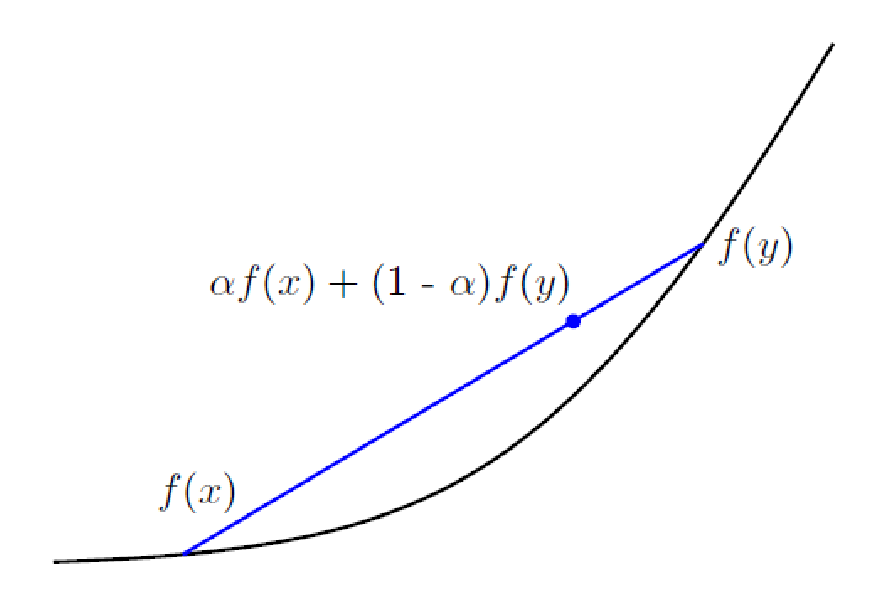
so $\alpha x + (1-\alpha)y \in C$.

Convex functions

- Def:

A function $f : \mathbb{R}^n \to \mathbb{R}$ is convex if for $x, y \in \mathrm{dom} f$ and any $a \in [0, 1]$,

$$f(ax + (1-a)y) \leq af(x) + (1-a)f(y)$$

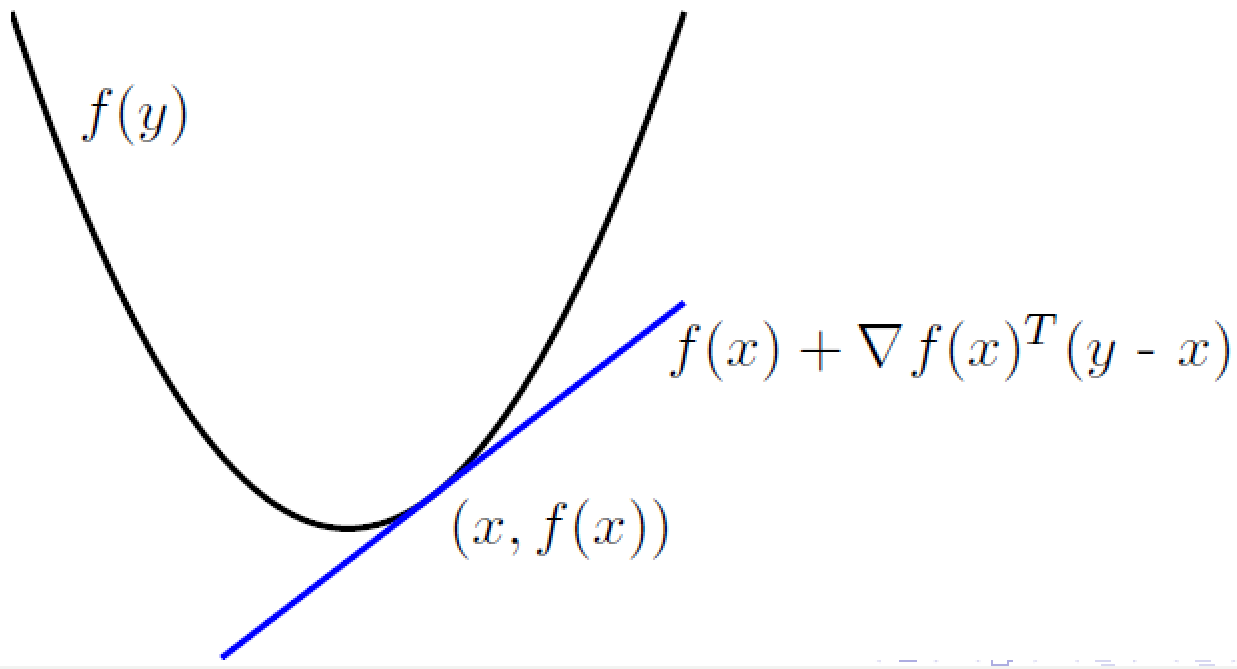


Convexity condition 1

- Theorem

Suppose $f : \mathbb{R}^n \to \mathbb{R}$ *is differentiable. Then* f *is convex if and only if for all* $x, y \in \operatorname{dom} f$

$$f(y) \geq f(x) + \nabla f(x)^T (y - x)$$



Subgradient

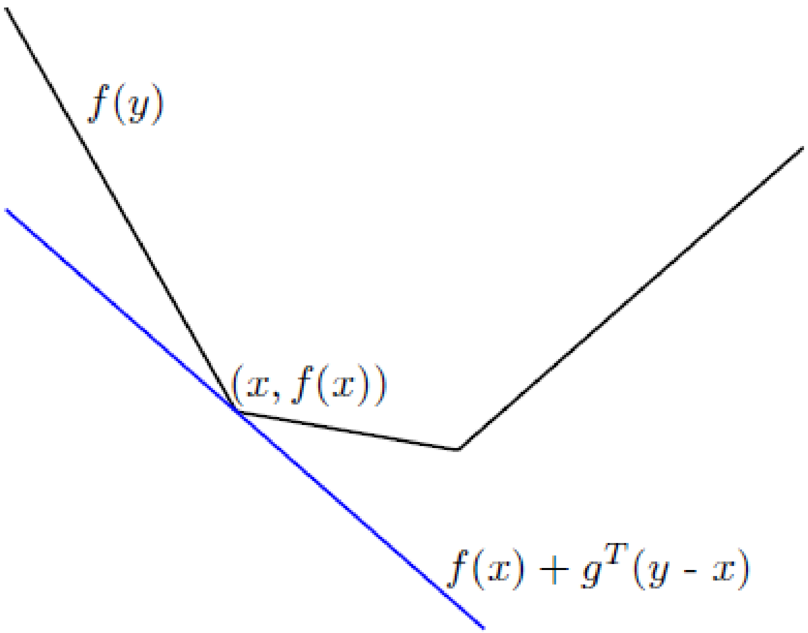
Definition

The *subgradient set*, or subdifferential set, $\partial f(x)$ of f at x is

$$\partial f(x) = \{g : f(y) \geq f(x) + g^T(y - x) \ \text{ for all } y\} .$$

Theorem

$f : \mathbb{R}^n \to \mathbb{R}$ is convex if and only if it has non-empty subdifferential set everywhere.

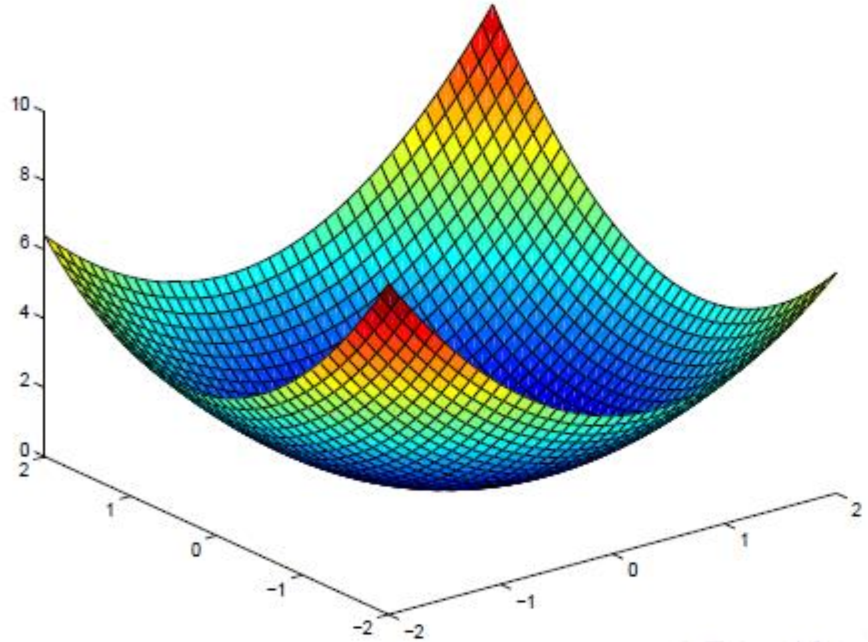


Convexity condition 2

Theorem

Suppose $f : \mathbb{R}^n \to \mathbb{R}$ is twice differentiable. Then f is convex if and only if for all $x \in \mathrm{dom}\, f$,

$$\nabla^2 f(x) \succeq 0.$$



Examples of convex functions

- Linear/affine functions:

$$f(x) = b^T x + c.$$

- Quadratic functions:

$$f(x) = \frac{1}{2} x^T A x + b^T x + c$$

for $A \succeq 0$. For regression:

$$\frac{1}{2} \|Xw - y\|^2 = \frac{1}{2} w^T X^T X w - y^T X w + \frac{1}{2} y^T y.$$

More examples

- Norms (like ℓ_1 or ℓ_2 for regularization):

$$\|\alpha x + (1-\alpha)y\| \leq \|\alpha x\| + \|(1-\alpha)y\| = \alpha \|x\| + (1-\alpha)\|y\| .$$

- Composition with an affine function $f(Ax+b)$:

$$\begin{aligned} f(A(\alpha x + (1-\alpha)y) + b) &= f(\alpha(Ax+b) + (1-\alpha)(Ay+b)) \\ &\leq \alpha f(Ax+b) + (1-\alpha) f(Ay+b) \end{aligned}$$

- Log-sum-exp (via $\nabla^2 f(x)$ PSD):

$$f(x) = \log\left(\sum_{i=1}^{n} \exp(x_i)\right)$$

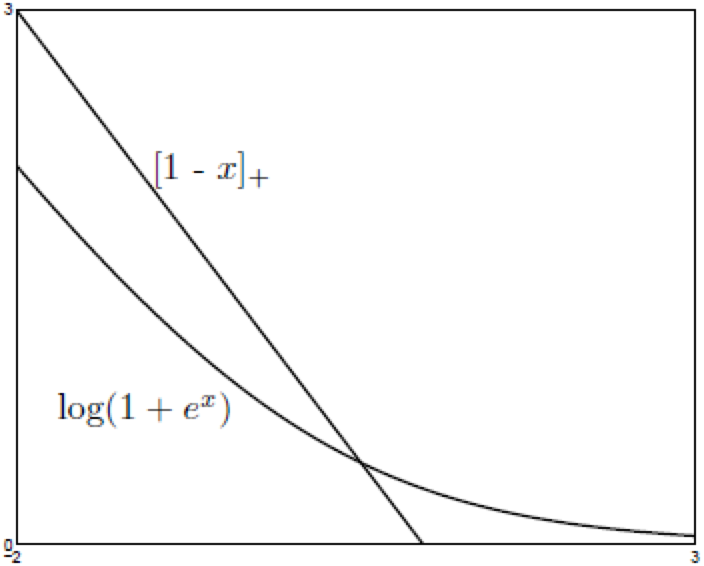
Examples in machine learning

- SVM loss:

$$f(w) = \left[1 - y_i x_i^T w\right]_+$$

- Binary logistic loss:

$$f(w) = \log\left(1 + \exp(-y_i x_i^T w)\right)$$



Convex optimization

- Def:

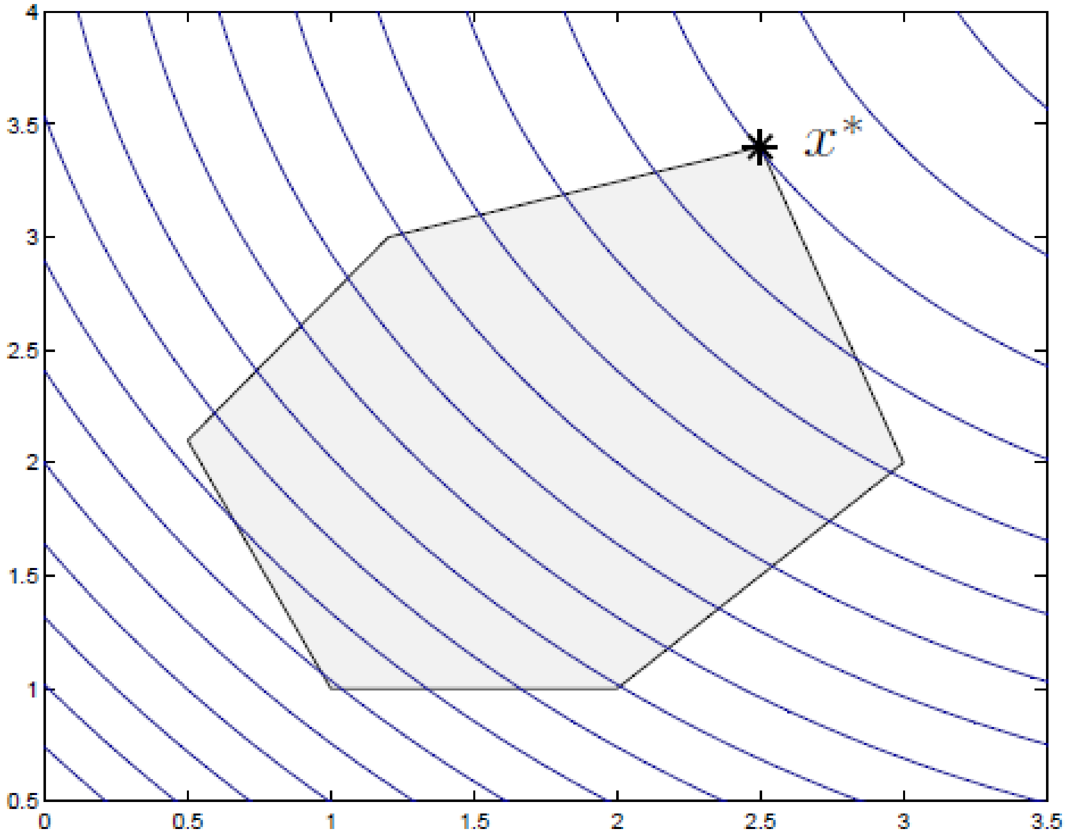
An optimization problem is *convex* if its objective is a convex function, the inequality constraints f_j are convex, and the equality constraints h_j are affine

$$
\begin{aligned}
\underset{x}{\text{minimize}}\ & f_0(x) && \text{(Convex function)} \\
\text{s.t.}\quad & f_i(x) \le 0 && \text{(Convex sets)} \\
& h_j(x) = 0 && \text{(Affine)}
\end{aligned}
$$

Convex problems are nice….

Theorem

If $\hat{x}$ is a local minimizer of a convex optimization problem, it is a global minimizer.



For smooth functions

Theorem

$\nabla f(x) = 0$ if and only if x is a global minimizer of $f(x)$.

Proof.

- $\nabla f(x) = 0$. We have

$$f(y) \geq f(x) + \nabla f(x)^T (y - x) = f(x).$$

- $\nabla f(x) \neq 0$. There is a direction of descent.

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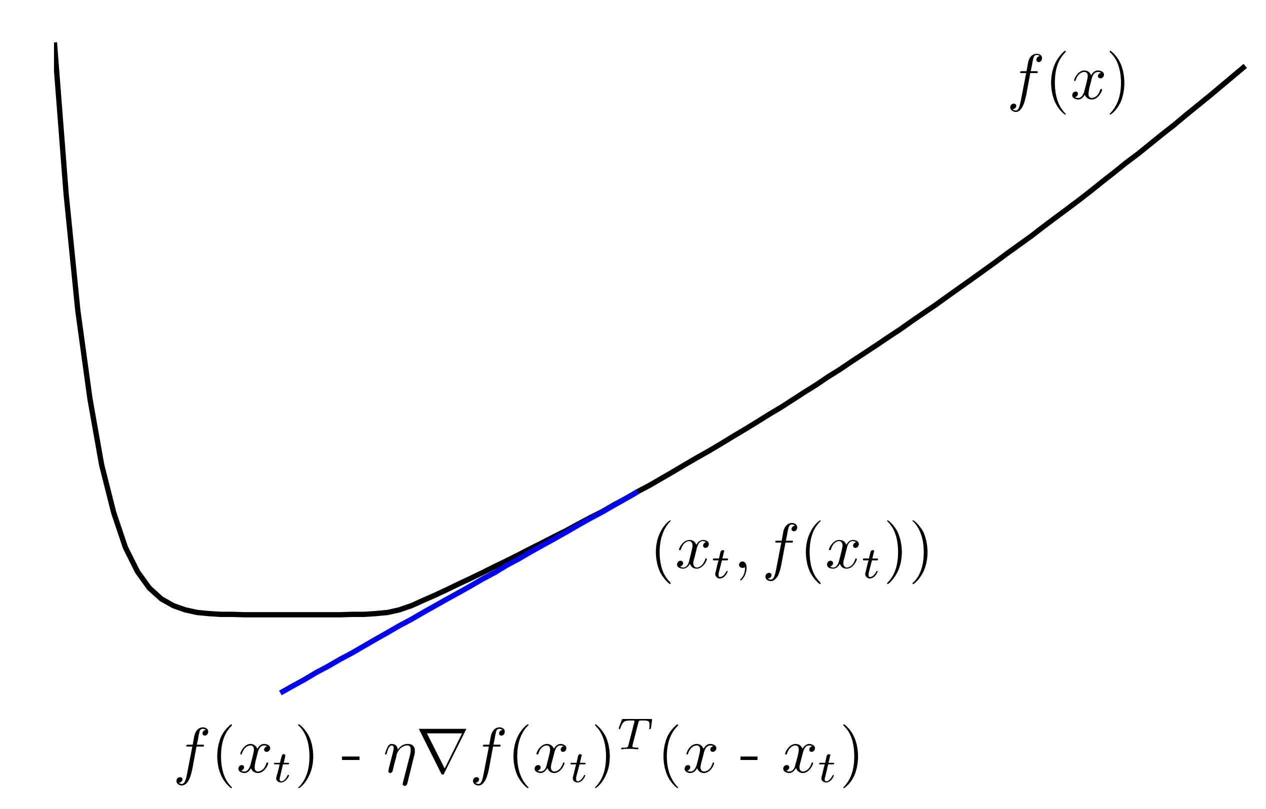
Gradient descent

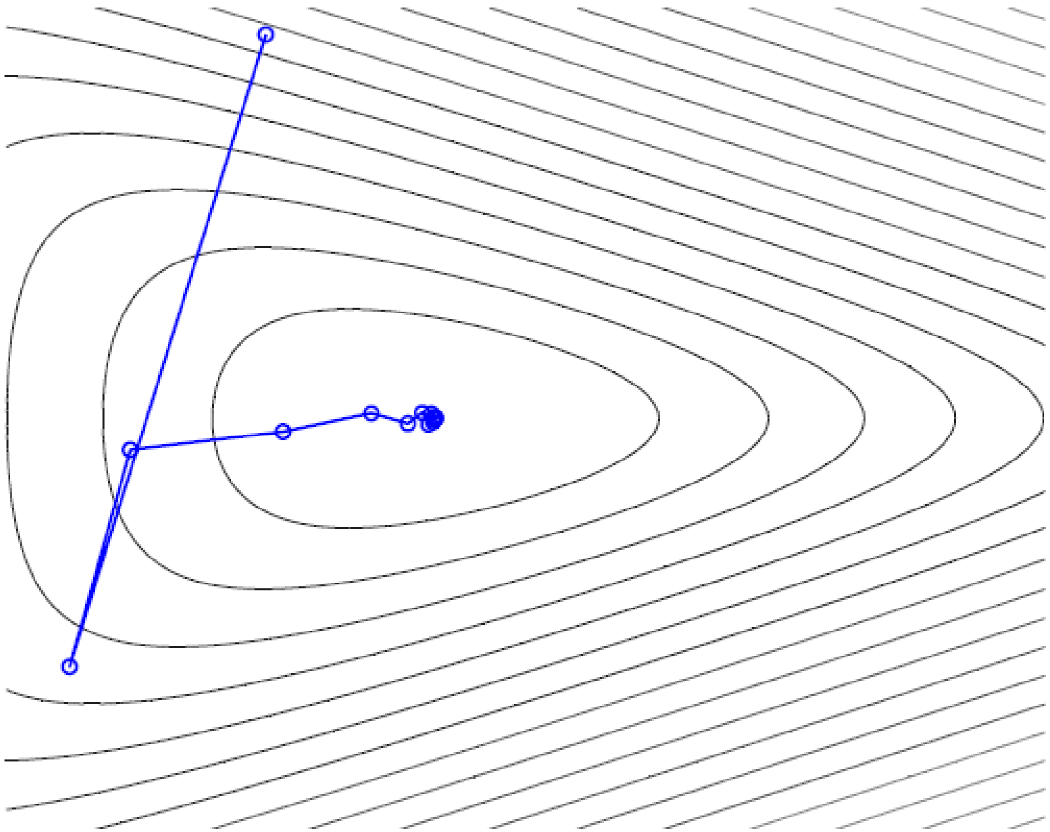
- Consider convex and unconstrained optimization.
- Solve $\min_x f(x)$
- One of the simplest approach:
  - For t = 1, … , T
    - $x_{t+1} \leftarrow x_t - \eta_t \nabla f(x_t)$
  - Until convergence
  - η_t is called step-size or learning rate.

Single step in gradient descent



Full gradient descent

$$f(x) = \log(\exp(x_1 + 3x_2 - .1) + \exp(x_1 - 3x_2 - .1) + \exp(-x_1 - .1))$$



How to choose step size ?

- Idea 1: exact line search

$$\eta_t = \operatorname*{argmin}_{\eta} f\left(x - \eta \nabla f(x)\right)$$

  Too expensive to be practical.

- Idea 2: backtracking (Armijo) line search. Let $\alpha \in (0, \frac{1}{2})$, $\beta \in (0, 1)$. Multiply $\eta = \beta \eta$ until

$$f\left(x - \eta \nabla f(x)\right) \leq f(x) - \alpha \eta \left\|\nabla f(x)\right\|^2$$

  Works well in practice.

Newton's method

Idea: use a second-order approximation to function.

$$f(x + \Delta x) \approx f(x) + \nabla f(x)^T \Delta x + \frac{1}{2} \Delta x^T \nabla^2 f(x) \Delta x$$

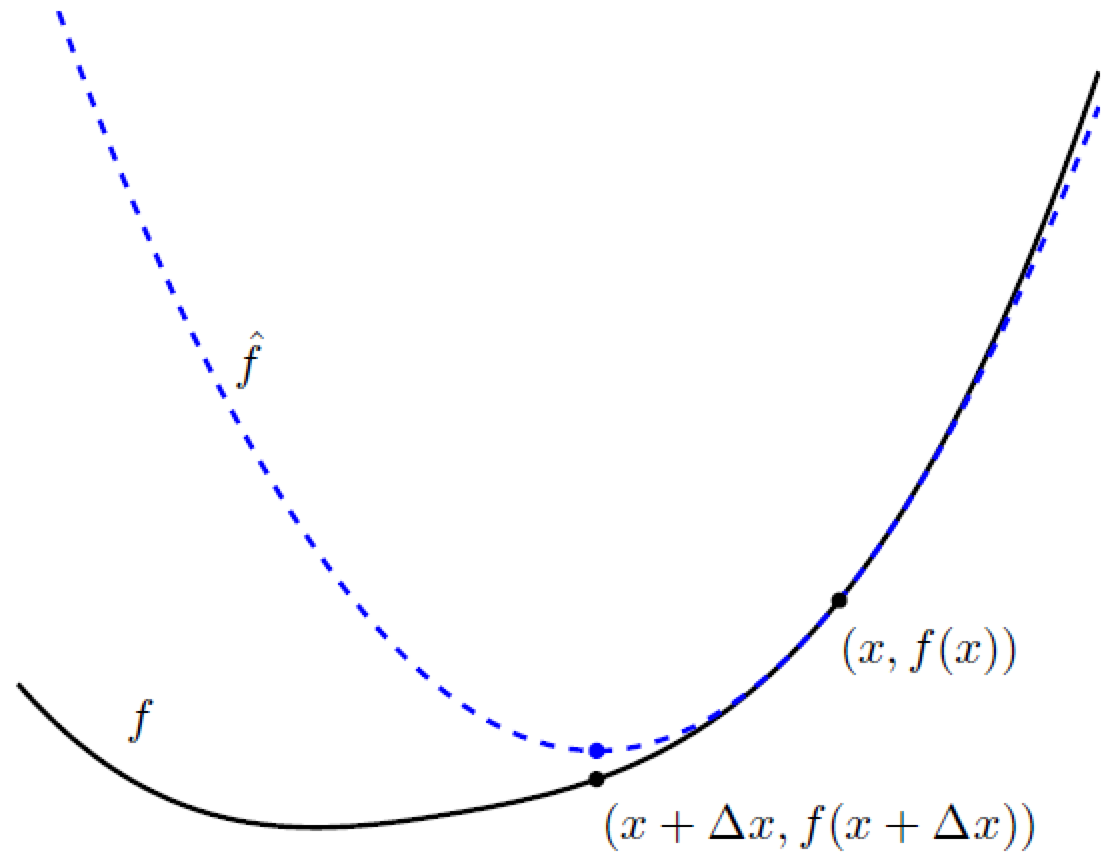
Choose Δx to minimize above:

$$\Delta x = - \left[\nabla^2 f(x)\right]^{-1} \nabla f(x)$$

This is descent direction:

$$\nabla f(x)^T \Delta x = -\nabla f(x)^T \left[\nabla^2 f(x)\right]^{-1} \nabla f(x) < 0.$$

Single step in Newton's method



$\hat{f}$ is 2^{nd}-order approximation, f is true function.

Convergence rate

- Strongly convex case: $\nabla^2 f(x) \succeq mI$, then "Linear convergence." For some $\gamma \in (0,1)$, $f(x_t) - f(x^*) \leq \gamma^t$, $\gamma < 1$.

$$f(x_t) - f(x^*) \leq \gamma^t \quad \text{or} \quad t \geq \frac{1}{\gamma} \log \frac{1}{\varepsilon} \;\Rightarrow\; f(x_t) - f(x^*) \leq \varepsilon.$$

- Smooth case: $\|\nabla f(x) - \nabla f(y)\| \leq C \|x - y\|$.

$$f(x_t) - f(x^*) \leq \frac{K}{t^2}$$

- Newton's method often is faster, especially when f has "long valleys"

Newton's method

- Inverting a Hessian is very expensive: $O(d^3)$
- Approximate inverse Hessian
  - BFGS, Limited-memory BFGS
- Or use Conjugate Gradient Descent
- For unconstrained problems, you can use these off-the-shelf optimization methods
- For unconstrained non-convex problems, these methods will find local optima

Optimization for machine learning

- Goal of machine learning
  - Minimize expected loss $L(h) = \mathbf{E}\left[\text{loss}(h(x), y)\right]$
    given samples $(x_i, y_i)\ i = 1, 2 \ldots m$
  - But we don't know $P(x,y)$, nor can we estimate it well
- Empirical risk minimization
  - Substitute sample mean for expectation
  - Minimize empirical loss: $L(h) = 1/n \sum_i \text{loss}(h(x_i), y_i)$
  - A.K.A. Sample Average Approximation

Batch gradient descent

- Let's put our knowledge into use
- Minimize empirical loss, assuming it's convex and unconstrained
  - Gradient descent on the empirical loss:
  - At each step,

$$w^{(k+1)} \leftarrow w^{(k)} - \eta_t \left(\frac{1}{n} \sum_{i=1}^{n} \frac{\partial L(w, x_i, y_i)}{\partial w} \right)$$

  - Note: at each step, gradient is the average of the gradient for all samples (*i* =1,...,*n*)
  - Very slow when *n* is very large

Stochastic gradient descent

- Alternative: compute gradient from just one (or a few samples)
- Known as stochastic gradient descent:
  - At each step,

$$w^{(k+1)} \leftarrow w^{(k)} - \eta_t \frac{\partial L(w, x_i, y_i)}{\partial w}$$

(choose one sample *i* and compute gradient for that sample only)

Cont'd

- The gradient of one random sample is not the gradient of the objective function
- Q1: Would this work at all?
- Q2: How good is it?
- A1: SGD converges to not only the empirical loss minimum, but also to the expected loss minimum!
- A2: Convergence (to expected loss) is slow
  - $f(w_t) - E[f(w^*)] \leq O(1/t)$ or $O(1/\sqrt{t})$

Practically speaking....

- If the training set is small:
  - batch learning using quasi-Newton or conjugate gradient descent
- If the training set is large:
  - stochastic gradient descent
- Somewhere in between
  - mini-batch
- Convergence is very sensitive to learning rate
  - Basically, it needs to be determined by trial-and-error (model selection or cross-validation)

Constrained optimization

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Lagrangian function

Start with optimization problem:

$$\begin{aligned} \underset{x}{\text{minimize}} \ & f_0(x) \\ \text{s.t.} \ & f_i(x) \leq 0, \ i = \{1, \dots, k\} \\ & h_j(x) = 0, \ j = \{1, \dots, l\} \end{aligned}$$

Form *Lagrangian* using Lagrange multipliers $\lambda_i \geq 0, \ \nu_i \in \mathbb{R}$

$$\mathcal{L}(x, \lambda, \nu) = f_0(x) + \sum_{i=1}^{k} \lambda_i f_i(x) + \sum_{j=1}^{l} \nu_j h_j(x)$$

Con't

- Original/primal problem

$$\begin{aligned} \underset{x}{\text{minimize}} \quad & f_0(x) \\ \text{s.t.} \quad & f_i(x) \le 0, \; i = \{1, \ldots, k\} \\ & h_j(x) = 0, \; j = \{1, \ldots, l\} \end{aligned}$$

  is equivalent to min-max optimization

$$\underset{x}{\text{minimize}} \left[\sup_{\lambda \succeq 0, \nu} \mathcal{L}(x, \lambda, \nu) \right]$$

- Why?
  - Consider a two-player game
  - If player 1 chooses x that violates a constraint $f_1(x)>0$, player 2 choose $\lambda_1 \rightarrow \infty$ so that $L(x,\lambda,v) = \ldots + \lambda_1 f_1(x) + \ldots \rightarrow \infty$
  - Therefore, player 1 is forced to satisfy constraints

Dual function and dual problem

- Dual function:

$$g(\lambda, \nu) = \inf_x \mathcal{L}(x, \lambda, \nu) = \inf_x \left\{ f_0(x) + \sum_{i=1}^{k} \lambda_i f_i(x) + \sum_{j=1}^{l} \nu_j h_j(x) \right\}$$

- Dual problem (cf: Primal problem)

$$\underset{\lambda \succeq 0, \nu}{\text{maximize}} \left[\inf_x \mathcal{L}(x, \lambda, \nu) \right].$$

$$\underset{x}{\text{minimize}} \left[\sup_{\lambda \succeq 0, \nu} \mathcal{L}(x, \lambda, \nu) \right]$$

- Q: How are primal and dual solutions related?

Weak duality

- Dual function lower-bounds the primal optimal value!

Lemma (Weak Duality)

If $\lambda \succeq 0$*, then*

$$g(\lambda, \nu) \leq f_0(x^*).$$

Proof.

We have

$$\begin{aligned} g(\lambda, \nu) = \inf_x \mathcal{L}(x, \lambda, \nu) \leq \mathcal{L}(x^*, \lambda, \nu) \\ = f_0(x^*) + \sum_{i=1}^{k} \lambda_i f_i(x^*) + \sum_{j=1}^{l} \nu_j h_j(x^*) \leq f_0(x^*). \end{aligned}$$

Strong duality

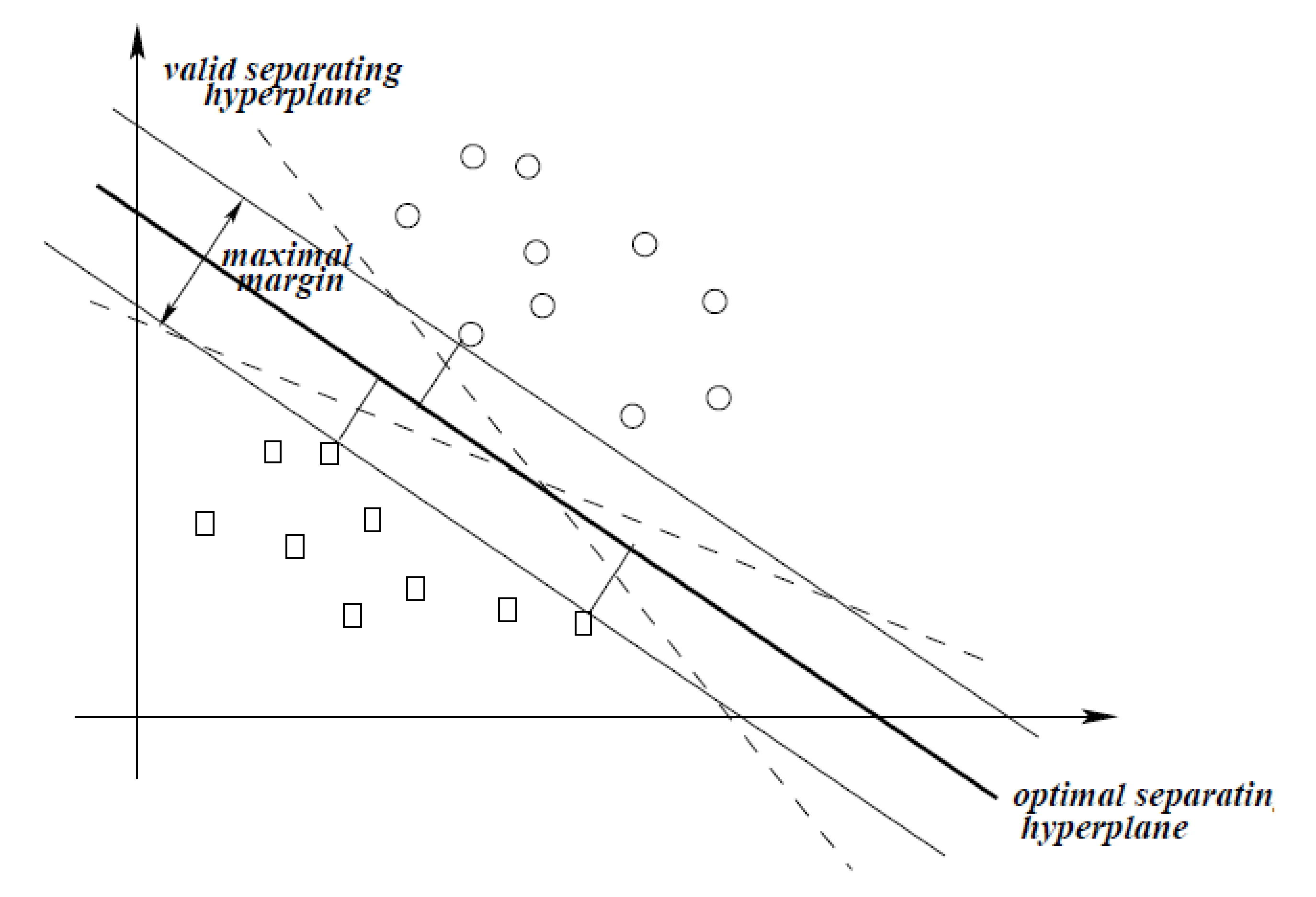
- For convex problems, primal and dual solutions are equivalent!

$$\sup_{\lambda \succeq 0, \nu} g(\lambda, \nu) = f_0(x^*)$$

- Equivalently, *max min L(x,λ,v) = min max L(x,λ,v)*

- What does the theorem mean in practice?
  - You had a constrained minimization problem, which may be hard to solve
  - Dual problem may be easier to solve (simpler constrains)
  - When you solve the dual problem, it also gives the solution for the primal problem!

SVM Recap



valid separating hyperplane
maximal margin
optimal separatin hyperplane

SVM in primal form

- Primal SVM

$$\begin{array}{ll} \textit{minimize} & \frac{1}{2}||w||^2 \\ \textit{subject to} & y_i(w \cdot x_i + w_0) \geq 1 \textbf{ for } i = 1, \ldots, m \end{array}$$

  - for linearly separable cases.
  - It is a linearly constrained QP, and therefore a convex problem

SVM in dual form

The Lagrangean function associated to the primal form of the given QP is

$$L_P(w, w_0, \alpha) = \frac{1}{2}||w^2|| - \sum_{i=1}^{m} \alpha_i(y_i(w \cdot x_i + w_0) - 1)$$

with $\alpha_i \geq 0, i = 1, \ldots, m$. Finding the minimum of L_P implies

$$\frac{\partial L_P}{\partial w_0} = -\sum_{i=1}^{m} y_i \alpha_i = 0$$

$$\frac{\partial L_P}{\partial w} = w - \sum_{i=1}^{m} y_i \alpha_i x_i = 0 \Rightarrow w = \sum_{i=1}^{m} y_i \alpha_i x_i$$

$$\text{where } \frac{\partial L_P}{\partial w} = (\frac{\partial L_P}{\partial w_1}, \ldots, \frac{\partial L_P}{\partial w_d})$$

By substituting these constraints into L_P we get its dual form

$$L_D(\alpha) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} \alpha_i \alpha_j y_i y_j \; x_i \cdot x_j$$

Constrained optimization methods

- Log barrier method
- Projected (sub)gradient
- Interior point method
- Specialized methods
  - SVM: Sequential Minimal Optimization
  - Structured-output SVM: cutting-plane method

- Other optimization not covered in this lecture:
  - Bayesian models: EM, variational methods
  - Discrete optimization
  - Graph optimization