Optimization for Machine Learning

CS 406

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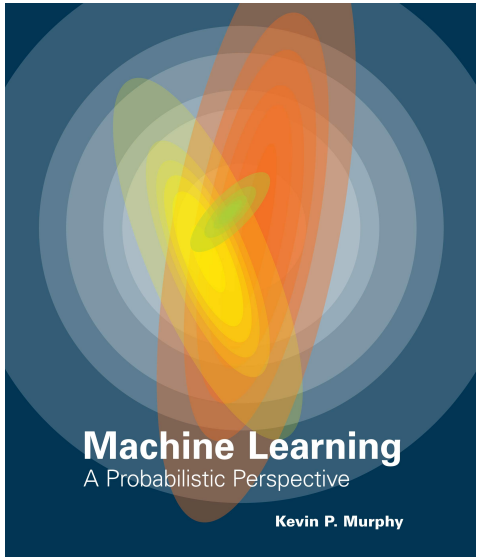
UBC Computer Science

Term 2, 2014-15

Goals of this Lecture

1. Give an overview and motivation for the machine learning technique of supervised learning.
2. Generalize convergence rates of gradient methods for solving linear systems to general smooth convex optimization problems.
3. Introduce the proximal-gradient algorithm, one of the most efficient algorithms for solving special classes of non-smooth convex optimization problems.
4. Introduce the stochastic-gradient algorithm, for solving data-fitting problems when the size of the data is very large.

Machine Learning



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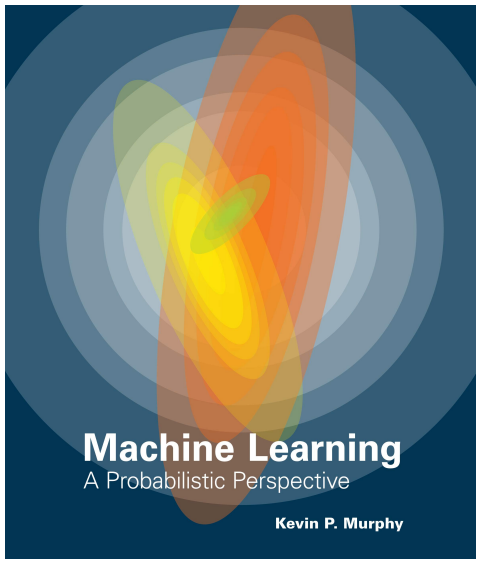

- *Study of using computers to automatically detect patterns in data, and use these to make predictions or decisions*.
- One of the fastest-growing areas of science/engineering.
- Recent successes: Kinect, book/movie recommendation, spam detection, credit card fraud detection, face recognition, speech recognition, object recognition, self-driving cars.

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  - Given input and output examples.
  - Build a model that predicts the output from the inputs.
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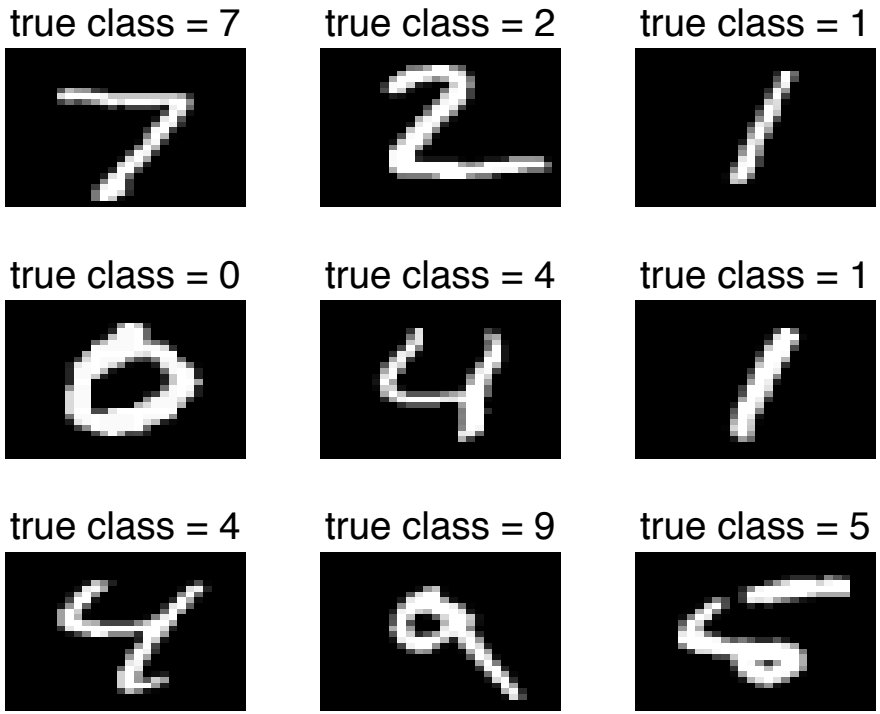
- Canonical example: hand-written digit recognition:



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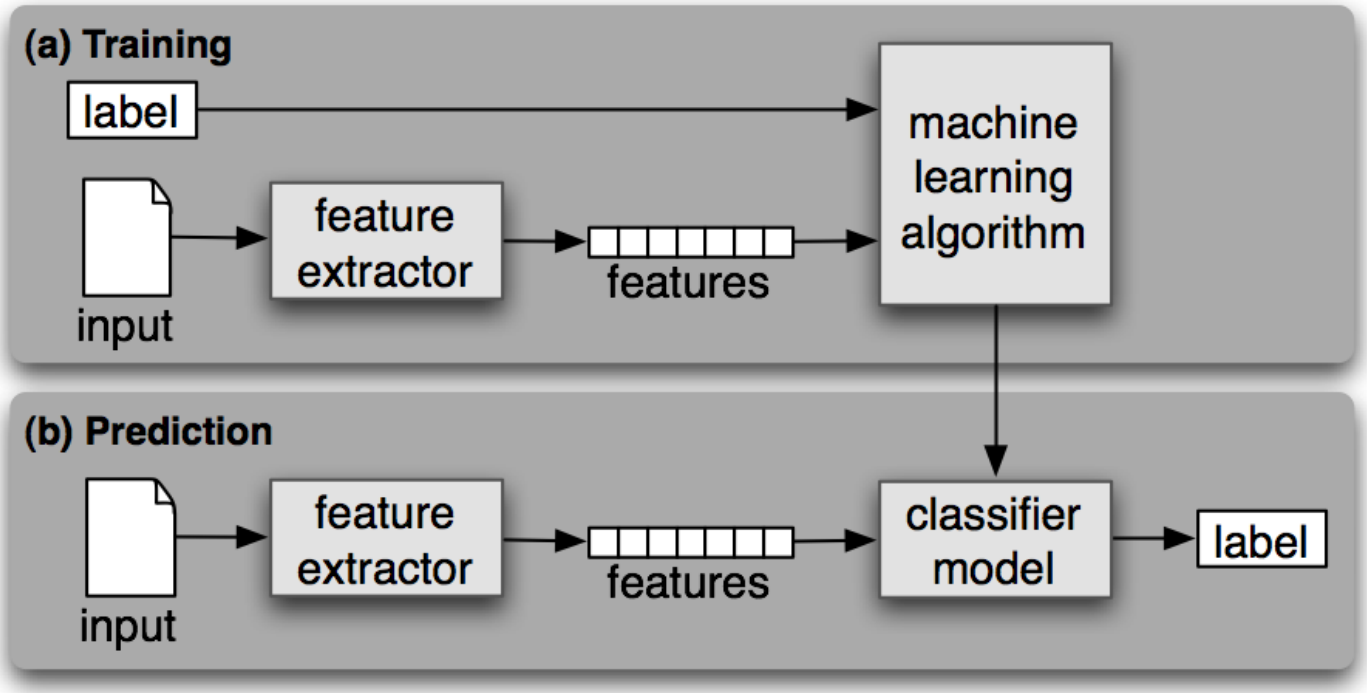
- But don't know how to write a program to solve it.
- And you have lots of labeled data.
- Key reason for machine learning's popularity and success.

Training and Testing

- Steps for supervised learning:
  1. Training phase: build model that maps from input features to labels. (based on many examples of the correct behaviour)
  2. Testing phase: model is used to label new inputs.



Connection to Numerical Optimization

- Typically, the training phase is formulated as an optimization problem,

$$\min_{\mathbf{x}} \quad \sum_{i=1}^{m} f_i(\mathbf{x}) \quad + \quad \lambda r(\mathbf{x}).$$

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- Squared ℓ_2-norm regularization:

$$r(\mathbf{x}) = \|\mathbf{x}\|^2.$$

Outline

Motivation for First-Order Methods

- We first consider the unconstrained optimization problem,

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

- In typical ML models the dimension, dimension n is very large.
- We will focus on matrix-free methods, as in the previous lecture:
  - Allows n to be in the billions or more.
  - We can show dimension-independent convergence rates.

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- We will focus on matrix-free methods, as in the previous lecture:
  - Allows n to be in the billions or more.
  - We can show dimension-independent convergence rates.
- As before, the simplest case is gradient descent,

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \alpha_k \nabla f(\mathbf{x}_k).$$

- How many iterations are needed?

Strongly-Convex and Strongly-Smooth

- Consider special case of least squares:

$$\min_{\mathbf{x}} f(\mathbf{x}) = \frac{1}{2}\|\mathbf{b} - A\mathbf{x}\|^2.$$

- Recall that

$$\nabla^2 f(\mathbf{x}) = A^T A,$$

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- Functions f with eigenvalues of Hessian bounded between positive constants for all f are called 'strongly smooth' and 'strongly convex'.
- These assumptions are sufficient to show a linear convergence rate.

Implication of Strong-Smoothness

- From Taylor's theorem, for some $\mathbf{z}$ we have:

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

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$$f(\mathbf{y}) \leq f(\mathbf{x}) + \nabla f(\mathbf{x})^T(\mathbf{y}-\mathbf{x}) + \frac{\lambda_1}{2}\|\mathbf{y}-\mathbf{x}\|^2$$

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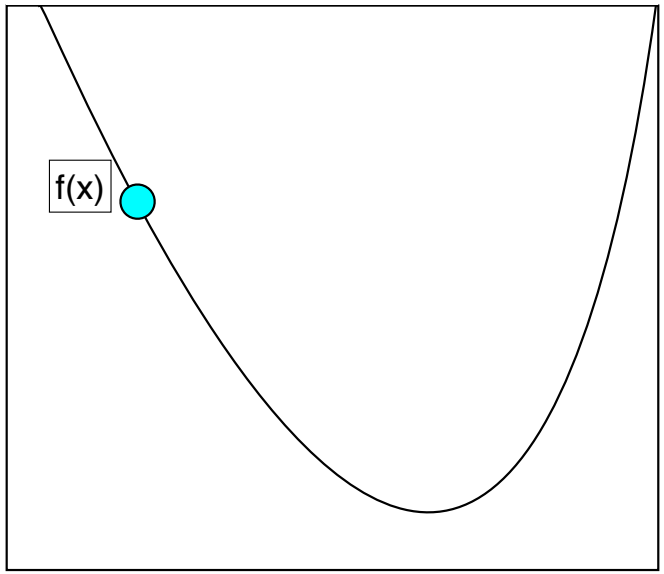

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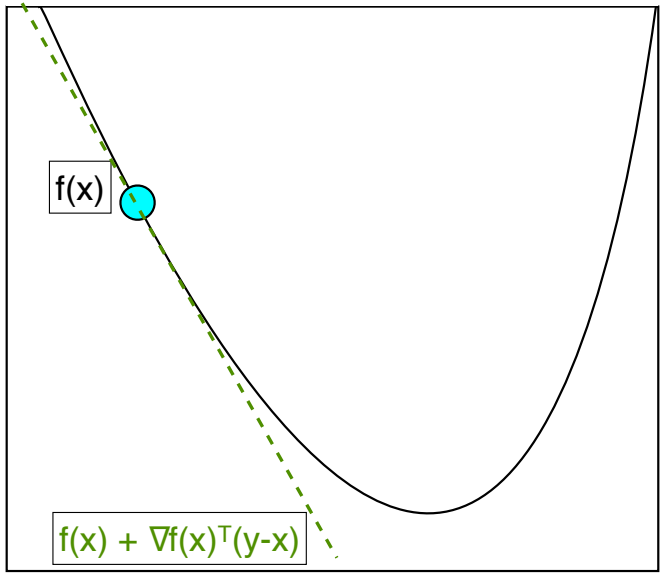

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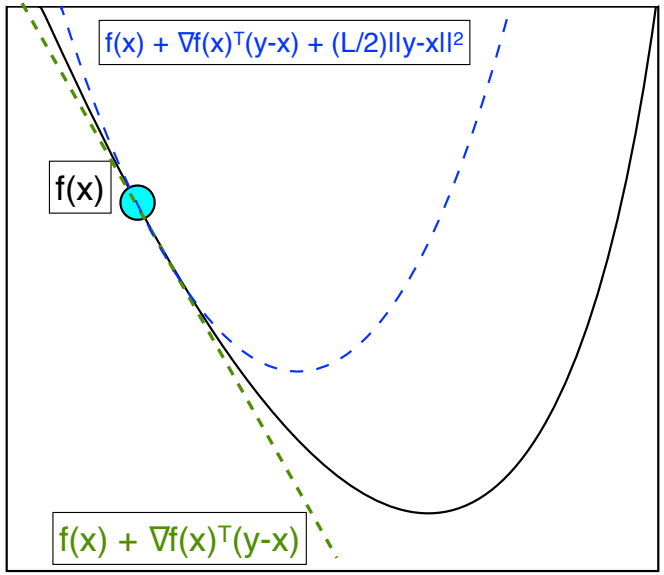

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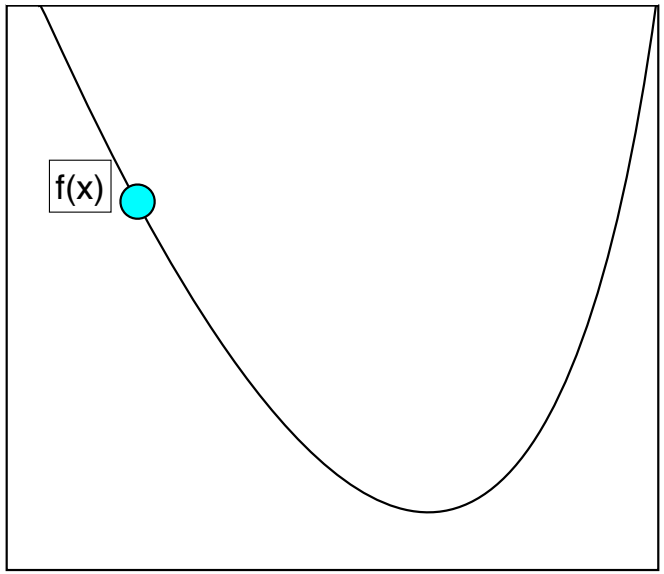

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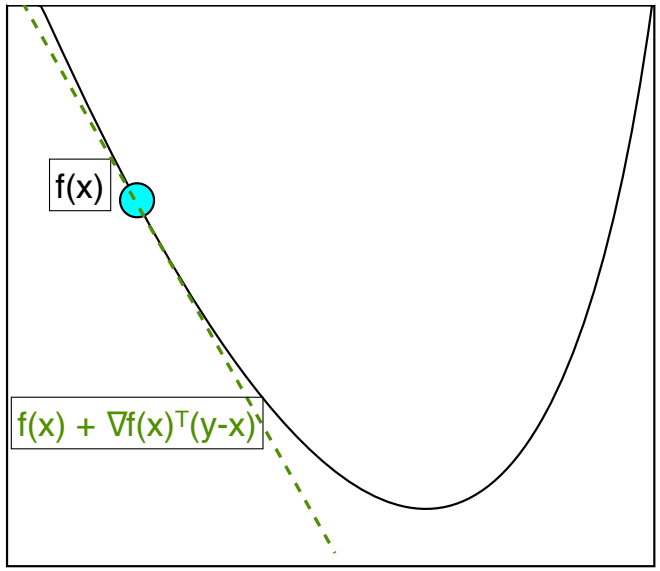

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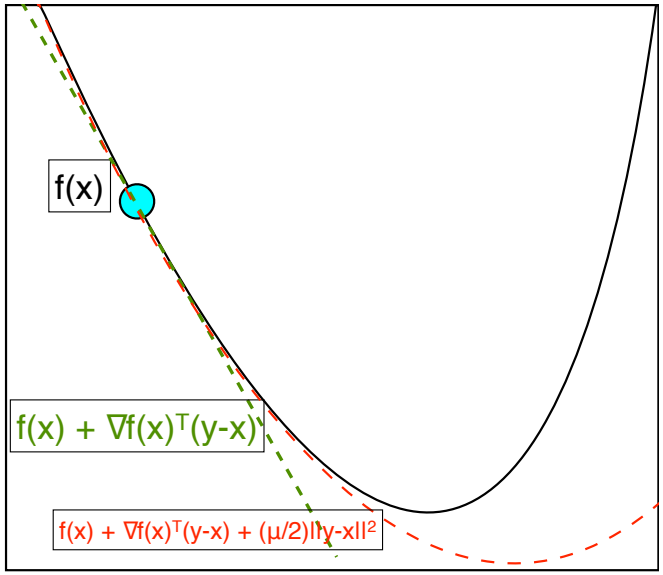

Bounds on Progress and Sub-Optimality

- We have the upper bound

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  and minimizing both sides in terms of y gives

$$f(\mathbf{x}^*) \geq f(\mathbf{x}_k) - \frac{1}{2\lambda_n}\|\nabla f(\mathbf{x}_k)\|^2,$$

  which bounds how far $\mathbf{x}_k$ is from the solution $\mathbf{x}^*$.

Linear Convergence of Gradient Descent

- We have bounds on $\mathbf{x}_{k+1}$ and $\mathbf{x}^*$:

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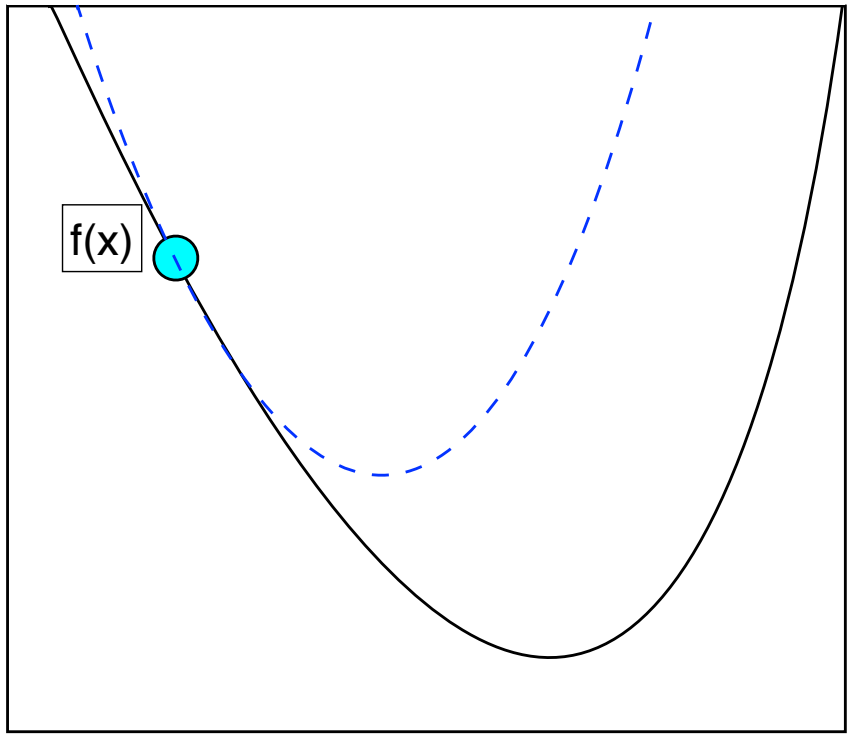

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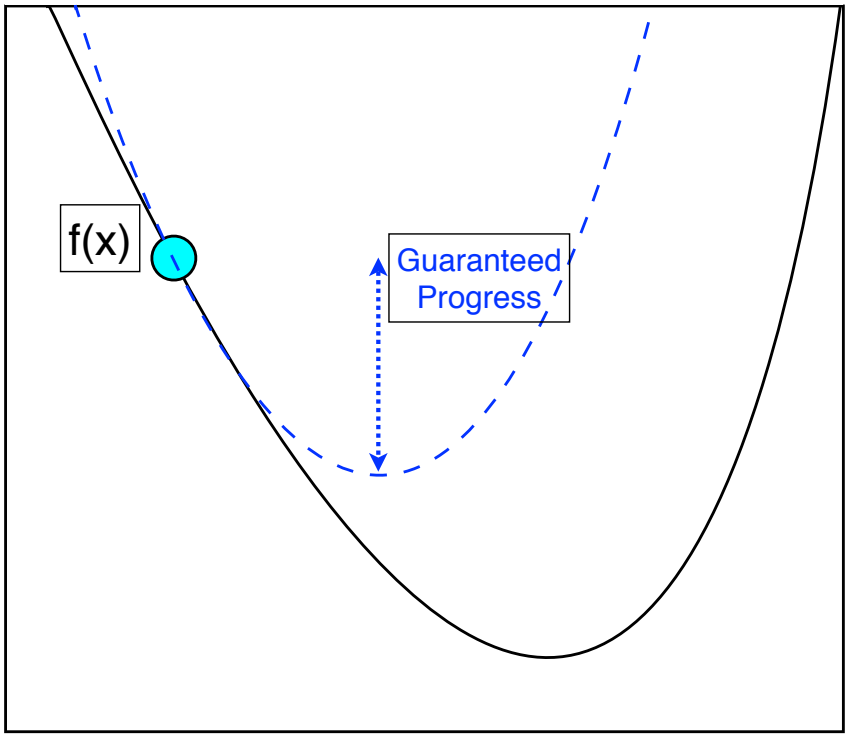

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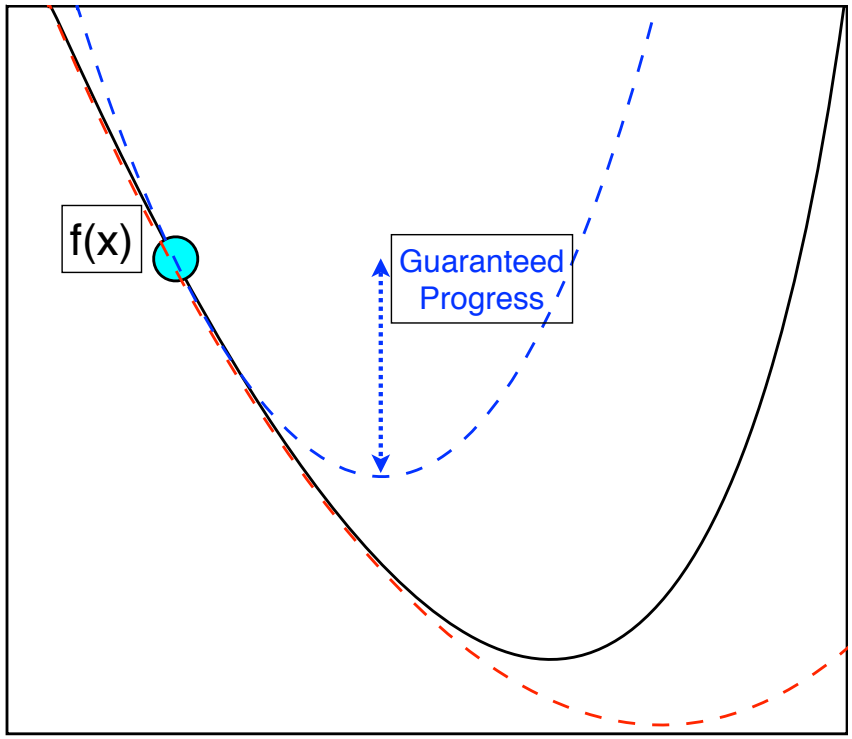

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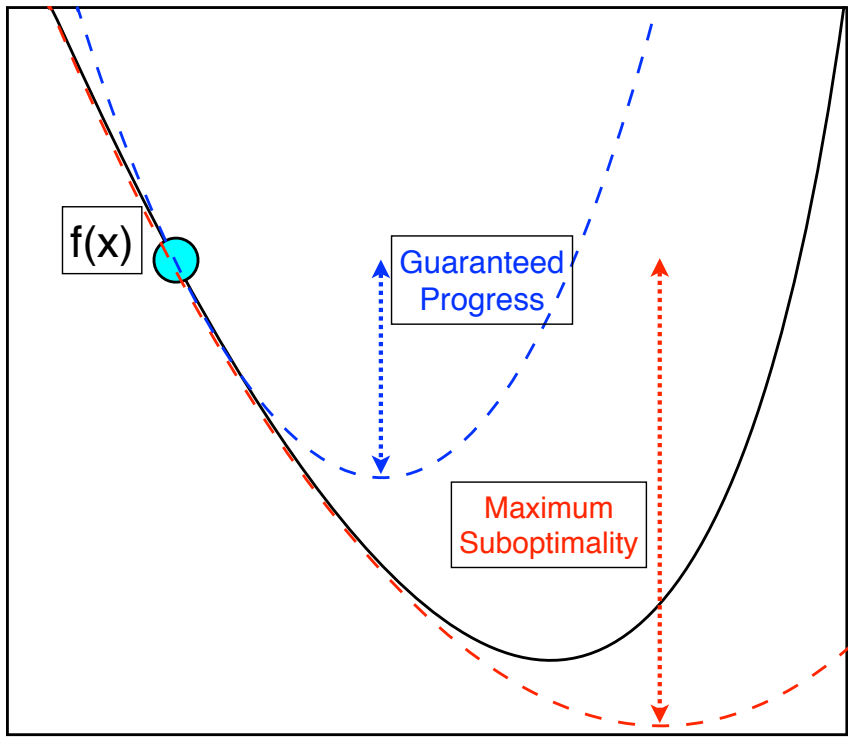

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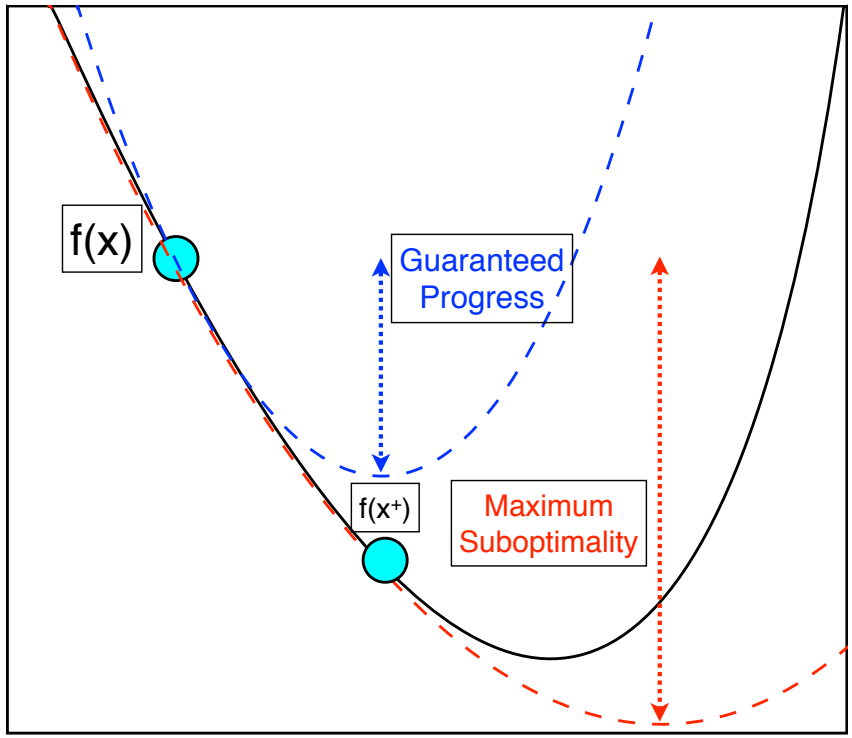

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- Applying recursively gives a linear convergence rate:

$$f(\mathbf{x}_k) - f(\mathbf{x}^*) \leq \left(1 - \frac{\lambda_n}{\lambda_1}\right)^k [f(\mathbf{x}_0) - f(\mathbf{x}^*)]$$

- We say that the condition number for f is given by $\kappa_f = \frac{\lambda_1}{\lambda_n}$.

Convergence Rate of Gradient Descent

- What about line-search?
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- Similar to the rate for solving linear systems (last lecture).
- Can we derive a method with the faster rate of conjugate gradient?

  ('Non-linear' conjugate gradient methods don't actually have a faster rate.)

Nesterov's accelerated gradient method

- There is a method similar to conjugate gradient,

$$\mathbf{x}_{k+1} = \mathbf{y}_k - \alpha_k \nabla f(\mathbf{y}_k),$$
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- It has a faster rate of

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- Slower in practice than non-linear conjugate gradient and quasi-Newton methods, but does not depend on dimension and generalizes to non-smooth problems...

Outline

Motivation: Spam Filtering

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- We will look at phrases in the e-mail messages:
  - "CPSC 406".
  - "Meet singles in your area now'
- There are too many possible phrases (model would be huge).
- But some are more helpful than others: feature selection.

LASSO: Sparse Regularization

- Consider the ℓ_1-regularized least squares problem (LASSO),

$$\min_{\mathbf{x}} \frac{1}{2}\|\mathbf{b} - A\mathbf{x}\|^2 + \lambda\|\mathbf{x}\|_1.$$

- Recall the definition of the ℓ_1-norm,

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- The challenge is that $|x_j|$ is non-differentiable.

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- Use a special class of methods called proximal-gradient methods.

Example: Non-Negative Least Squares

- Consider non-negative least squares,

$$\min_{\mathbf{x} \geq 0} \sum_{i=1}^{m} (b_i - \sum_{j=1}^{n} a_{ij} x_j)^2,$$

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- Gradient projection:
  - Alternates between gradient step and projection step:

$$\mathbf{x}_{k+1} = \text{project}[\mathbf{x}_k - \alpha_k \nabla f(\mathbf{x}_k)],$$

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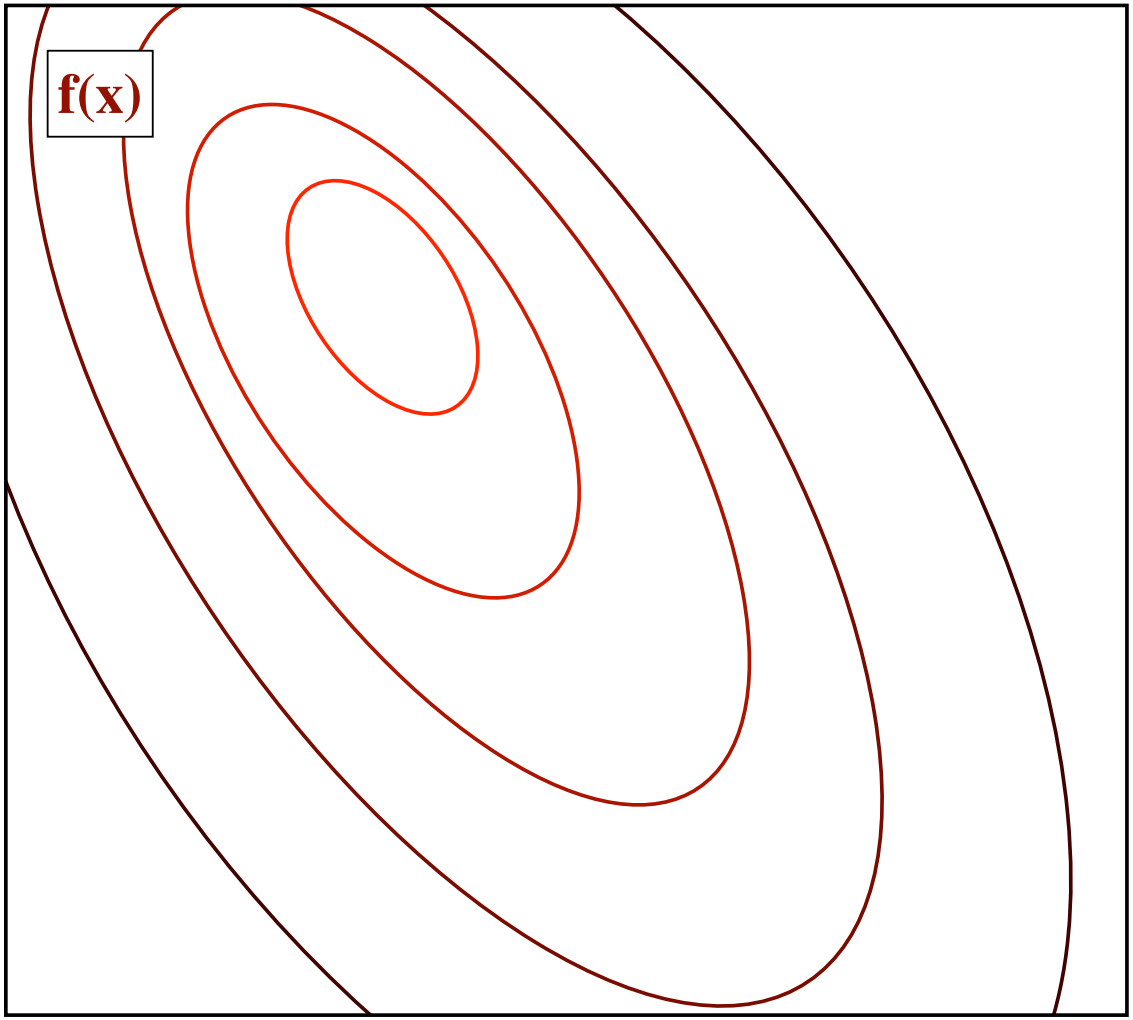
Gradient Projection



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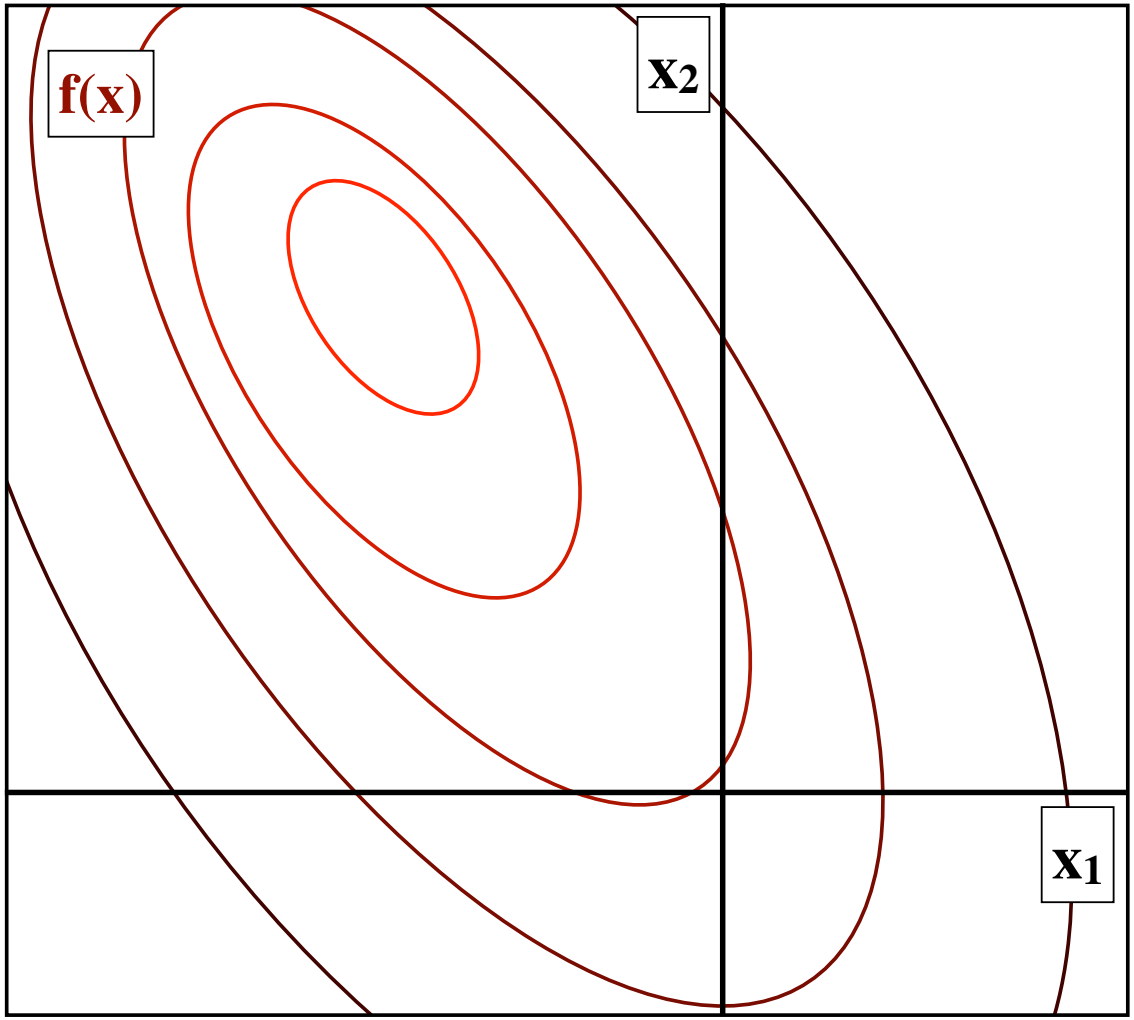

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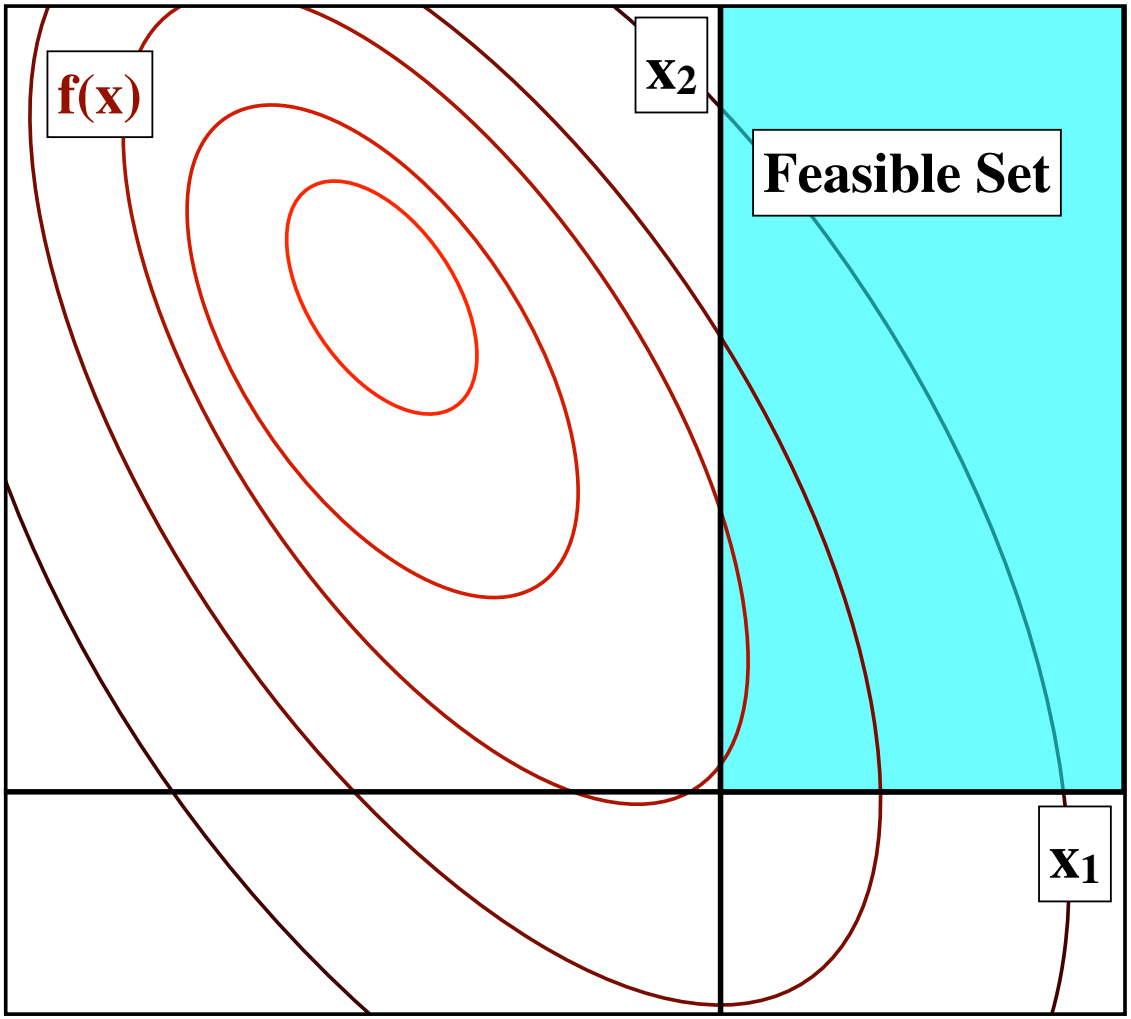

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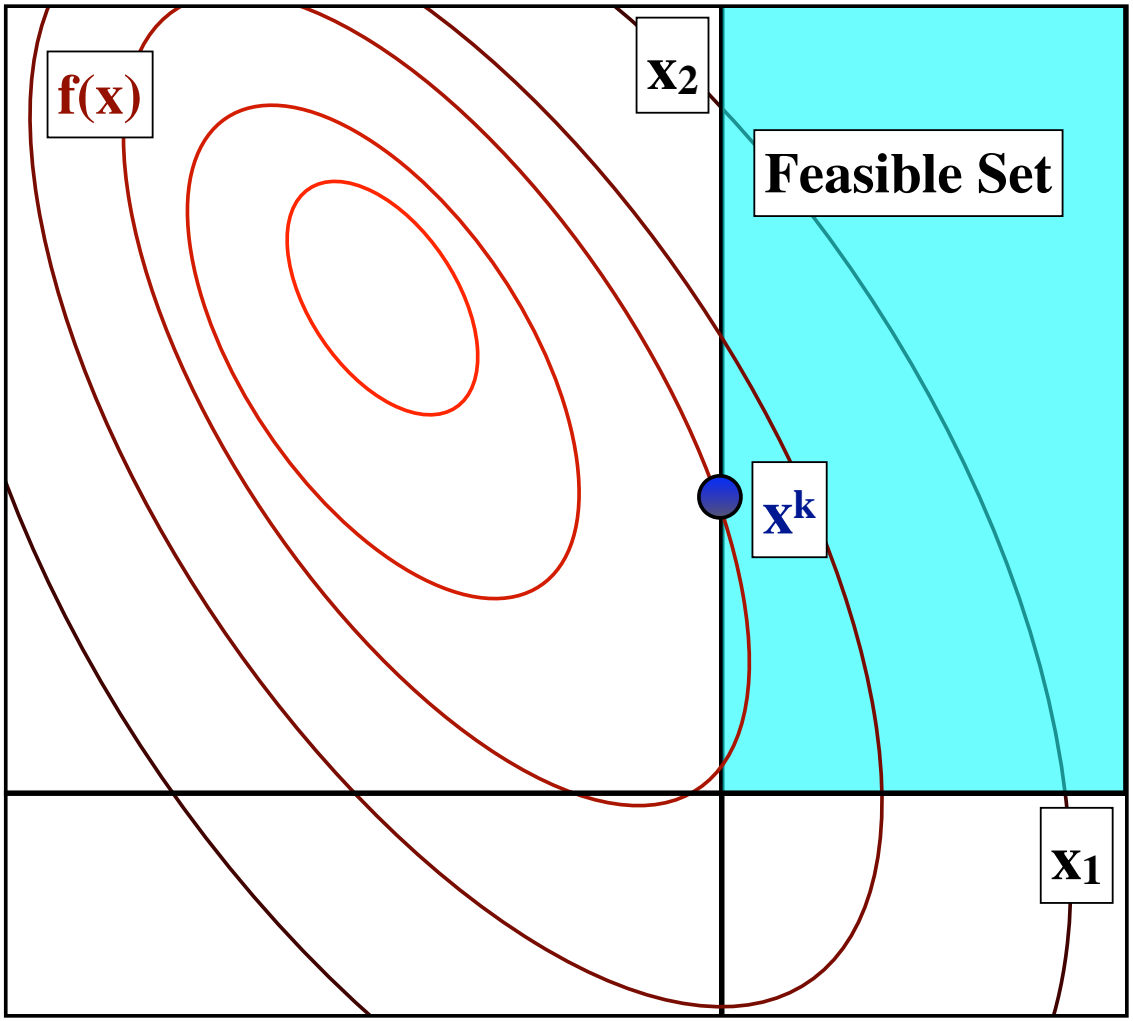

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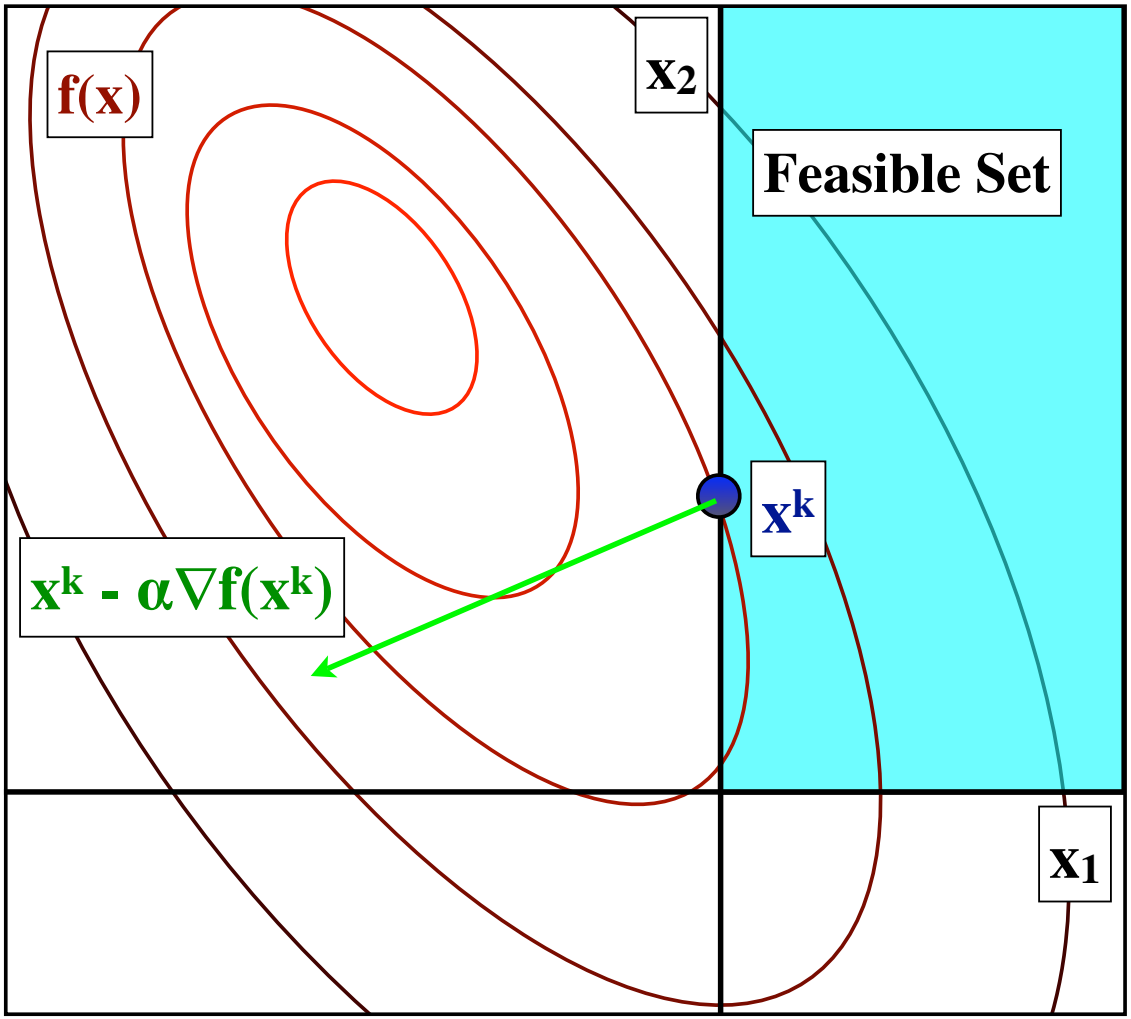

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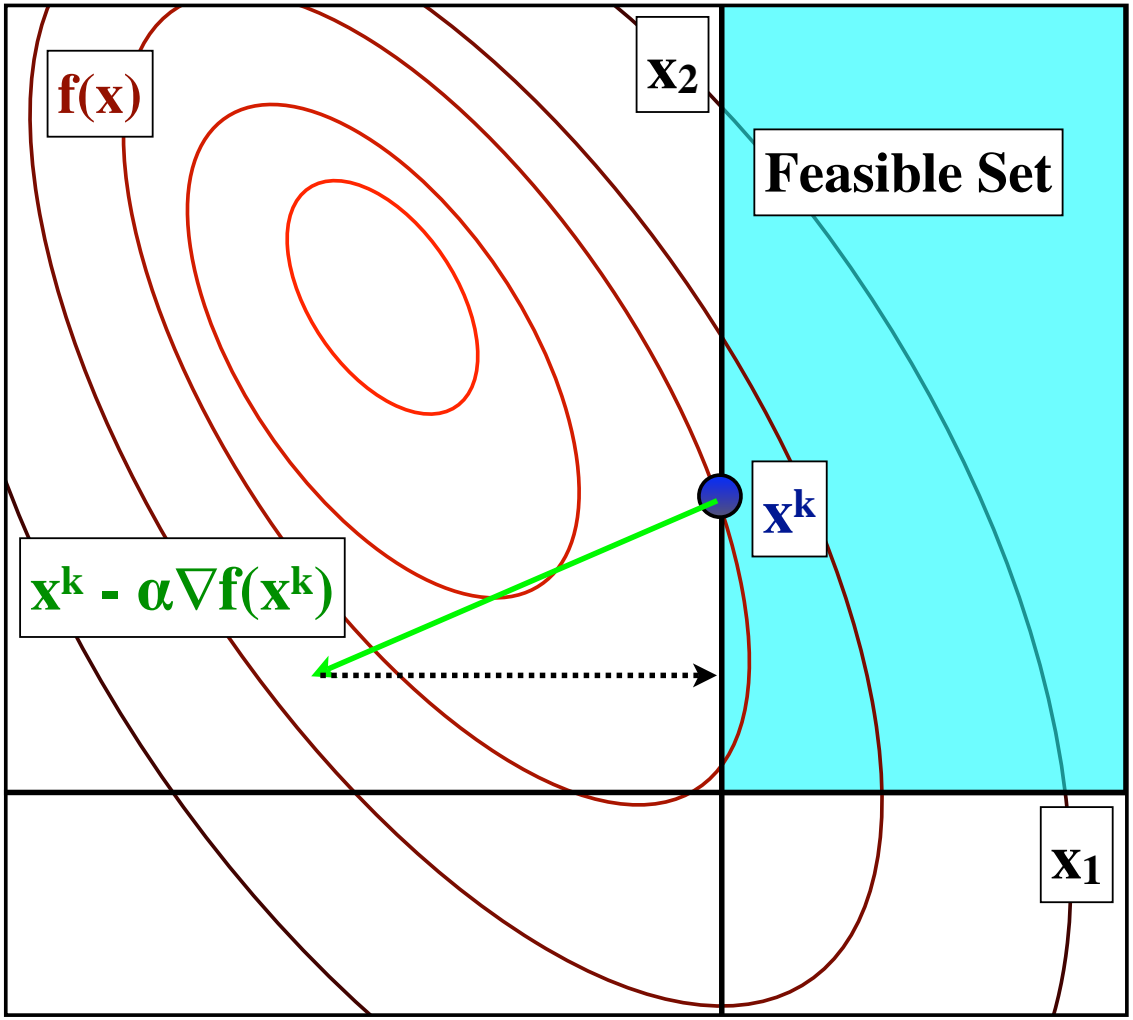

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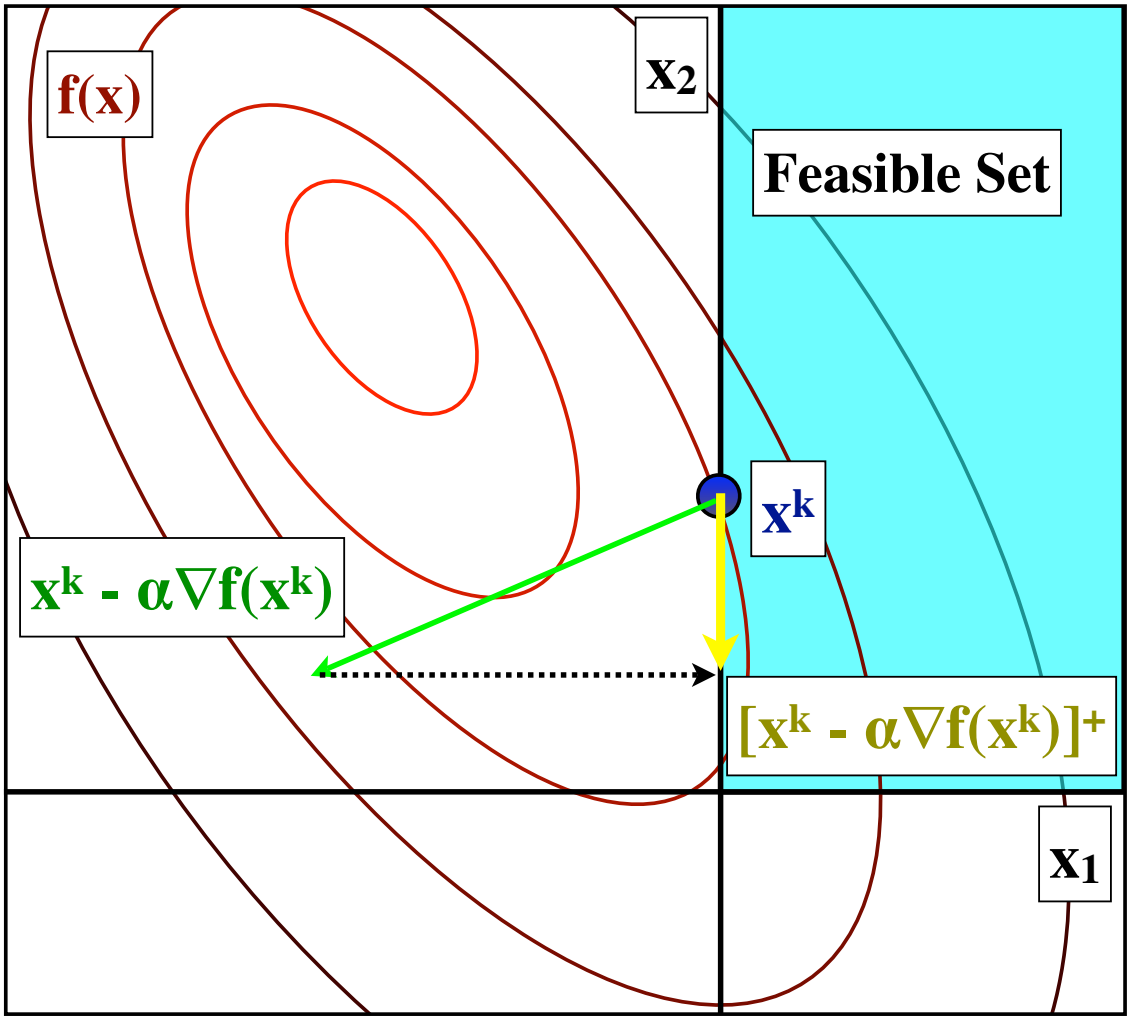

Simple Constraints

- Gradient projection has the same convergence rate as the unconstrained gradient method,

$$f(\mathbf{x}_k) - f(\mathbf{x}^*) \leq \left(1 - \frac{1}{\kappa_f}\right)[f(\mathbf{x}_0) - f(\mathbf{x}^*)].$$

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gives a better dependence on the condition number,

$$f(\mathbf{x}_k) - f(\mathbf{x}^*) \leq \left(1 - \frac{1}{\sqrt{\kappa_f}}\right)[f(\mathbf{x}_0) - f(\mathbf{x}^*)].$$

Proximal-Gradient Method

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- Convergence rates are still the same as for minimizing f alone.

Special case of Projected-Gradient Methods

- Projected-gradient methods are a special case:

$$r(\mathbf{x}) = \begin{cases} 0 & \text{if } \mathbf{x} \in \mathcal{C} \\ \infty & \text{if } \mathbf{x} \notin \mathcal{C} \end{cases},$$

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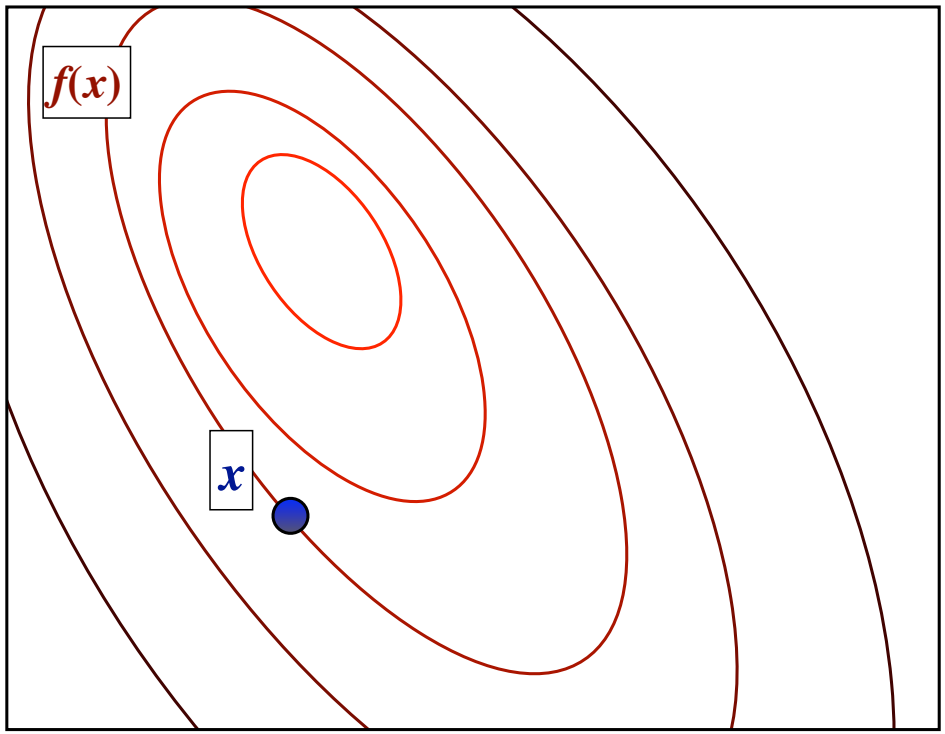

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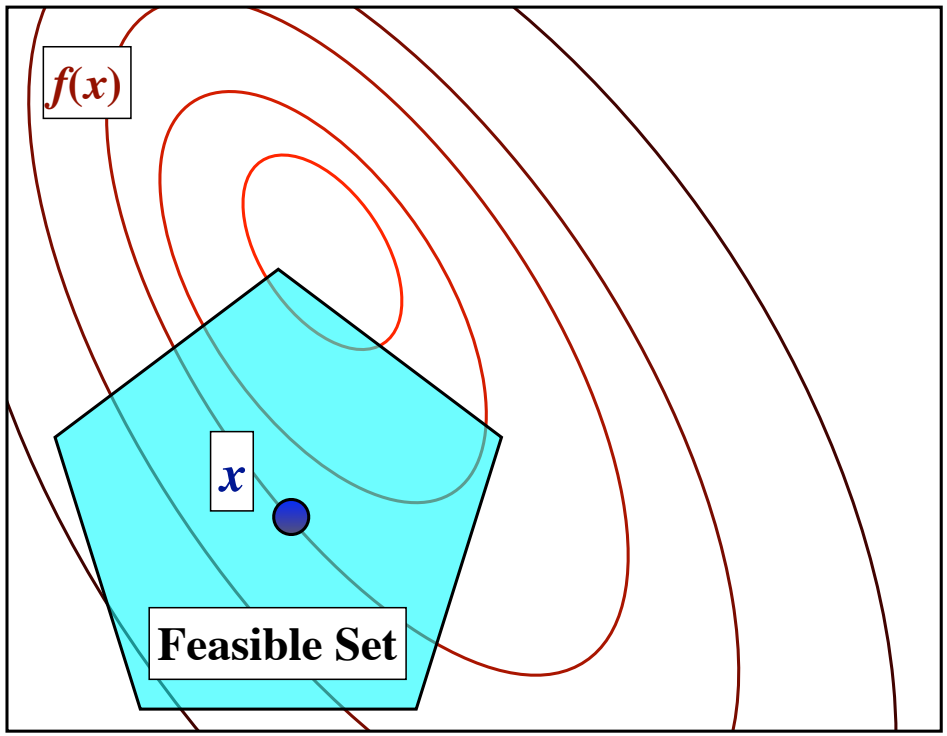

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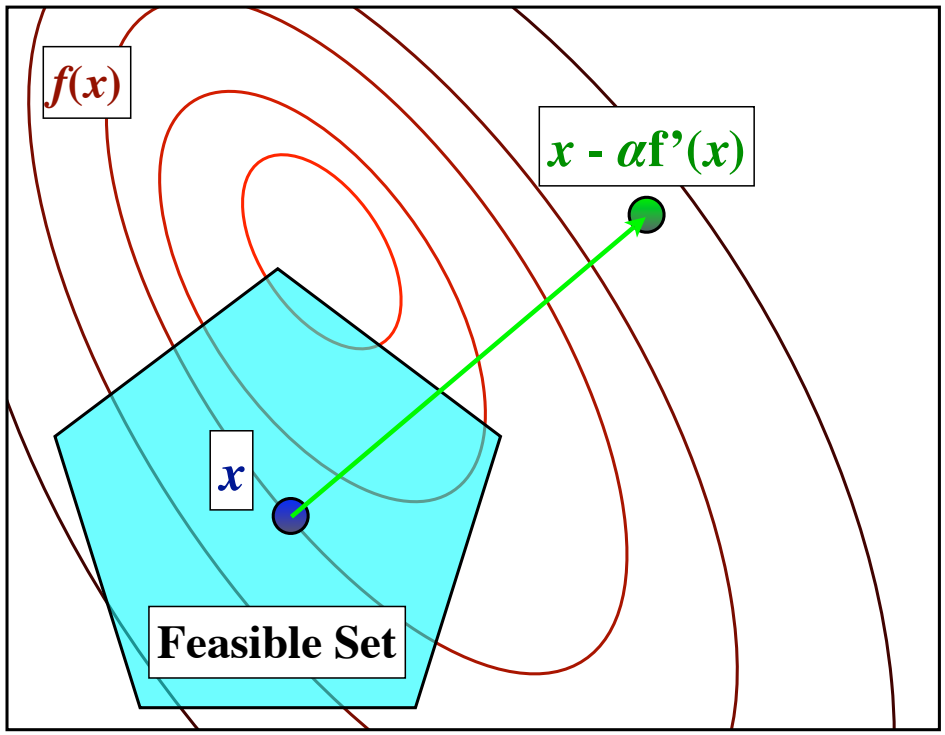

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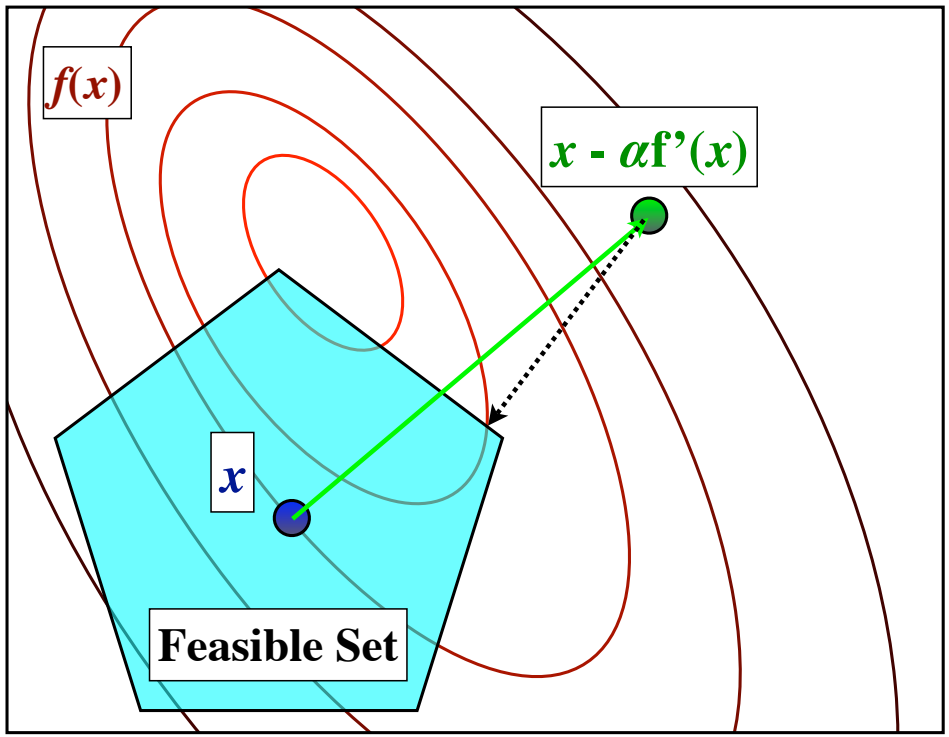

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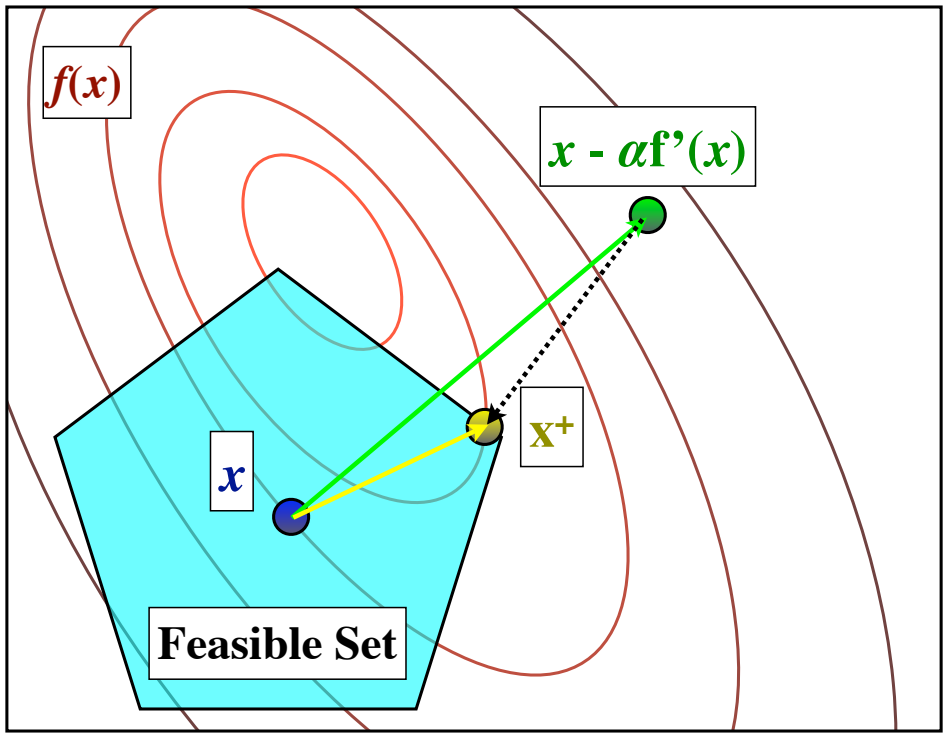

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- Can solve huge instances of these constrained/non-smooth problem.

Outline

Big-N Problems

- Consider the problem of minimizing a finite sum,

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- Examples:
  - Each i is a Facebook user.
  - Each i is a product on Amazon.
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- We can't afford to go through all m examples many times.
- One way to deal with this restriction is stochastic gradient methods.

Stochastic Gradient Methods

- Stochastic gradient methods consider minimizing expectations,

$$\min_{\mathbf{x}} \mathbb{E}[f(\mathbf{x})].$$

- They assume we can generate a random vector $\mathbf{p}_k$ whose expectation is the gradient

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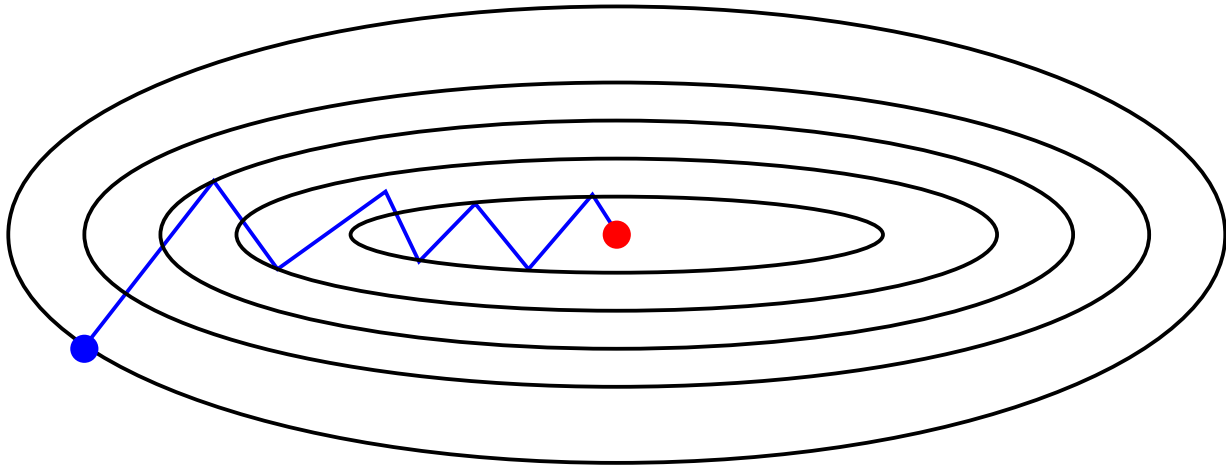
- For convergence, usually require the step-sizes α_k to converge to 0.
  - E.g., Robbins-Munro conditions,

$$\sum_{k=1}^{\infty} \alpha_k = \infty, \quad \sum_{k=1}^{\infty} \alpha_k^2 < \infty,$$

suggests using $\alpha_k = \gamma/k$ for some constant γ.

Gradient Method vs. Stochastic Gradient Method

Gradient method:



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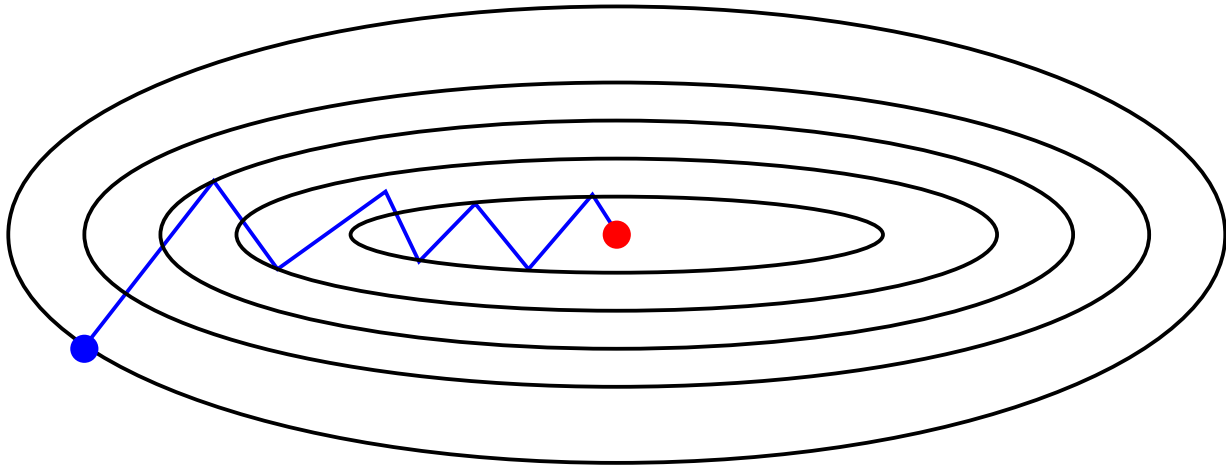

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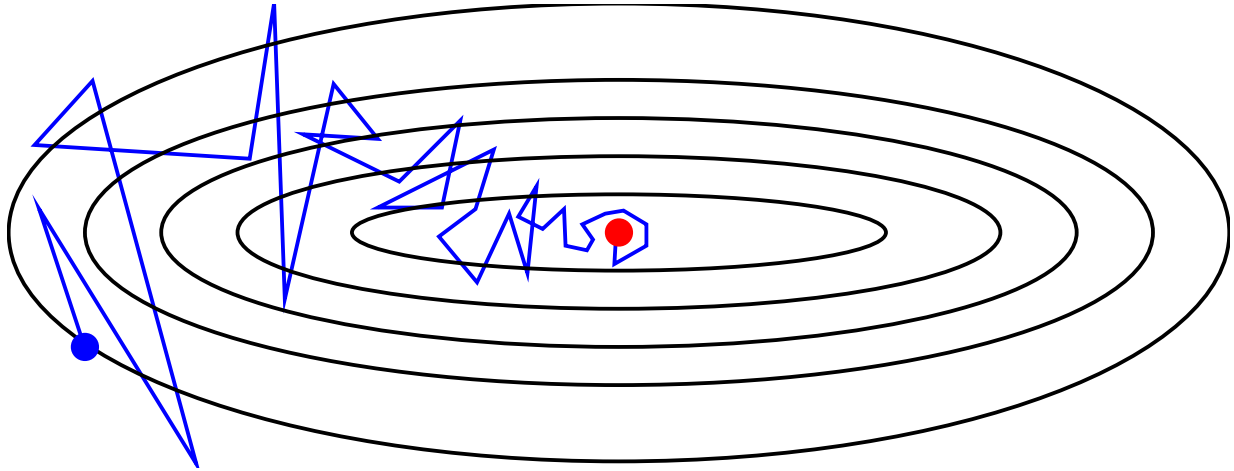

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$$\begin{aligned}\mathbb{E}[\mathbf{p}_k] &= \mathbb{E}_i[\nabla f_i(\mathbf{x}_k)] \\ &= \sum_{i=1}^{m} p(i) \nabla f_i(\mathbf{x}_k) \\ &= \frac{1}{m} \sum_{i=1}^{m} \nabla f_i(\mathbf{x}_k).\end{aligned}$$

Application to Finite Sums

- Returning to the problem of minimizing a finite sum,

$$\min_{\mathbf{x}} \frac{1}{m}\sum_{i=1}^{m} f_i(\mathbf{x}).$$

- Set $\mathbf{p}_k$ to the gradient of a random function f_{i_k},

$$\begin{aligned}\mathbb{E}[\mathbf{p}_k] &= \mathbb{E}_i[\nabla f_i(\mathbf{x}_k)] \\ &= \sum_{i=1}^{m} p(i)\nabla f_i(\mathbf{x}_k) \\ &= \frac{1}{m}\sum_{i=1}^{m} \nabla f_i(\mathbf{x}_k).\end{aligned}$$

- This gives us the stochastic gradient algorithm

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \alpha_k \nabla f_{i_k}(\mathbf{x}_k).$$

- The iteration cost is independent of m.

Convergence Rate of Stochastic Gradient

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Convergence Rate of Stochastic Gradient

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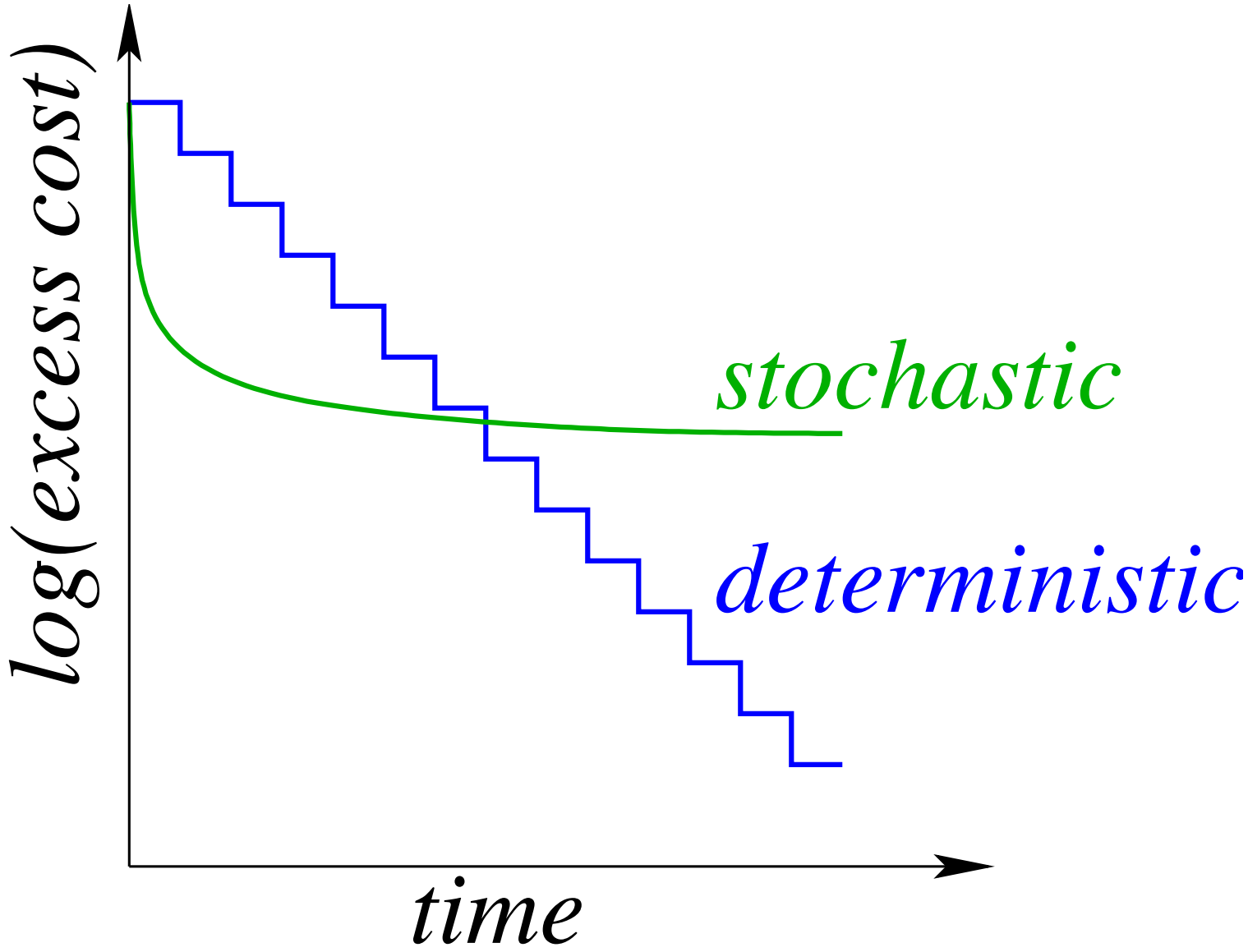
- But how many iterations are required?
- If we set $\alpha_k = 1/k\lambda_n$, we have that

$$\mathbb{E}[f(x^k) - f(x^*)] = O(1/k).$$

- This is a sublinear rate.
- Often works badly in practice:
  - Initial α_k might be huge.
  - Later α_k might be tiny.
- Nesterov/Newton-like variations can only improve the constant.

(even in low dimensions)

Comparison of Gradient and Stochastic Gradient



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  2. Constant step-sizes: If you use a constant step-size $\alpha_k = \alpha$, you can show

$$\mathbb{E}[f(x^k) - f(x^*)] = (1 - 2\alpha\lambda_n)^k[f(x^0) - f(x^*)] + O(\alpha),$$

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  3. Use special problem structures: For certain problems, you can show faster rates.
- Since 2012, large focus on better algorithms for finite sum structure.

Stochastic Average Gradient

- The stochastic average gradient (SAG) algorithm uses,

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \frac{\alpha_k}{m} \sum_{i=1}^{m} \mathbf{y}_k^i,$$

and evaluates a random $\nabla f_i(x^k)$, with $\mathbf{y}_k^i$ the last evaluation of ∇f_i.

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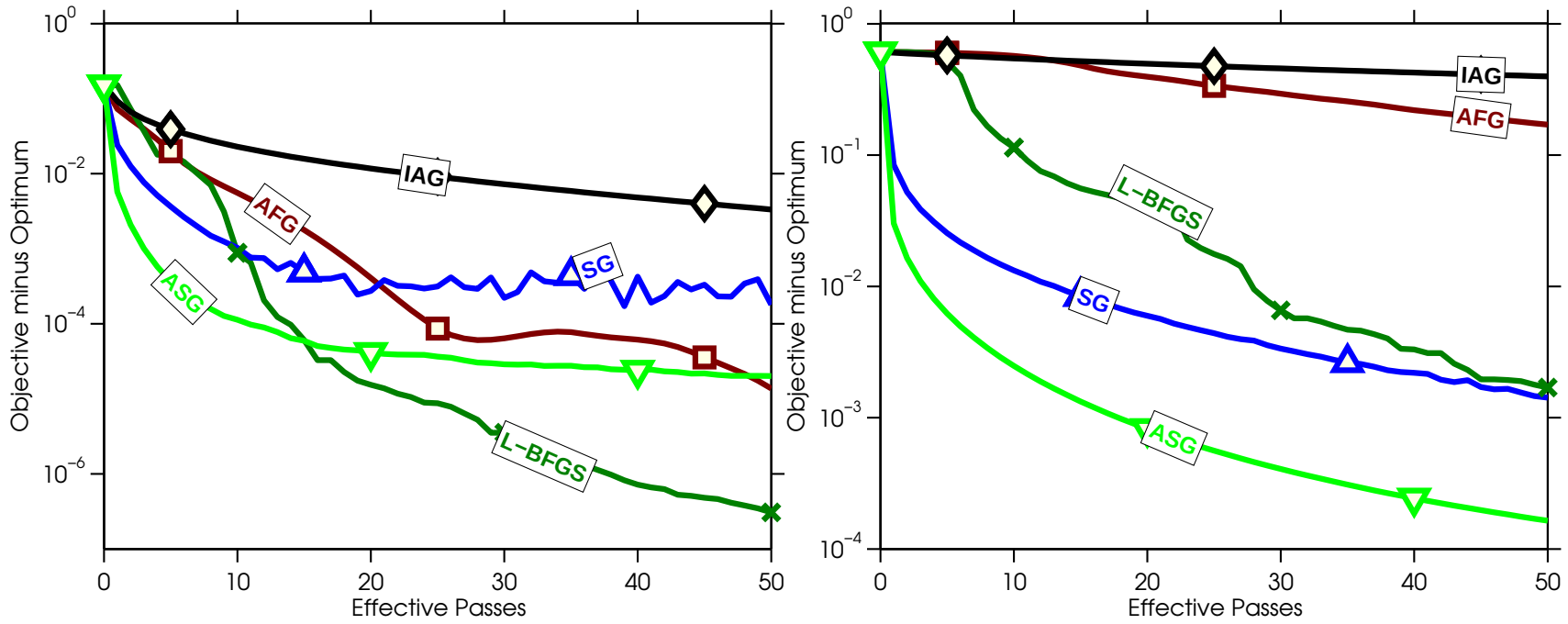
  and evaluates a random $\nabla f_i(x^k)$, with $\mathbf{y}_k^i$ the last evaluation of ∇f_i.
- With $\alpha_k = 1/16\Lambda_1$, the SAG algorithm has linear rate,

$$\mathbb{E}[f(\mathbf{x}_k)] - f(\mathbf{x}^*) \leq \left(1 - \min\left\{\frac{1}{8m}, \frac{\lambda_n}{16\Lambda_1}\right\}\right)^k [f(\mathbf{x}_0) - f(\mathbf{x}^*)],$$

  where Λ_1 bounds eigenvalues of *each* $\nabla^2 f_i(\mathbf{x})$.
- Iteration cost independent of m, rate similar to gradient method.

Comparing FG and SG Methods

- quantum ($n = 50000$, $p = 78$) and rcv1 ($n = 697641$, $p = 47236$)



SAG Compared to FG and SG Methods

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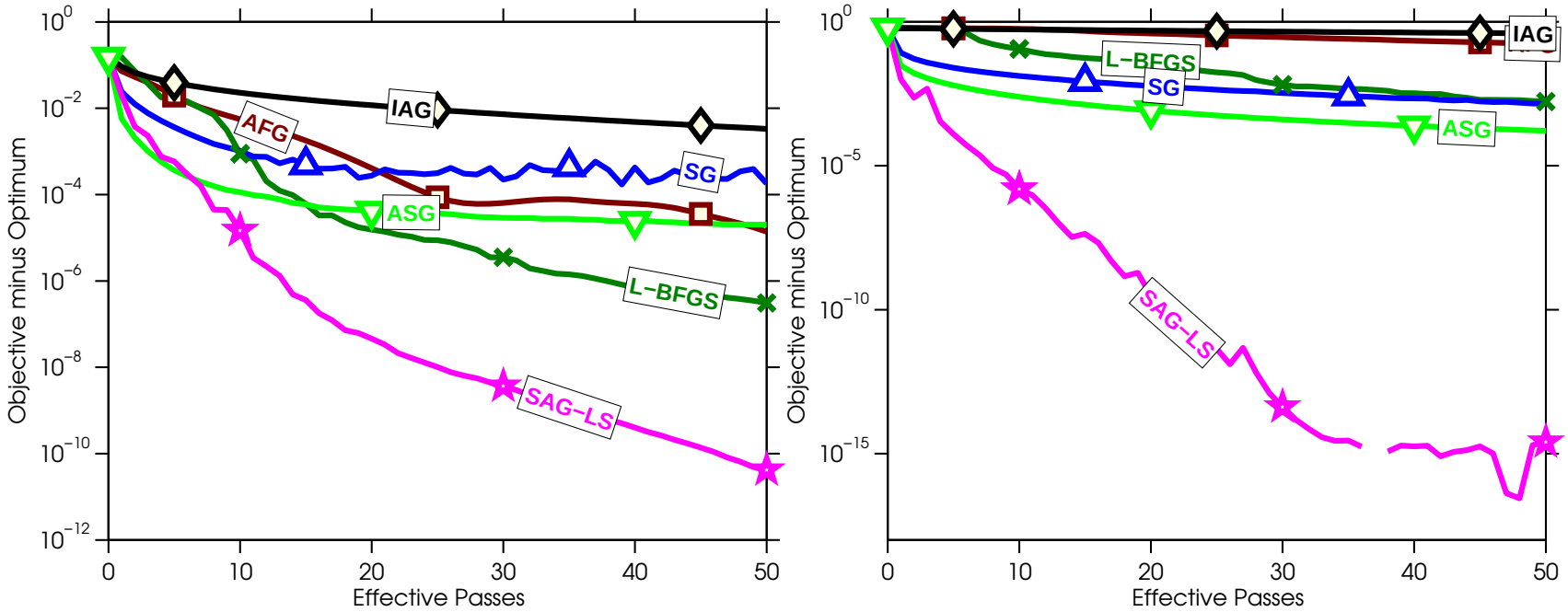

Summary

- Part 1: Numerical optimization is at the core of many modern machine learning applications.
- Part 2: Gradient-based methods allow elegant scaling with dimensionality for smooth problems.
- Part 3: Proximal-gradient methods allow the same scaling for many non-smooth problems.
- Part 4: Stochastic gradient methods allow scaling to a huge number of data samples.