COMP 545: Advanced topics in optimization
From simple to complex ML systems

Lecture 3

Overview

- In the last lecture, we:
    - Talked about a bit of smooth non-convex and convex optimization
    - Worked in practice and theory with gradient descent
    - Discussed the limits and convergence rates of gradient descent

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  - Talked about a bit of smooth non-convex and convex optimization
  - Worked in practice and theory with gradient descent
  - Discussed the limits and convergence rates of gradient descent
- Often, gradient descent is not sufficient in practice. In this lecture, we will:
  - Discuss **alternatives to gradient descent**
  - Discuss cases where the above methods are problematic
  - Discuss gradient descent versions that somehow **accelerate convergence**

From previous lecture: lower bounds

- For objectives with Lipschitz continuous gradients:

$$f(x_t) - f(x^\star) \geq \frac{3L\|x_0 - x^\star\|_2^2}{32(t+1)^2}$$

(Under these assumptions, and using only gradients, we cannot achieve better than $o\left(\frac{1}{t^2}\right)$)

- In addition, for objectives that are strongly convex:

$$\|x_t - x^\star\|_2^2 \geq \left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^{2t} \|x_0 - x^\star\|_2^2 \qquad \kappa := \frac{L}{\mu}$$

(The case we described has near optimal exponent, but does not involve the square root of κ)

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Can we do better if we use more information?

The notorious Newton's method

- Remember the second-order Taylor expansion:

$$f(x + \Delta x) \approx f(x) + \langle \nabla f(x), \Delta x \rangle + \frac{1}{2} \left\langle \nabla^2 f(x) \Delta x, \Delta x \right\rangle$$

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- Taking the derivative and setting to zero:

$$\nabla_{\Delta x} f(x+\Delta x) = 0 \quad \Rightarrow \quad \nabla f(x) + \nabla^2 f(x) \Delta x = 0 \quad \Rightarrow \quad \Delta x = -\left(\nabla^2 f(x)\right)^{-1} \nabla f(x)$$

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$$x_{t+1} = x_t - \eta H_t^{-1} \nabla f(x_t), \quad H_t := \nabla^2 f(x_t)$$

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- Theory dictates even $\eta = 1$; often this is too optimistic, we use $\eta < 1$

(Damped Newton's method)

The notorious Newton's method

Demo

Guarantees of Newton's method

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

"Assume the objective is has Lipschitz continuous Hessians. Also, assume that the initial point is close enough to the optimal point:

$$\|x_0 - x^\star\|_2 < \frac{2\mu}{3M} \quad \textit{where} \quad \nabla^2 f(x^\star) \succeq \mu I \quad \textit{and} \quad \|\nabla^2 f(x) - \nabla^2 f(y)\|_2 \leq M\|x - y\|_2$$

$$x_{t+1} = x_t - \left(\nabla^2 f(x_t)\right)^{-1} \nabla f(x_t)$$

converges quadratically according to:

$$\|x_{t+1} - x^\star\|_2 \leq \frac{M\|x_t - x^\star\|_2^2}{2(\mu - M\|x_t - x^\star\|_2)} \quad "$$

Guarantees of Newton's method

Local convergence guarantees
Assumes no convexity – but assumes good initialization

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Guarantees of Newton's method

Whiteboard

General comments of Newton's method

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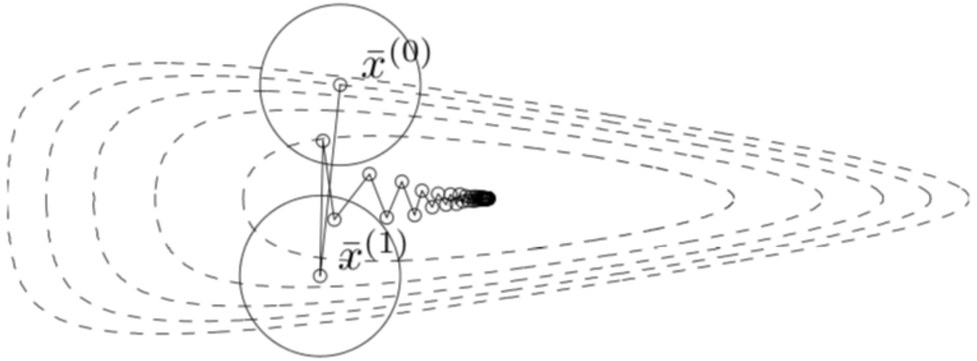
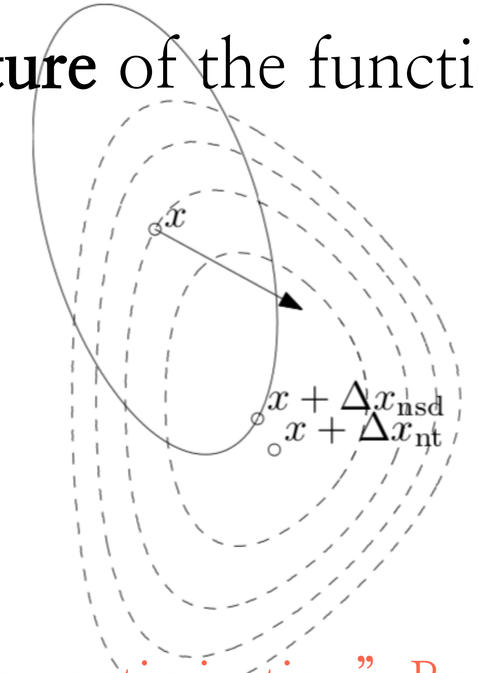
- Newton's method exploits the **local curvature** of the function





"Convex optimization", Boyd and Vandenberghe

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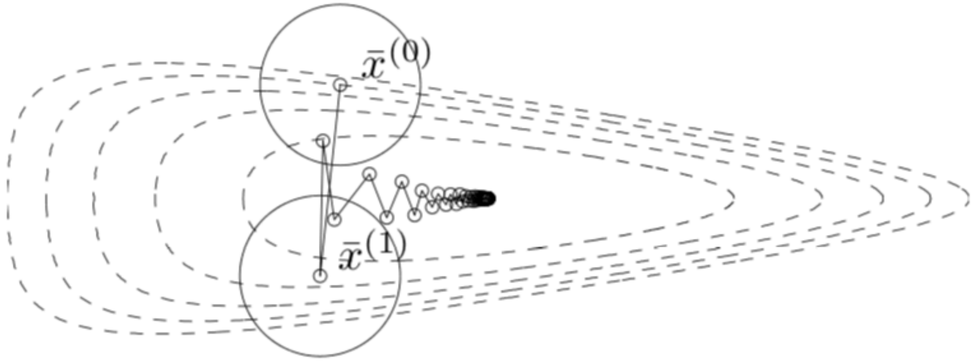

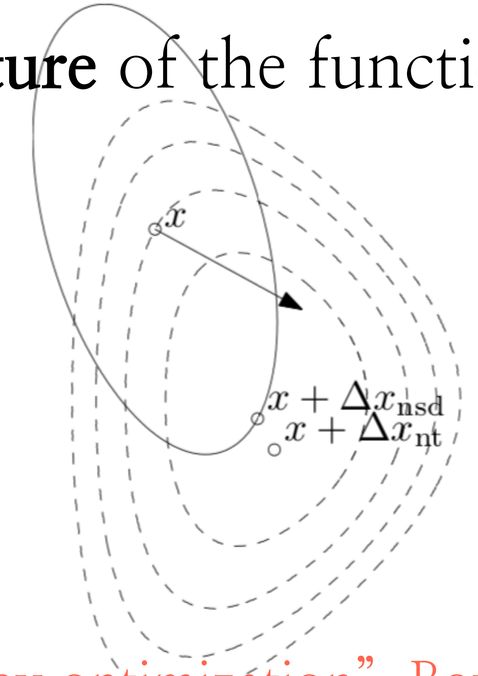

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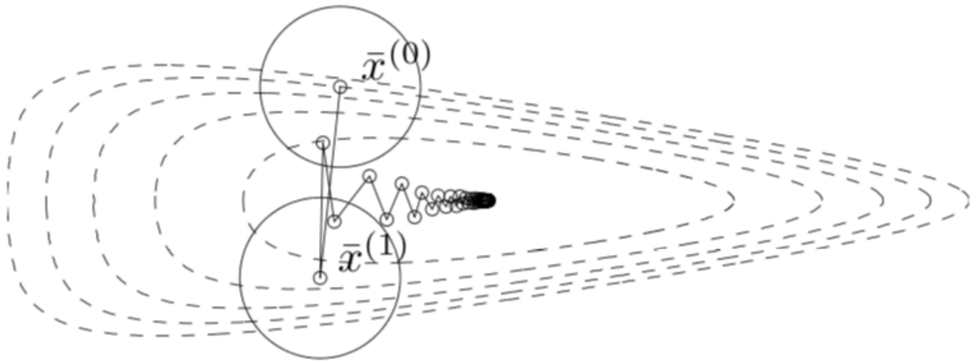

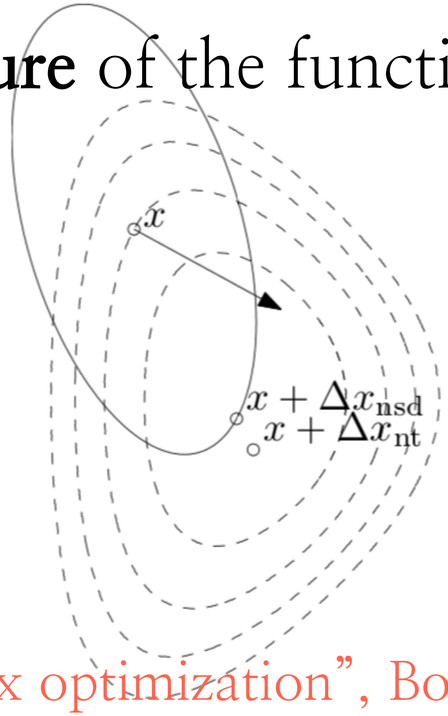

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(We often observe a two-phase behavior: A linear convergence at first, and then a quadratic one)

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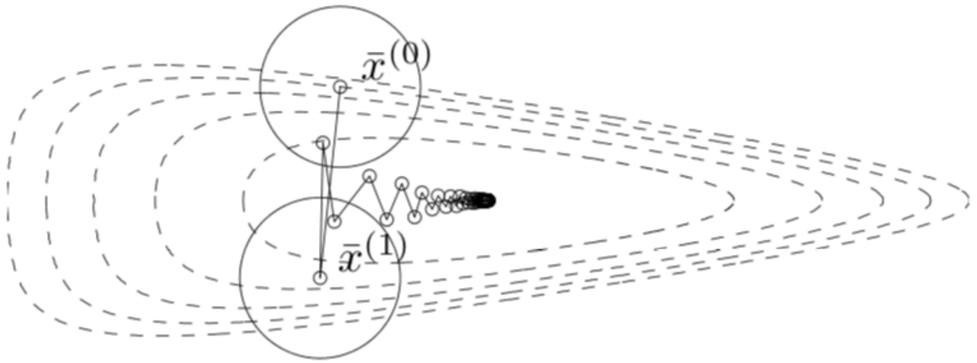

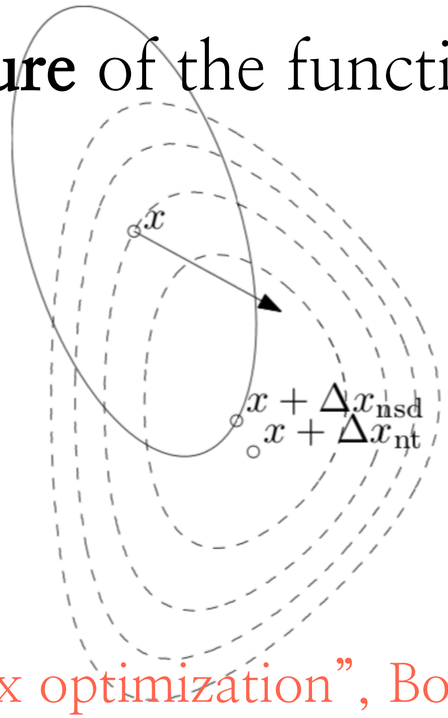

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- Useful for exact solutions; not often the situation in machine learning

Between gradient descent and Newton's method

- Quasi-Newton methods

$$x_{t+1} = x_t - \eta B_t \nabla f(x_t)$$

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Approximation of the inverse Hessian

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- "Quasi-Newton" reveals that we want to avoid second-order calculations

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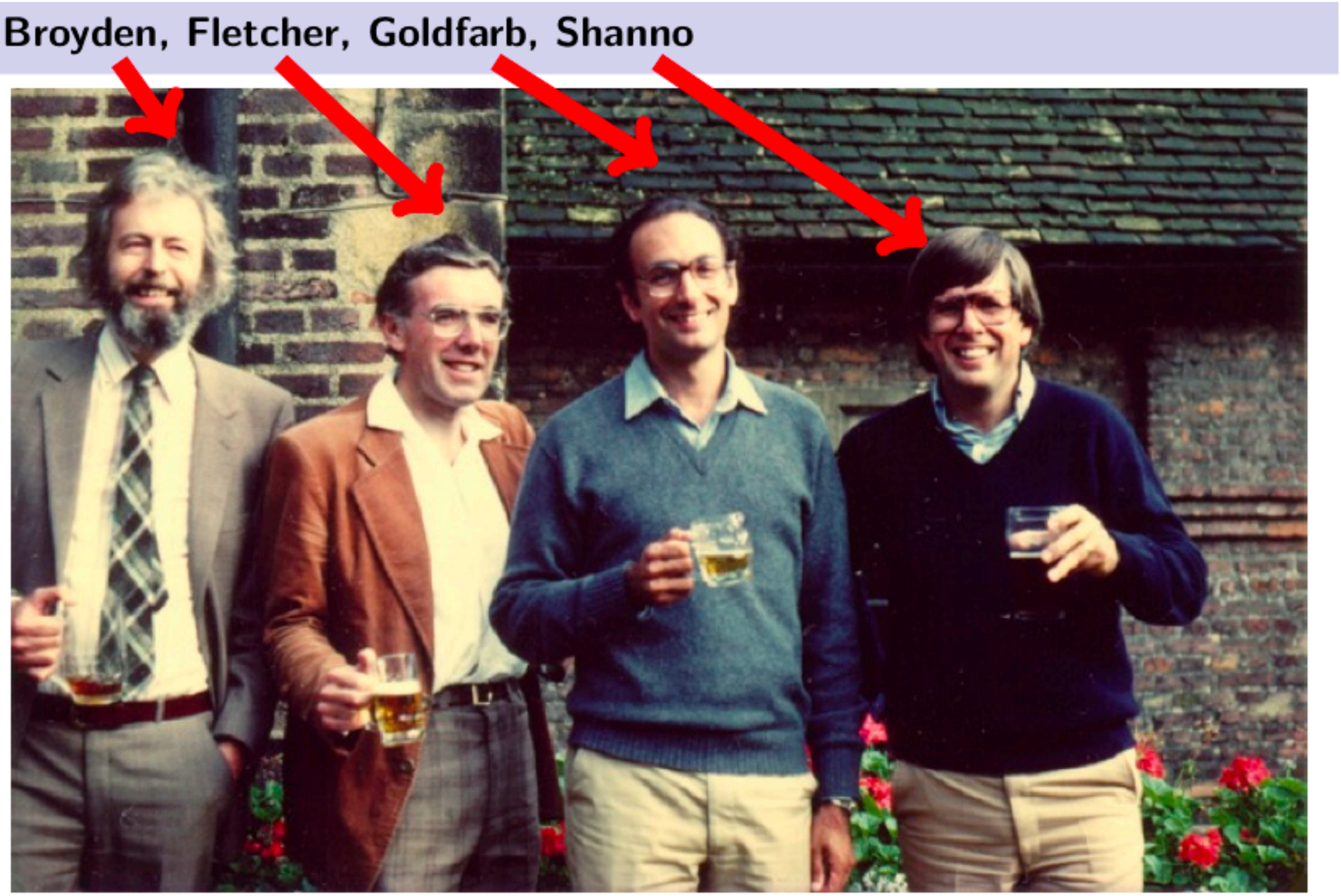
Approximation of the inverse Hessian

- "Quasi-Newton" reveals that we want to avoid second-order calculations
- There are various ways to construct this approximation
  - **(L)-BFGS approximation**
  - **SR1 approximation**

The BFGS method

Paying tribute to these gentlemen



The BFGS method

- Quadratic approximations around current point

$$g_t(\Delta x) := f(x_t) + \langle \nabla f(x_t), \Delta x \rangle + \tfrac{1}{2} \langle H_t \Delta x, \Delta x \rangle$$

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- Instead of estimating from scratch H_{t+1}, we require the new model $g_{t+1}(\cdot)$ satisfy two gradient conditions:

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$$\nabla g_{t+1}(-\Delta x) = \nabla f(x_t)$$ (i.e., we take the opposite step and compute the gradient, the latter should match the gradient of the previous quad. approx.)

The BFGS method

- Secant equation

$$\nabla g_{t+1}(-\Delta x) = \nabla f(x_t) \longrightarrow H_{t+1}\Delta x = \nabla f(x_{t+1}) - \nabla f(x_t)$$

(Some of you might have seen the expression $H_{t+1}s_t = y_k$)

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- Requirement: $H_{t+1} \succ 0 \longrightarrow \Delta x^\top (\nabla f(x_{t+1}) - \nabla f(x_t)) > 0$

(Why?)

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(How do we choose which one?)

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- By solving:

$$\begin{aligned} \min_{\boldsymbol{H} \succ 0} \ & \|H - H_t\|_F^2 \\ \text{s.t.} \quad & H = H^\top, \\ & H\Delta x = \nabla f(x_t) - \nabla f(x_{t-1}) \end{aligned}$$

(Intuition?)

The BFGS method

- The BFGS method goes a bit further:

Approximates directly the inverse!

$$\begin{aligned} \min_{\boldsymbol{B} \succ 0} \quad & \|B - B_t\|_F^2 \\ \text{s.t.} \quad & B = B^\top, \\ & \Delta x = B\left(\nabla f(x_t) - \nabla f(x_{t-1})\right) \end{aligned}$$

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- The BFGS method has an easy closed for solution:

$$B_{t+1} = \left(I - \frac{s_t y_t^\top}{s_t^\top y_t}\right) B_t \left(I - \frac{y_t s_t^\top}{s_t^\top y_t}\right) + \frac{s_t s_t^\top}{s_t^\top y_t}$$

$$s_t := \Delta x$$

$$y_t := \nabla f(x_{t+1}) - \nabla f(x_t)$$

(Only inner product/outer product computations!)
(Only uses gradient information)

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- **No guarantee for positive definiteness!**
  - Might be useful to generate indefinite Hessian approximations in non convex optimization

(Could be a project proposal)

For the sake of saving lecture time

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No theory or demo

(But willing to prepare some if people get interested)

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- Have in mind the formula:

$$x_{t+1} = x_t - \eta B_t \nabla f(x_t)$$

Preconditioner matrix

Instead of forming higher order approximations..

..can we use 0-th order information?

0-th order optimization

- Some examples: Bisection method, genetic algorithms, simulated annealing Metropolis methods..

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- Here we will briefly describe the **finite differences method**:

$$x_{t+1} = x_t - \eta \frac{f(x_t + \mu_t u) - f(x_t)}{\mu_t} \cdot u$$

(we have access to function evaluations)

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- Based on the approximation of the gradient:

$$f'(x) \approx \frac{f(x+\epsilon) - f(x)}{\epsilon}$$

Application: Adversarial examples in NN training

(A quick description)

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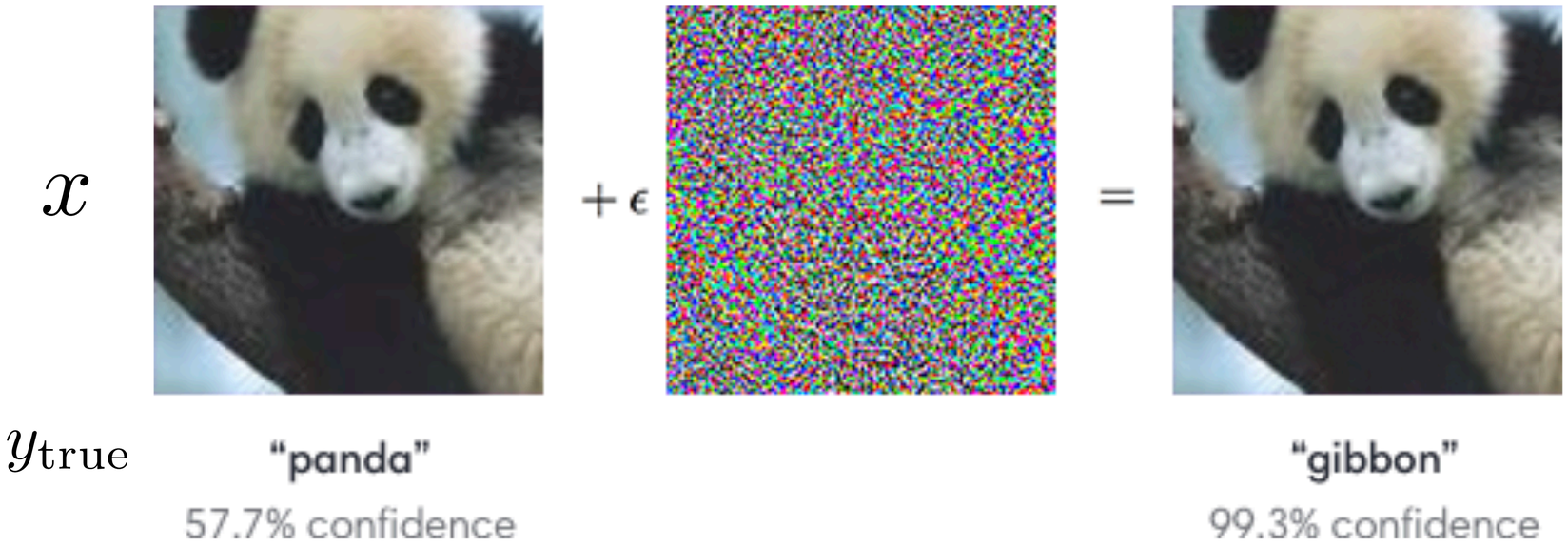


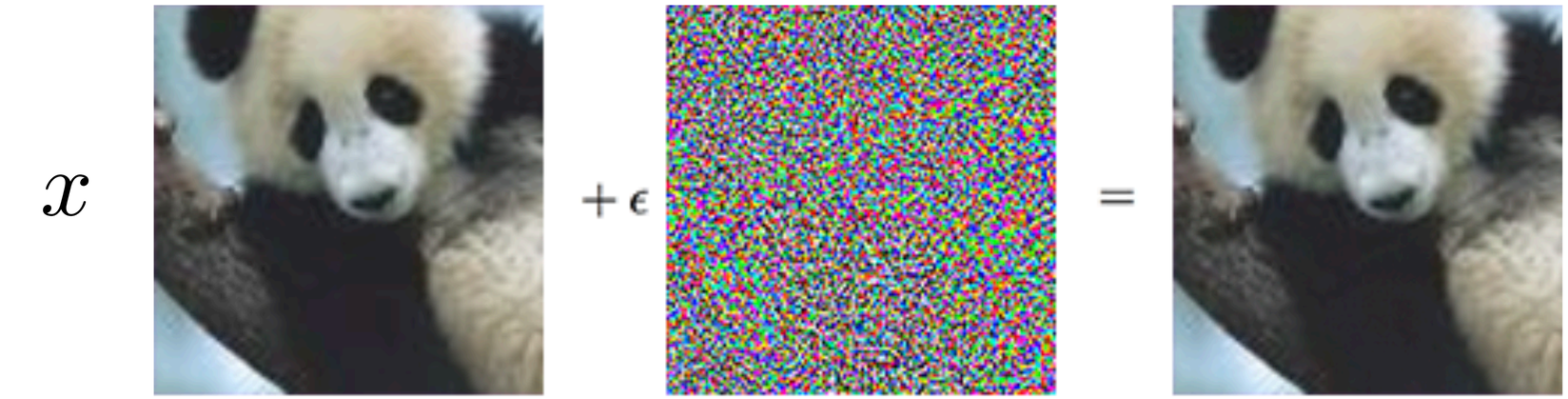
$$x_{\text{adv}} = x + \epsilon \cdot \texttt{sign}\left(\nabla f(x, y_{\text{true}})\right)$$

(The objective represents a complex model like a neural network)

Application: Adversarial examples in NN training

(A quick description)

- The idea of adversarial examples: small perturbations lead to misclassification



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We are looking into directions that move away from the minimum

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(A quick description)

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- However, **the forward operation remains intact**: this means that the function evaluations are normally computed

Application: Adversarial examples in NN training

(A quick description)

- SPSA attack (Simultaneous Perturbation Stochastic Approximation)

Algorithm 1 SPSA adversarial attack

Input: function to minimize f, initial image $x_0 \in \mathbb{R}^D$, perturbation size δ, step size $\alpha > 0$, batch size n

for $t = 0$ **to** $T - 1$ **do**

Sample $v_1, \ldots, v_n \sim \{1, -1\}^D$

Define $v_i^{-1} = [v_{i,1}^{-1}, \ldots, v_{i,D}^{-1}]$

Calculate $g_i = (f(x_t + \delta v_i) - f(x - \delta v_i))v_i^{-1}/(2\delta)$

Set $x'_t = x_t - \alpha(1/n)\sum_{i=1}^{n} g_i$

Project $x_{t+1} = \arg\min_{x \in N_\epsilon(x_0)} \|x'_t - x_0\|$

end for

"Adversarial Risk and the Dangers of Evaluating Against Weak Attacks", Uesato et al., 2018

From previous lecture: lower bounds

- For objectives with Lipschitz continuous gradients:

$$f(x_t) - f(x^\star) \geq \frac{3L\|x_0 - x^\star\|_2^2}{32(t+1)^2}$$

(Under these assumptions, and using only gradients, we cannot achieve better than $o\left(\frac{1}{t^2}\right)$)

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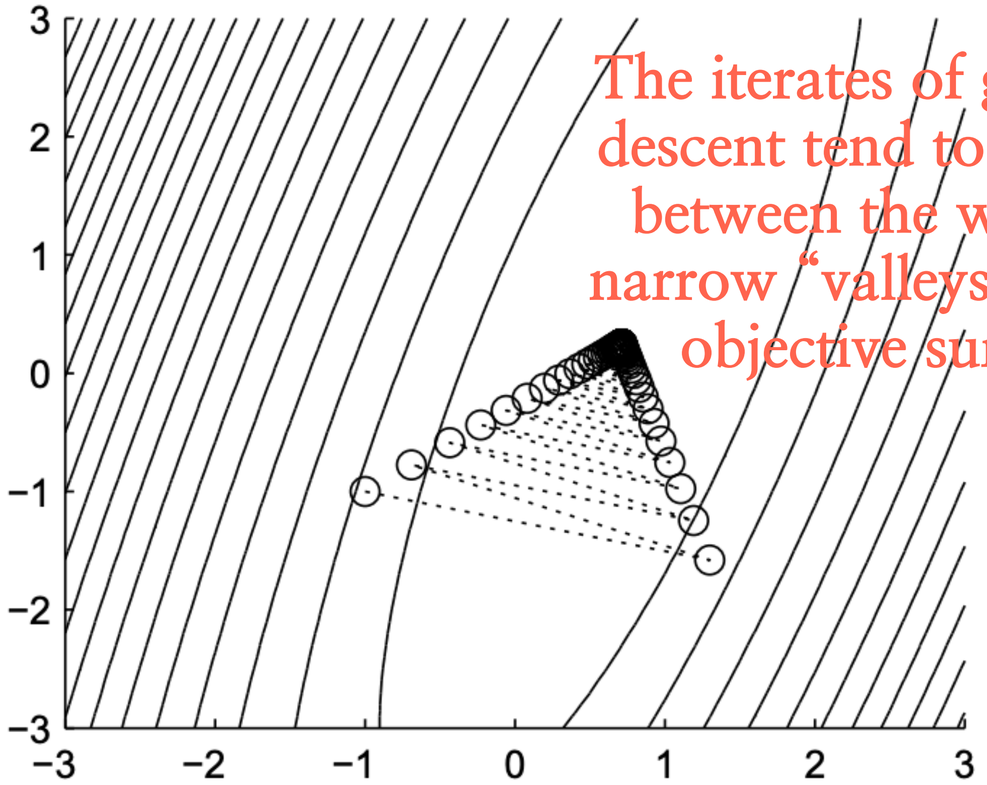
(The case we described has near optimal exponent, but does not involve the square root of κ)

So far, we are "cheating": use/approximate of higher-order information

“Can we accelerate having as our basis the standard gradient descent?”

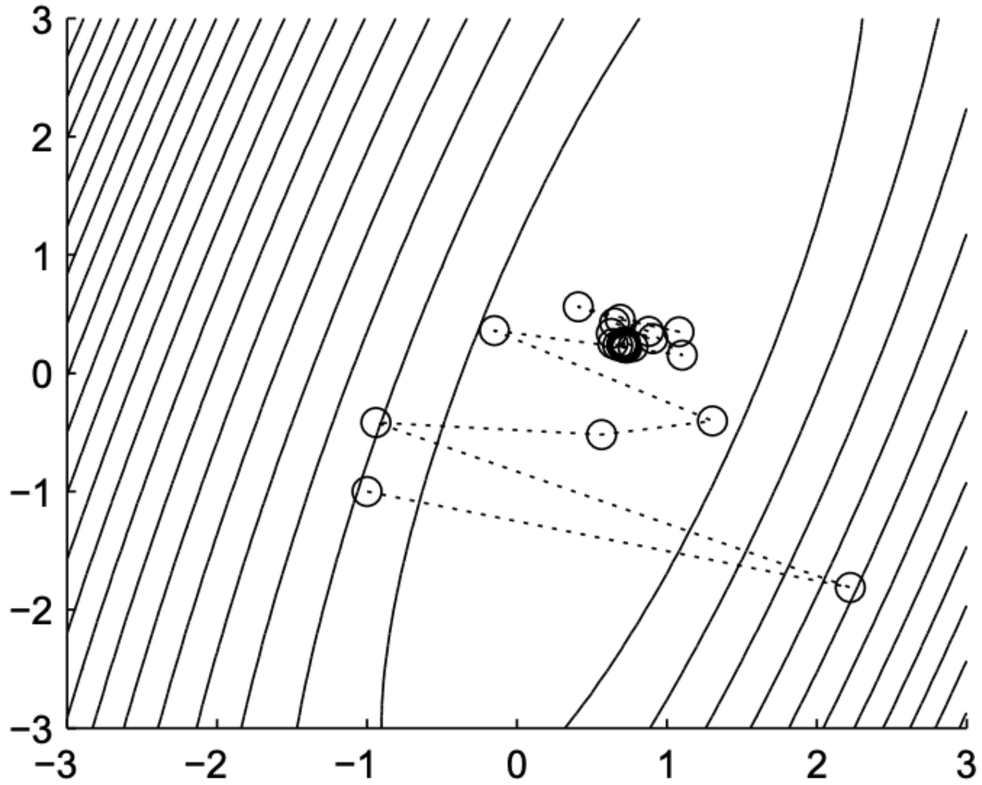
Acceleration #1: Momentum acceleration

- Heavy ball method



The iterates of gradient descent tend to bounce between the walls of narrow "valleys" on the objective surface

Gradient descent



Extrapolating previous directions

Acceleration #1: Momentum acceleration

Tribute to
Piotr Skalski

Acceleration #1: Momentum acceleration

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Acceleration #1: Momentum acceleration

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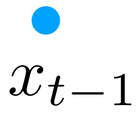

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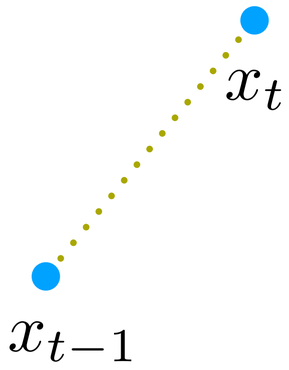

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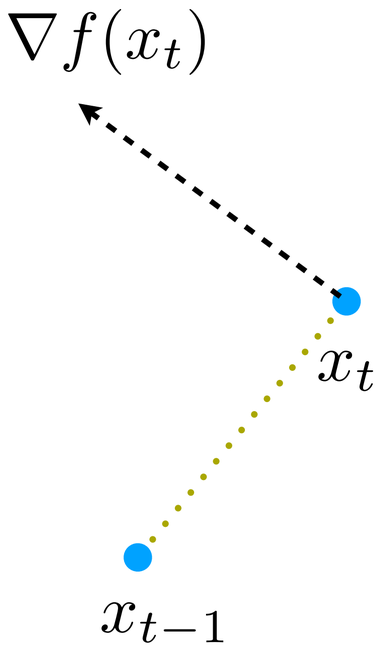

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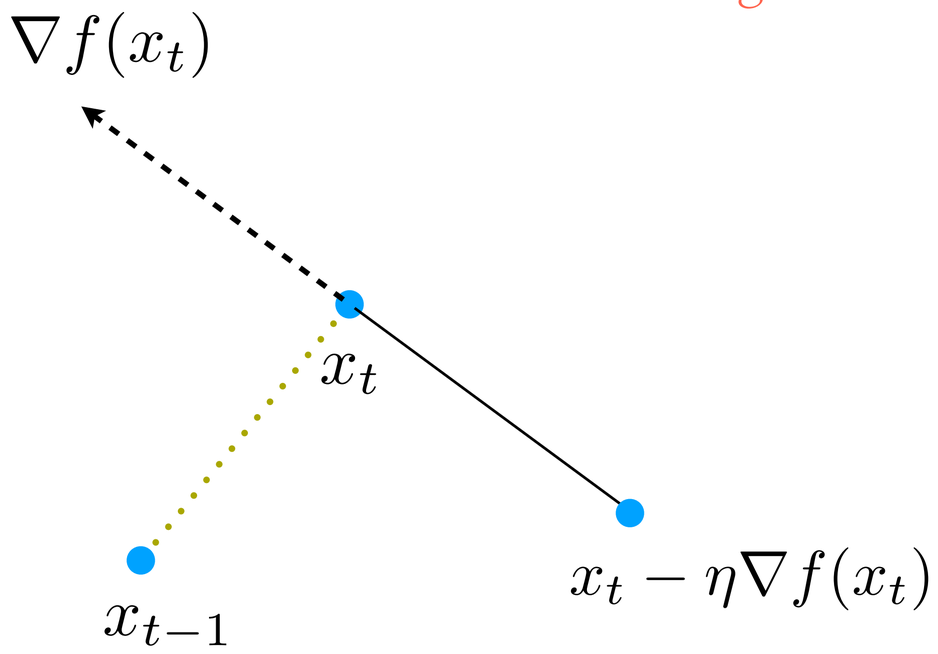

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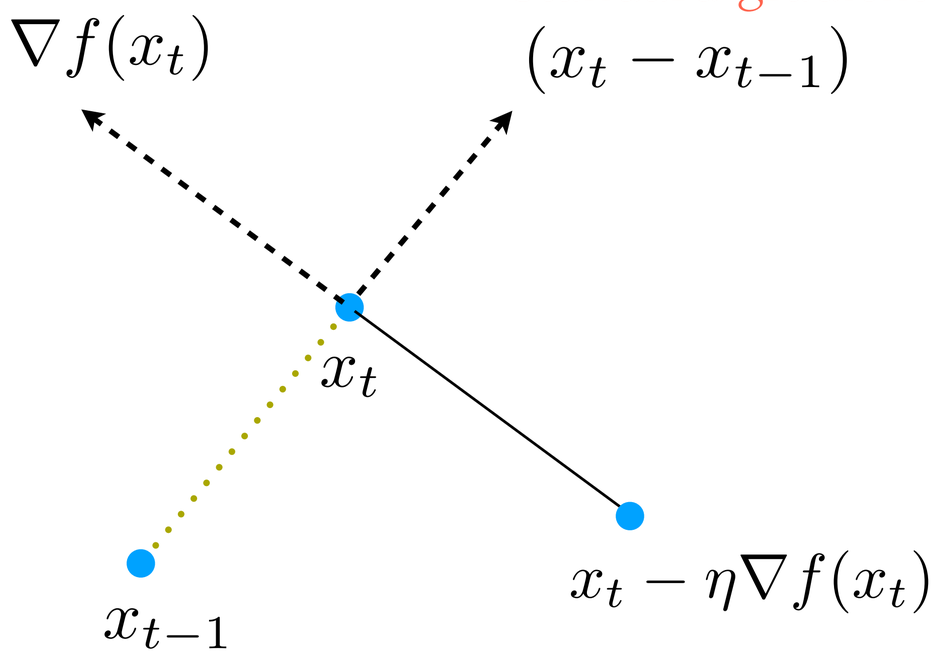

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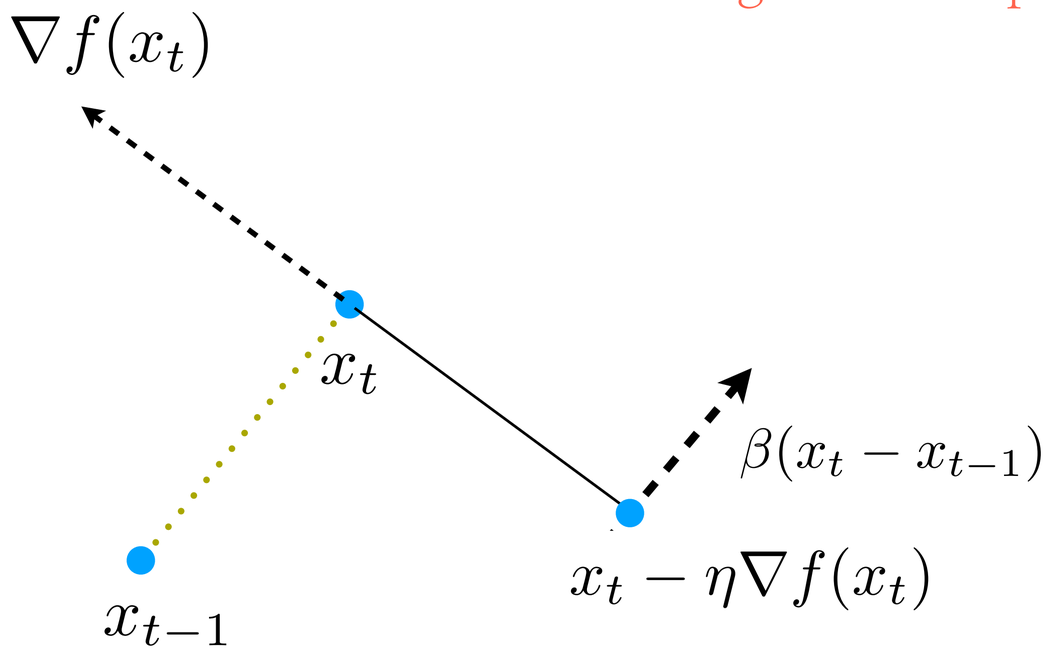

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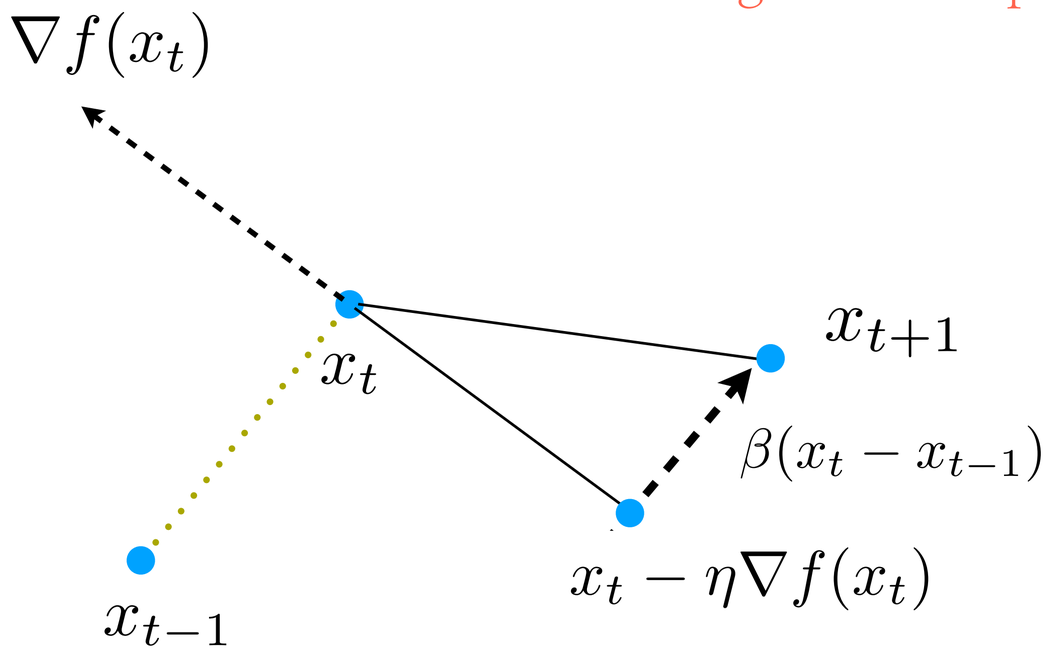

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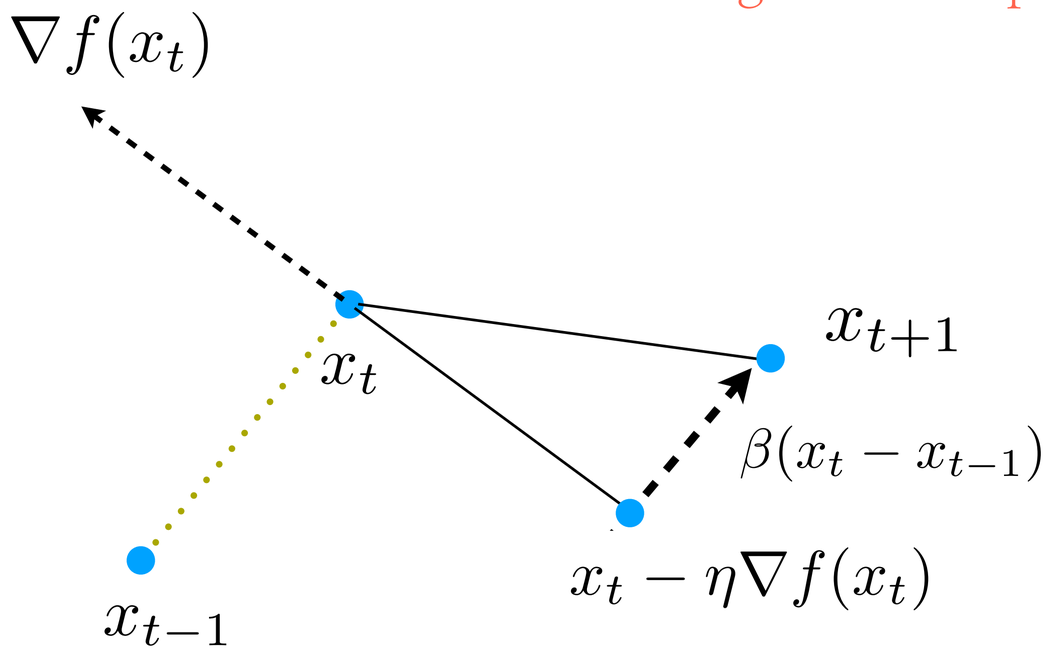

Any analogy in the physical world?

- If current gradient step is in same direction as previous step, then move a little further in that direction

Guarantees of Heavy Ball method

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

"Assume the objective is has Lipschitz continuous gradients, and it is strongly convex. Then:

$$x_{t+1} = x_t - \eta \nabla f(x_t) + \beta(x_t - x_{t-1})$$

for $\eta = \dfrac{4}{\sqrt{L} + \sqrt{\mu}}$ *and* $\beta = \max\{|1 - \sqrt{\eta\mu}|,\ |1 - \sqrt{\eta L}|\}^2$

converges linearly according to:

$$\|x_{t+1} - x^\star\|_2 \leq \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}\right)^t \|x_0 - x^\star\|_2$$ "

Guarantees of Heavy Ball method

Whiteboard

Guarantees of Heavy Ball method

- It achieves the lower bound for strongly convex cases!

$$\text{“} \quad \|x_t - x^\star\|_2^2 \geq \left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^{2t} \|x_0 - x^\star\|_2^2 \qquad \kappa := \frac{L}{\mu} \quad \text{“}$$

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- In comparison with simple gradient descent:

$$O\left(\kappa \log \tfrac{1}{\varepsilon}\right) \quad \text{vs} \quad O\left(\sqrt{\kappa} \log \tfrac{1}{\varepsilon}\right)$$

Performance of Heavy Ball method

Demo

Acceleration #1: Momentum acceleration

- Nesterov's work: a collection of acceleration methods

Constant Step Scheme, I

0. Choose $x_0 \in R^n$ and $\gamma_0 > 0$. Set $v_0 = x_0$.

1. kth iteration ($k \geq 0$).

a). Compute $\alpha_k \in (0,1)$ from the equation

$$L\alpha_k^2 = (1-\alpha_k)\gamma_k + \alpha_k\mu.$$

Set $\gamma_{k+1} = (1-\alpha_k)\gamma_k + \alpha_k\mu$.

b). Choose $y_k = \frac{\alpha_k\gamma_k v_k + \gamma_{k+1}x_k}{\gamma_k + \alpha_k\mu}$.
Compute $f(y_k)$ and $f'(y_k)$.

c). Set $x_{k+1} = y_k - \frac{1}{L}f'(y_k)$ and

$$v_{k+1} = \frac{1}{\gamma_{k+1}}[(1-\alpha_k)\gamma_k v_k + \alpha_k\mu y_k - \alpha_k f'(y_k)].$$

Constant Step Scheme, II

0. Choose $x_0 \in R^n$ and $\alpha_0 \in (0,1)$.
Set $y_0 = x_0$ and $q = \frac{\mu}{L}$.

1. kth iteration ($k \geq 0$).

a). Compute $f(y_k)$ and $f'(y_k)$. Set

$$x_{k+1} = y_k - \tfrac{1}{L}f'(y_k).$$

b). Compute $\alpha_{k+1} \in (0,1)$ from equation

$$\alpha_{k+1}^2 = (1-\alpha_{k+1})\alpha_k^2 + q\alpha_{k+}$$

and set $\beta_k = \frac{\alpha_k(1-\alpha_k)}{\alpha_k^2+\alpha_{k+1}}$,

$$y_{k+1} = x_{k+1} + \beta_k(x_{k+1} - x_k)$$

Constant step scheme, III

0. Choose $y_0 = x_0 \in R^n$.

1. kth iteration ($k \geq 0$).

$$x_{k+1} = y_k - \tfrac{1}{L}f'(y_k),$$

$$y_{k+1} = x_{k+1} + \frac{\sqrt{L}-\sqrt{\mu}}{\sqrt{L}+\sqrt{\mu}}(x_{k+1} - x_k).$$

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- Nesterov's work: a collection of acceleration methods

$$x_{t+1} = x_t - \eta \nabla f(x_t) + \beta(x_t - x_{t-1})$$

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$$\widetilde{x} = x_t - \eta \nabla f(x_t)$$

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Evaluate gradient at current point

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What if we evaluate the gradient at the point we end up?

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Nesterov's acceleration (1/2)

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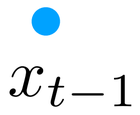

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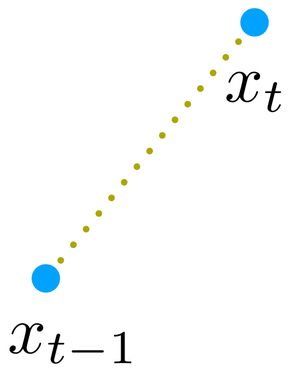

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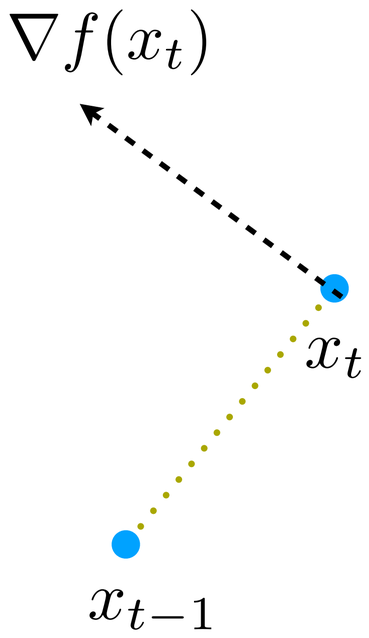

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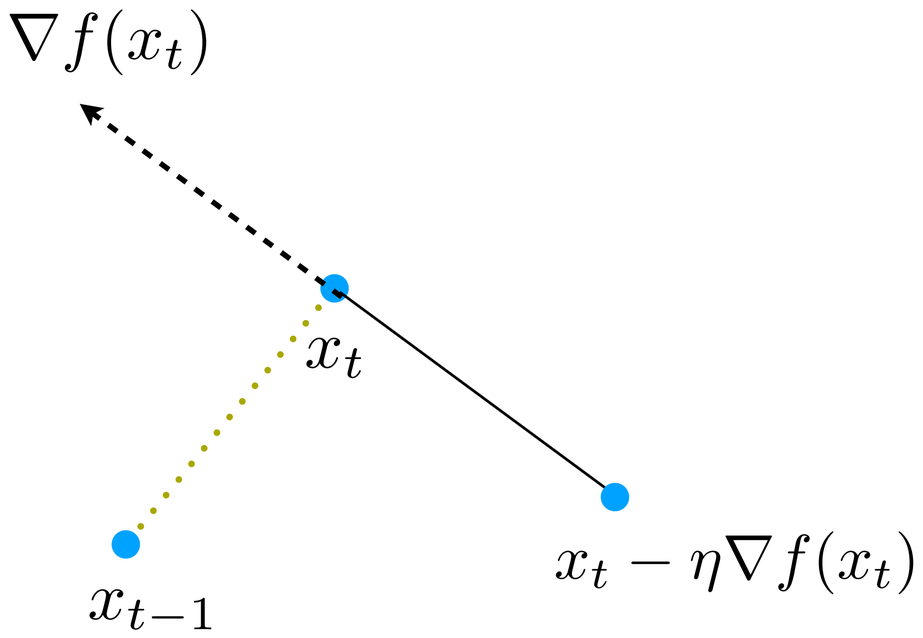

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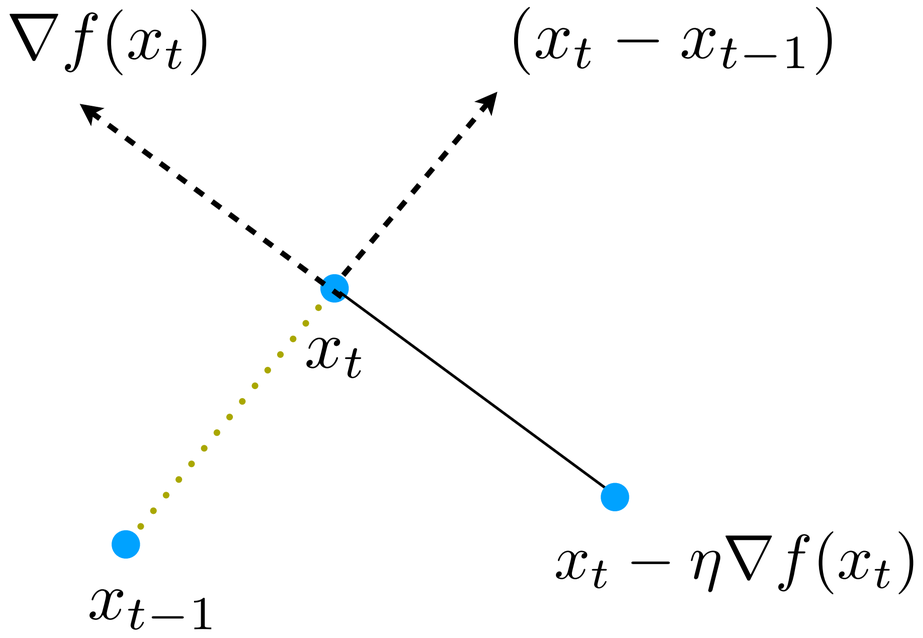

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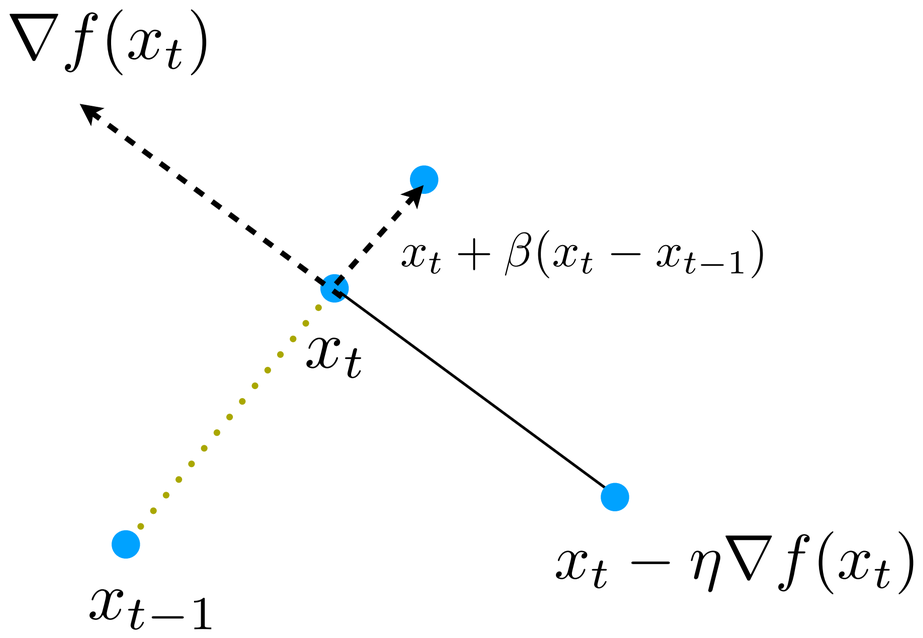

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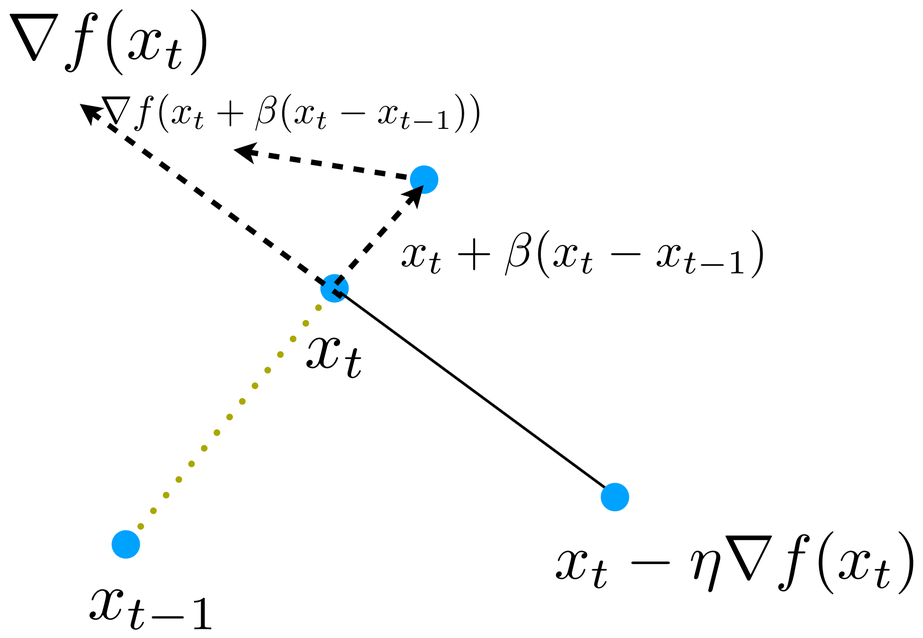

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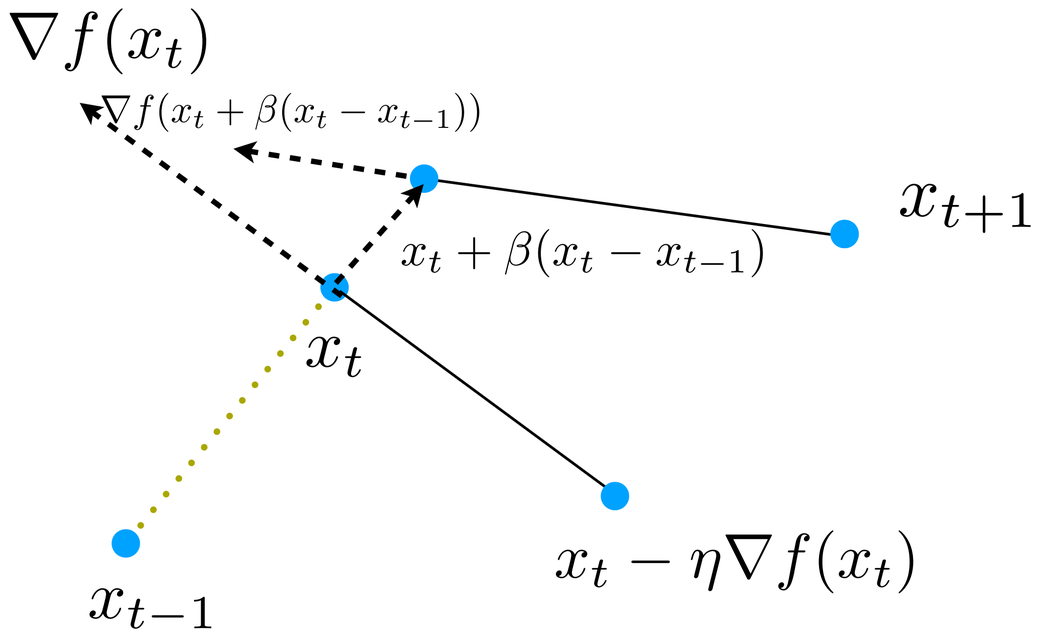

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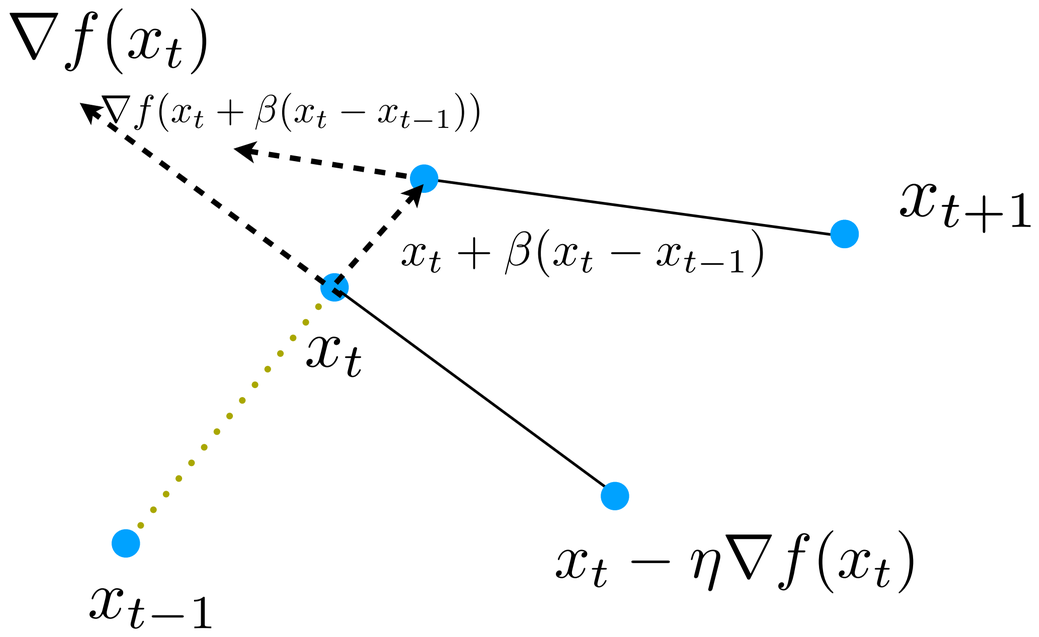

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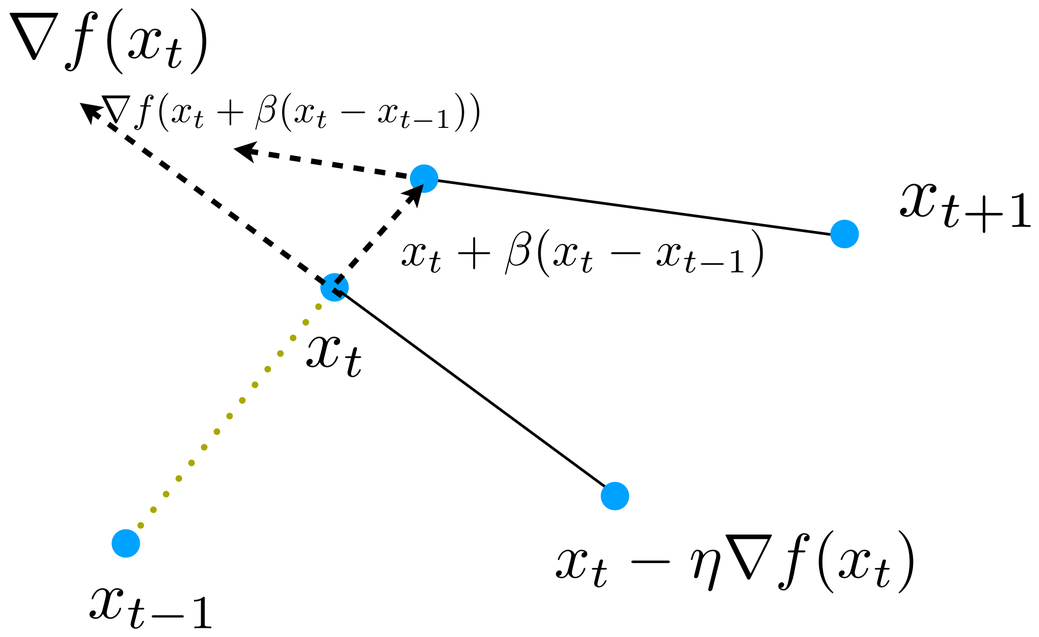

- Main difference: the point that we are calculating the gradient at.

- Heavy ball can fail converging in cases where Nesterov's scheme still succeeds

Acceleration #1: Momentum acceleration

- Nesterov's work: how do we set up the momentum parameter?

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One of the mysteries of optimization..

Performance of Nesterov's acceleration

Demo

Guarantees of Nesterov's acceleration

(No theory but willing to provide links for whoever is interested)

- Gradient descent in the absence of strong convexity

$$f(x_t) - f(x^\star) \leq \frac{2L\|x_0 - x^\star\|_2^2}{t+4}$$

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Optimal!

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Notes on Nesterov's acceleration

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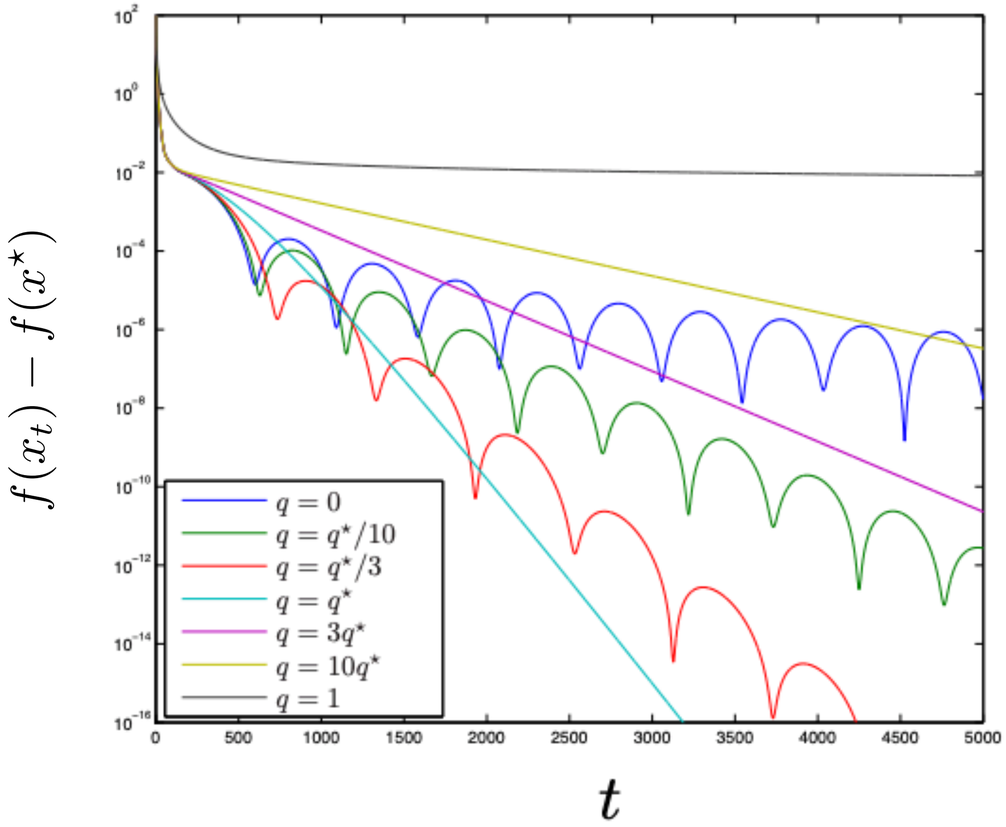
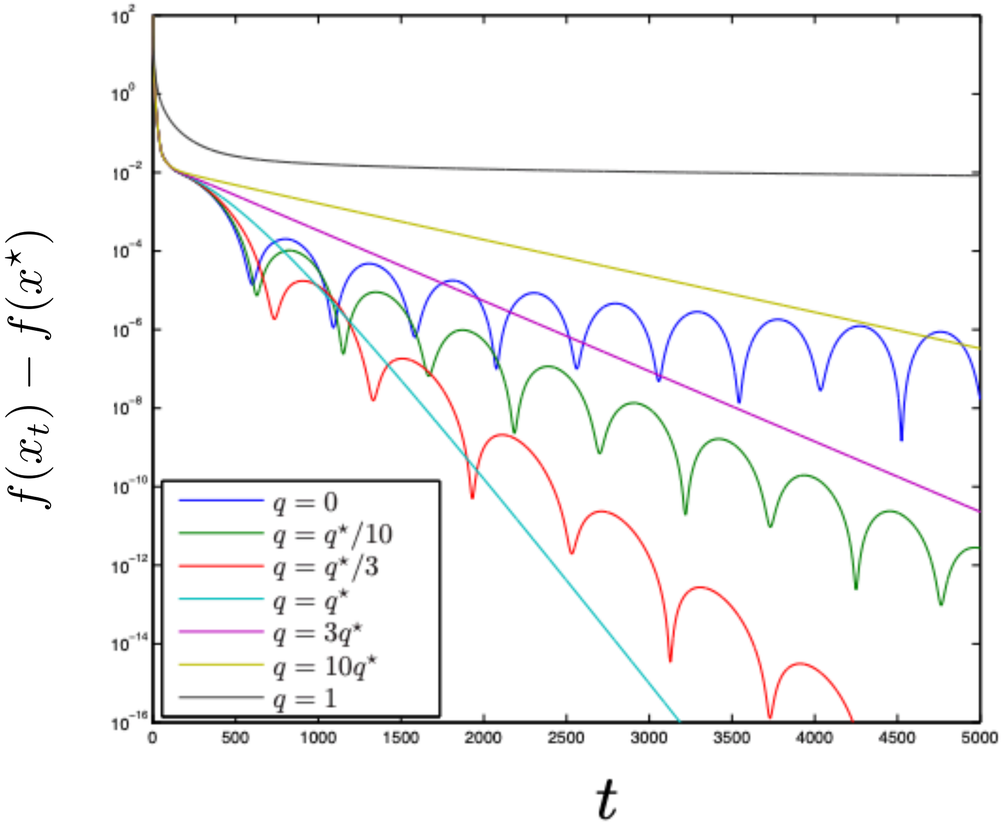


Notes on Nesterov's acceleration

- The original paper of 1983 does not converge linearly for strongly convex functions, but there is a fix to this
- It is a common observation to see ripples
- There are heuristics for resetting the momentum term to zero that improves the convergence rate.
- Often used even in cases where it is not guaranteed to work: deep learning



Acceleration #2: Cut-off complexity per iteration

- Common situation in machine learning/signal processing

$$f(x) = \frac{1}{n} \sum_{i=1}^{n} f_i(x)$$

(Empirical risk minimization)

where each $f_i(x)$ depends on, let's say, different part of input data.

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- Examples:
  - Least squares: $f_i(x) = \frac{1}{2}(y_i - \alpha_i^\top x)^2$
  - Logistic regression: $f_i(x) = \log(1 + \exp(-y_i \alpha_i^\top x))$

- Dimensions to worry about: $x \in \mathbb{R}^p$, number of samples n

Acceleration #2: Cut-off complexity per iteration

- **Stochastic gradient descent (SGD)**

$$x_{t+1} = x_t - \eta_t \nabla f(x_t) \quad \longrightarrow \quad x_{t+1} = x_t - \eta_t \nabla f_{i_t}(x_t), \quad i_t \in [n]$$

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$O(np)$ (Assume least-squares objective) $O(p)$

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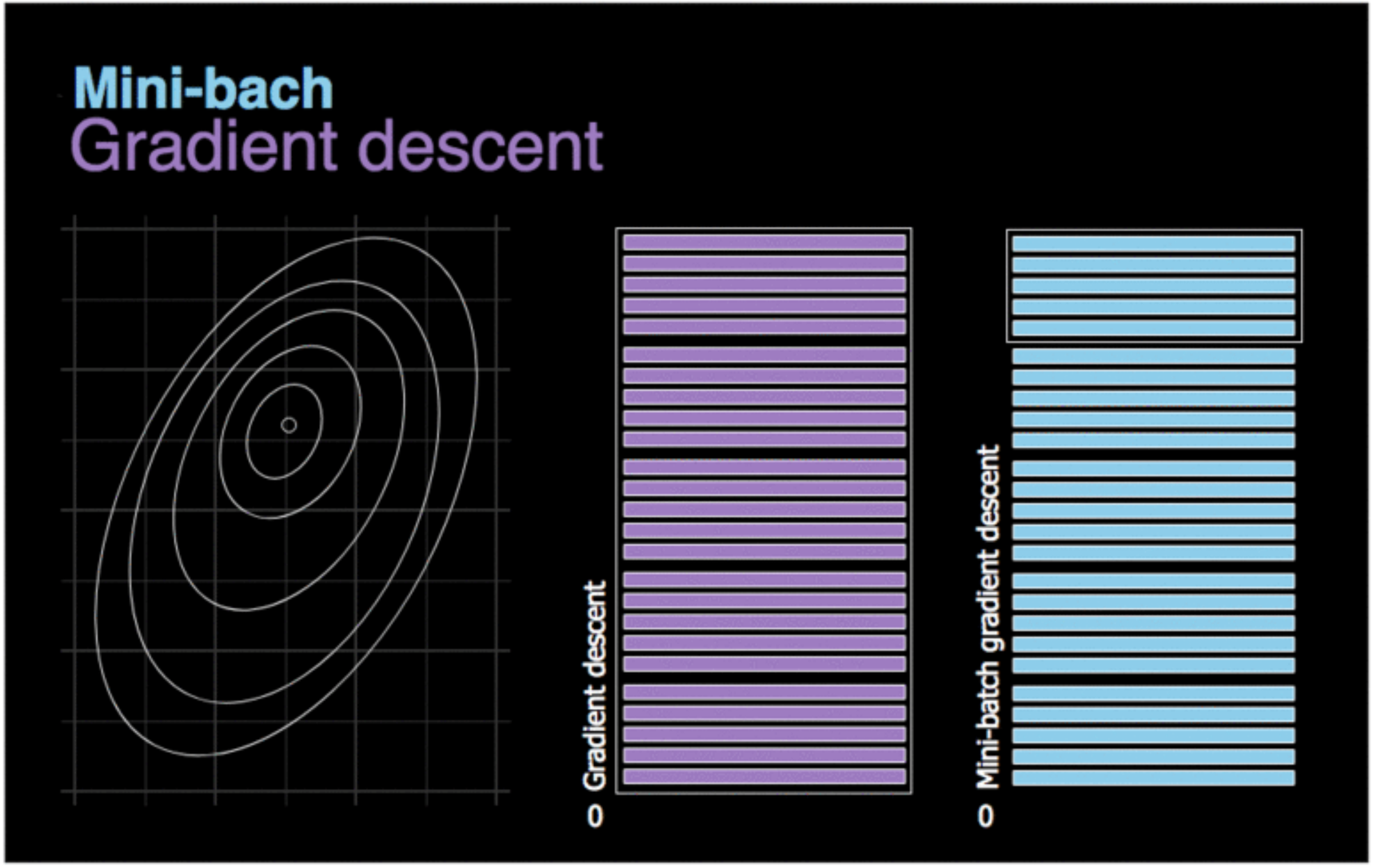
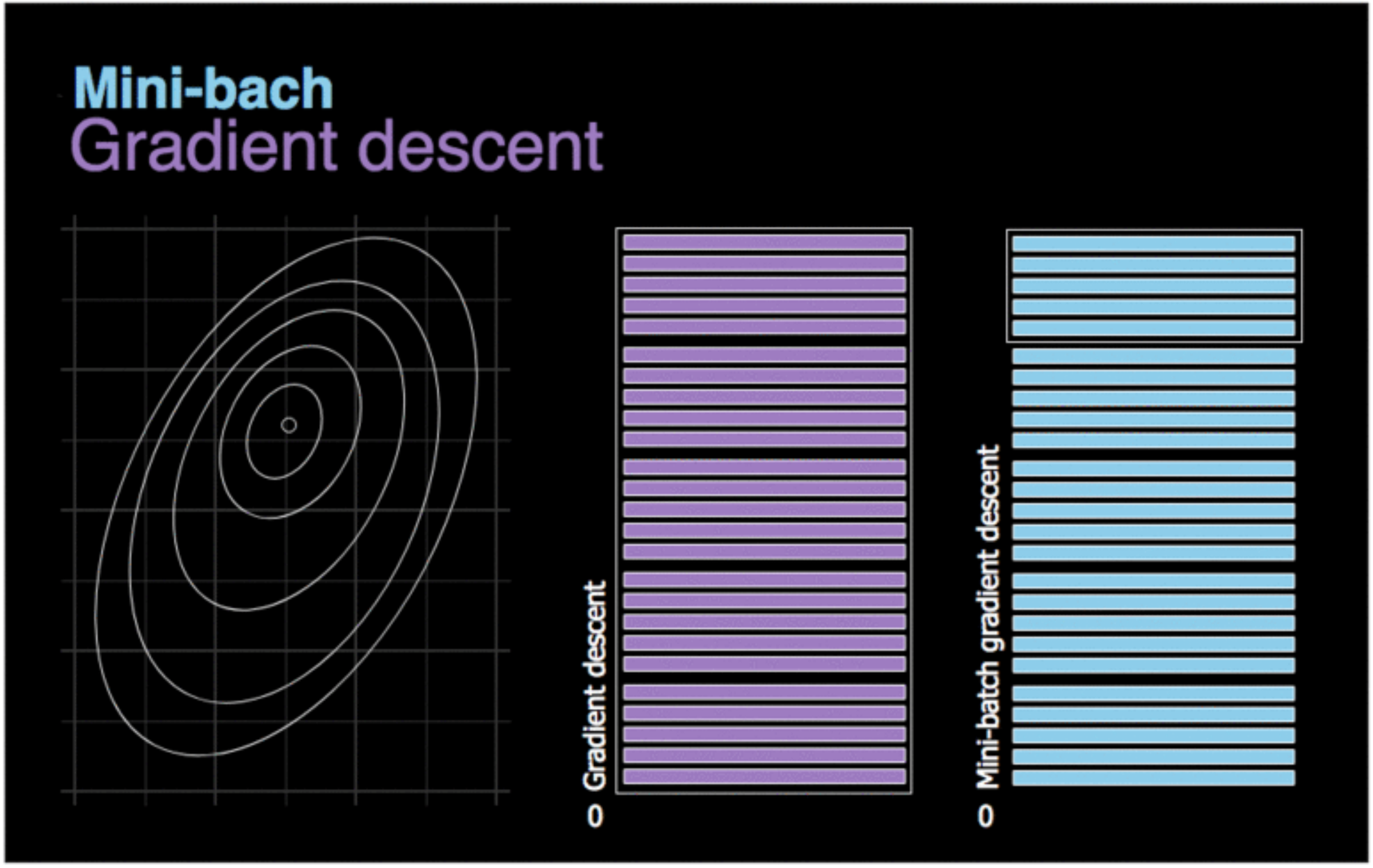
- When is $n \gg p$? Big-data regime!
  - There is redundancy in data
  - Far from the optimal, exact gradients might have small returns

Acceleration #2: Cut-off complexity per iteration



Tribute to
Piotr Skalski

Acceleration #2: Cut-off complexity per iteration



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(This means that some tools from deterministic optimization do not hold here)

3. The above lead to the intuition that if we have a descent direction in **expectation,** we probably will perform just fine

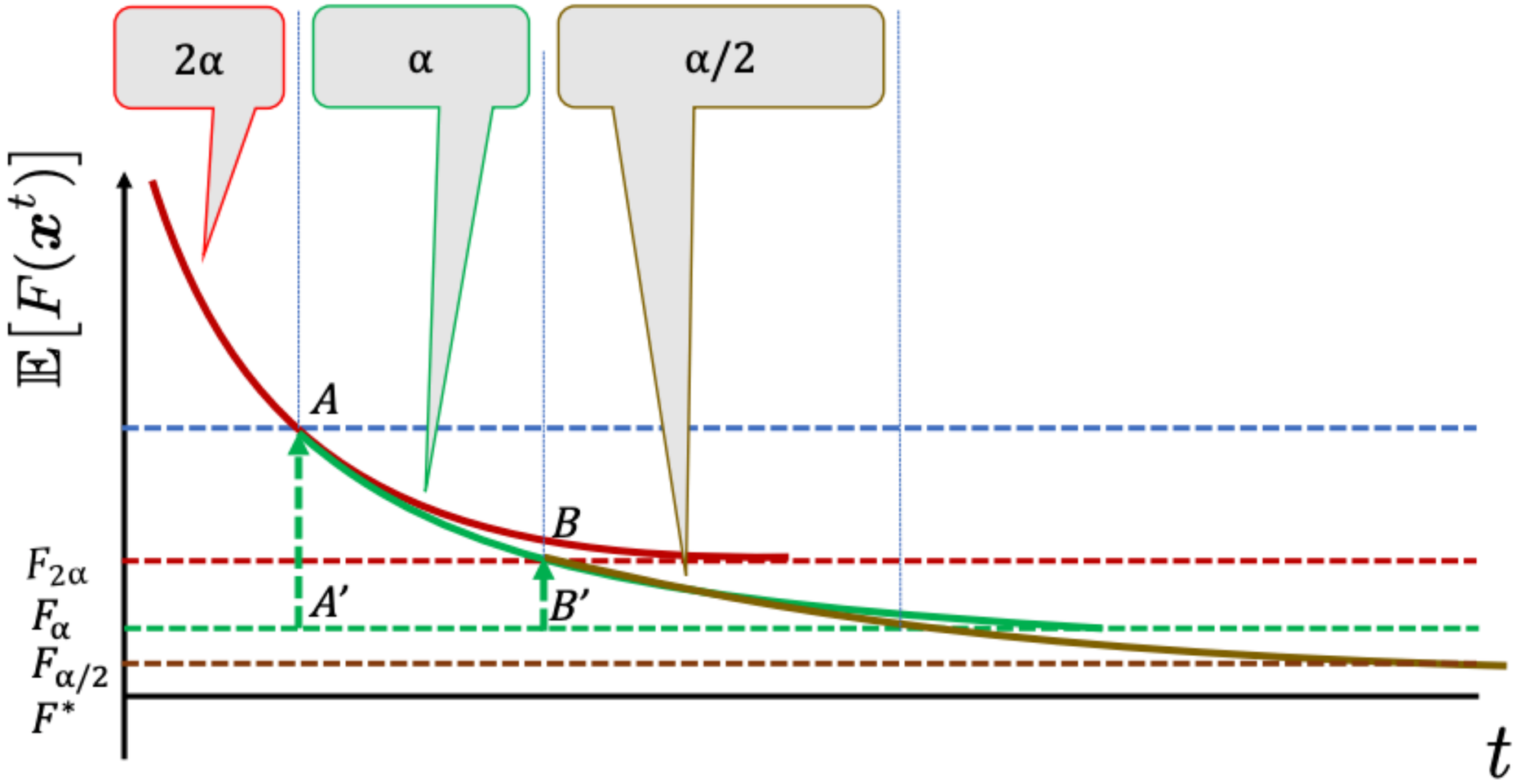
(This means that we will work with expectations w.r.t. the random sequence)

Guarantees of SGD

Whiteboard

Guarantees of SGD

Pic. from: "Optimization Methods for Large-Scale Machine Learning"



- Start with large step size; decrease it when SGD "stalls"

Guarantees of SGD

Whiteboard

Intuition behind preference for SGD

- Overall, for strongly convex and smooth functions

	iteration complexity	per-iteration cost	total comput. cost
batch GD	$\log \frac{1}{\varepsilon}$	n	$n \log \frac{1}{\varepsilon}$
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- The real comparison is between $n \log \frac{1}{\varepsilon} \; ? \; \frac{1}{\varepsilon}$
- In the big data regime, n can be huge!
- Gradient descent uses full dataset per iteration; there might be **redundancies**
- It actually works great in practice!

Intuition behind preference for SGD

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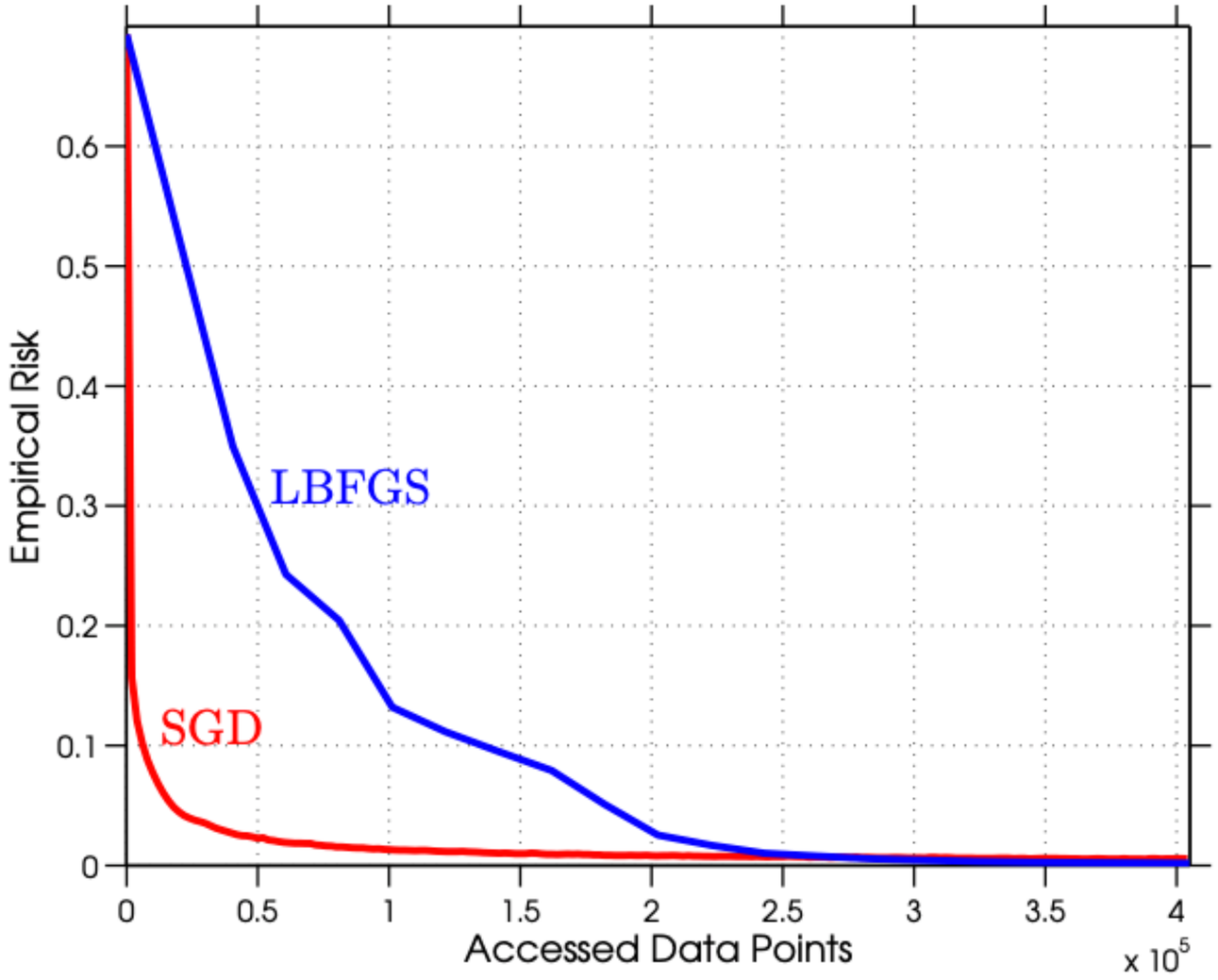

Variants of SGD

- Mini-batch SGD: instead of picking one sample, pick multiple

$$x_{t+1} = x_t - \eta_t \nabla f_{\mathcal{I}_t}(x_t) = x_t - \eta_t \cdot \sum_{j=1}^{|\mathcal{I}_t|} \nabla f_j(x_t)$$

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- SGD with importance sampling: select "carefully" the next sample

  - Select $i_t \in [n]$ according to distribution $p \in [0,1]^n$, $\sum_i p_i = 1$
  - Main question: can we compute a good probability distribution without too much effort?

Variants of SGD

- Stochastic variance-reduced gradient (SVRG)

$$x_{t+1} = x_t - \eta_t \left(\nabla f_{i_t}(x_t) - \left(\nabla f_{i_t}(\widetilde{x}_q) - \nabla f(\widetilde{x}_q) \right) \right)$$

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Correction term

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$$\mathbb{E}\left[\nabla f_{i_t}(x_t) - \nabla f_{i_t}(\widetilde{x}_q) + \nabla f(\widetilde{x}_q) \right] = \nabla f(x_t)$$

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- Theoretical guarantees:

$$\mathbb{E}\left[f(x_{t+1}) - f(x^\star) \right] \leq \rho \cdot \mathbb{E}\left[f(x_t) - f(x^\star) \right] \ , \quad \rho = O\left(\tfrac{1}{1-2\eta L} \cdot \left(\tfrac{1}{m\eta} + 2L\eta \right) \right) < 1$$

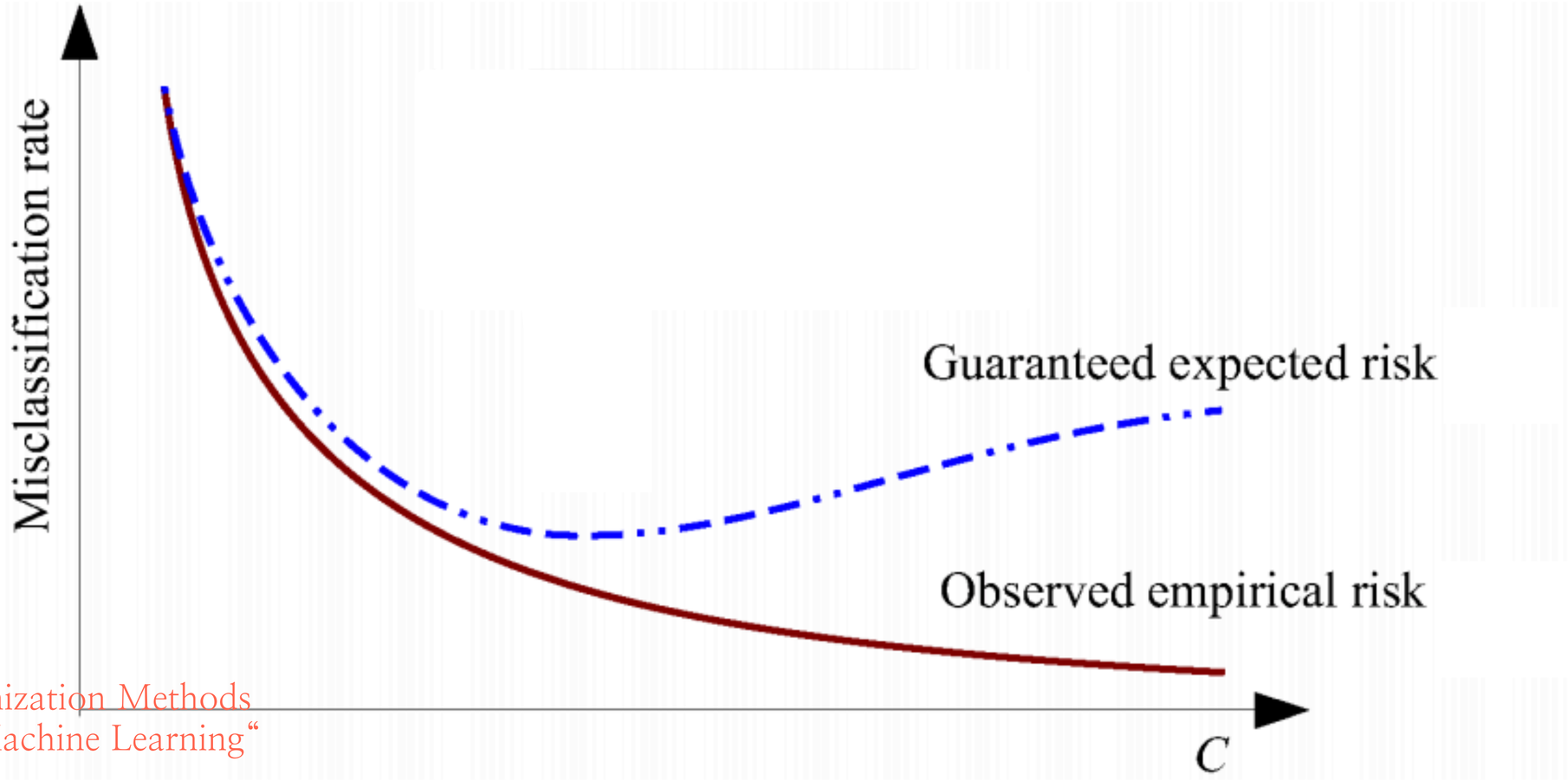
- Main drawback: Full gradient, but overall complexity $O\left((n+\kappa) \log \frac{1}{\varepsilon} \right)$

Performance of SGD

Demo

Why SGD is so important in machine learning?

(or some of the reasons)



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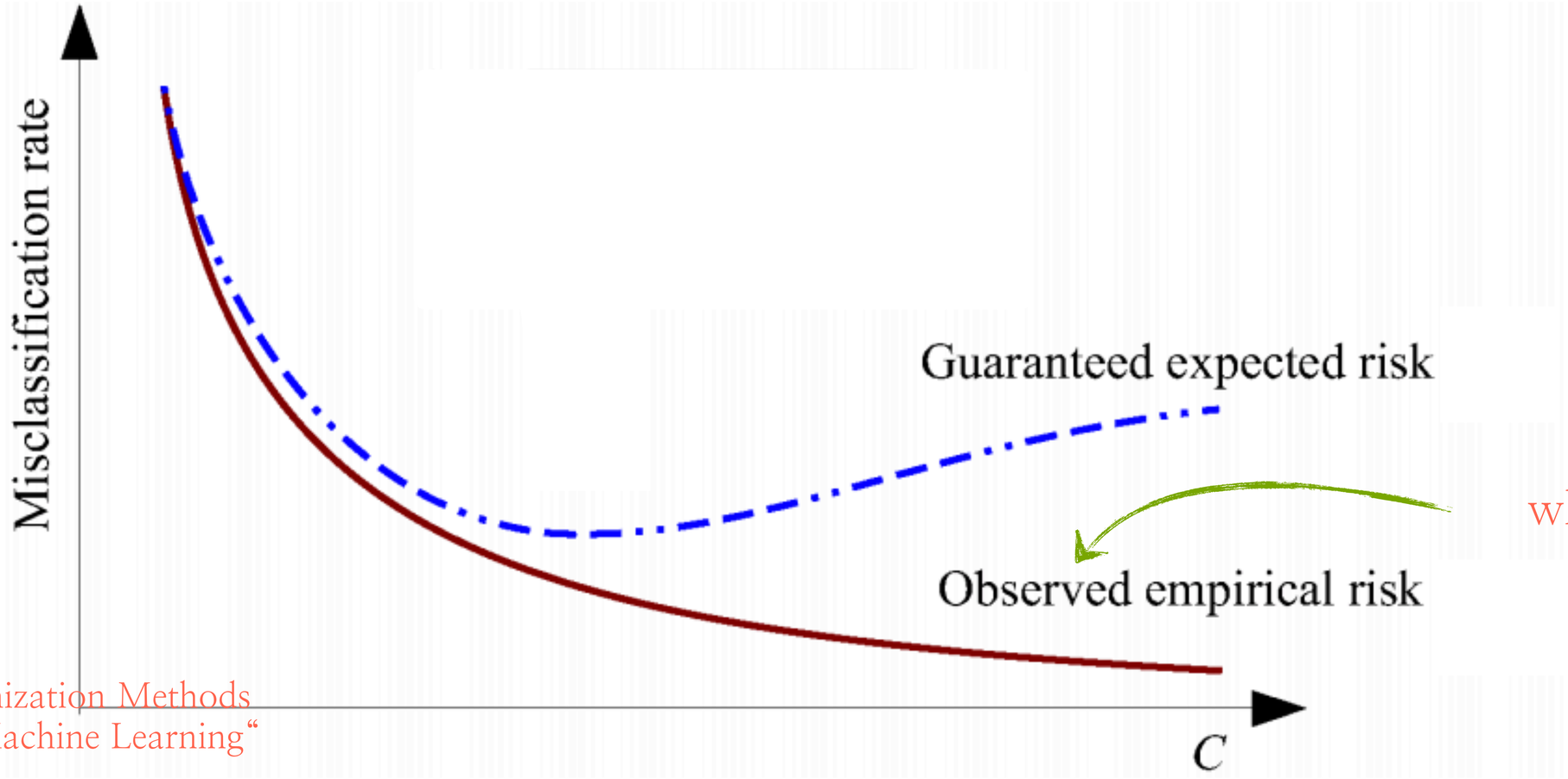

where batch methods thrive

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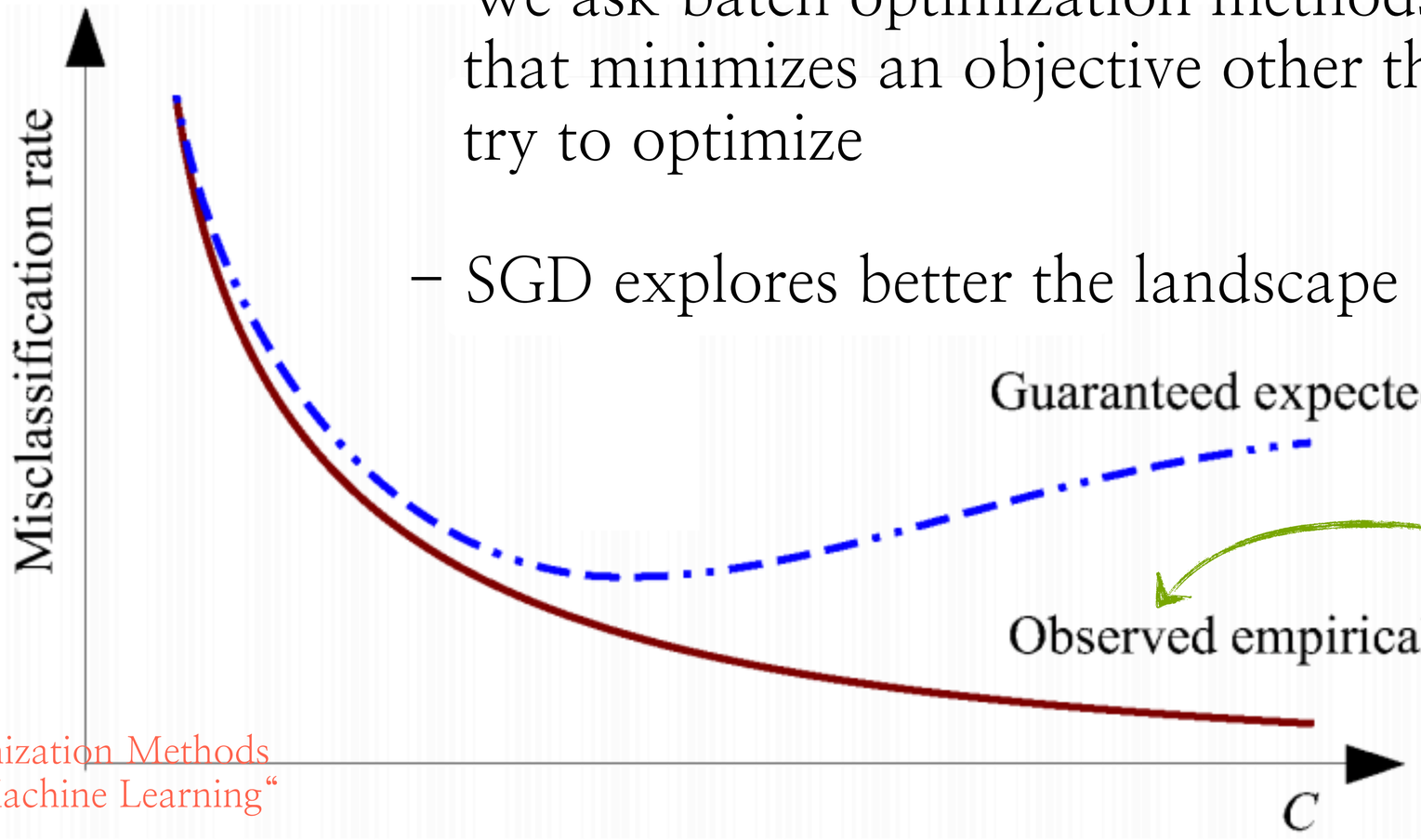
Why SGD is so important in machine learning?

(or some of the reasons)

- We ask batch optimization methods to find a model that minimizes an objective other than what they try to optimize

- SGD explores better the landscape

(more to come in future lectures)



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(but it is an active area of research, as things are not 100% clear)

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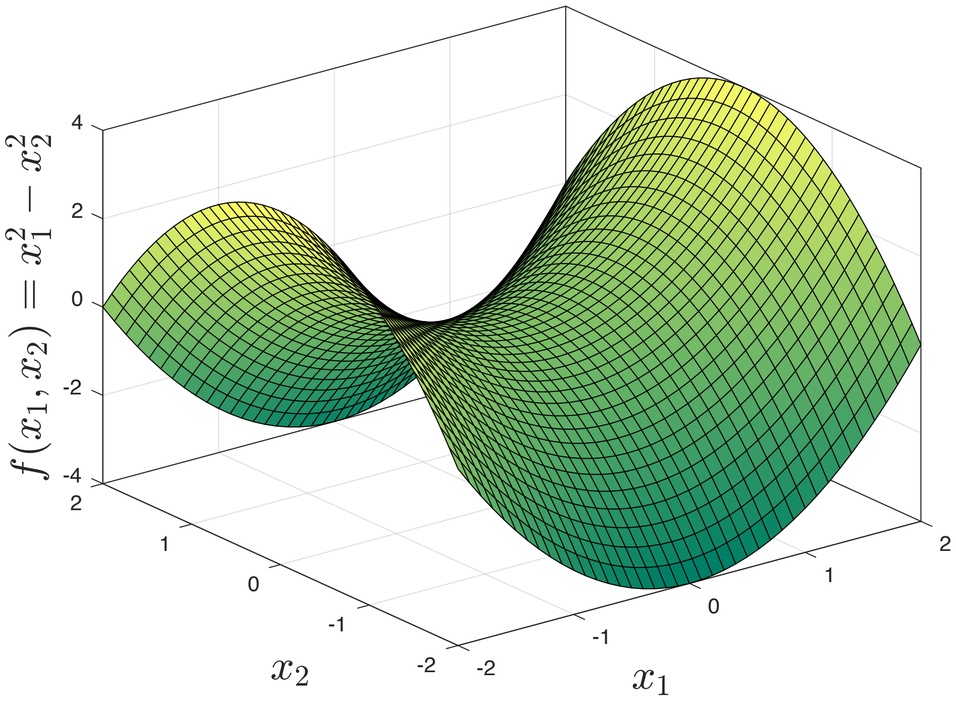

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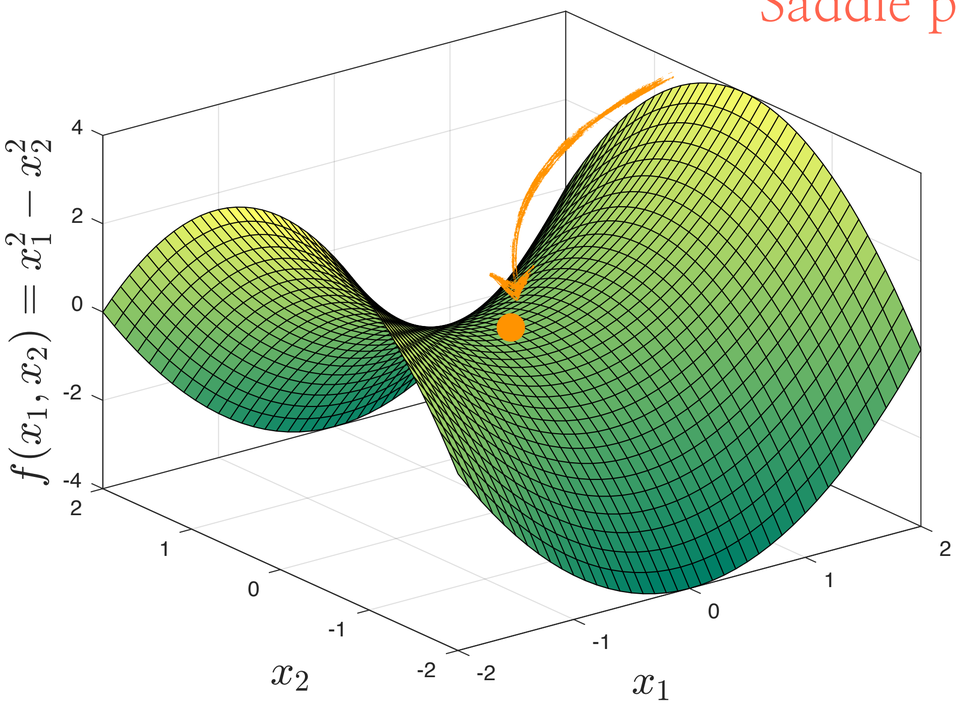

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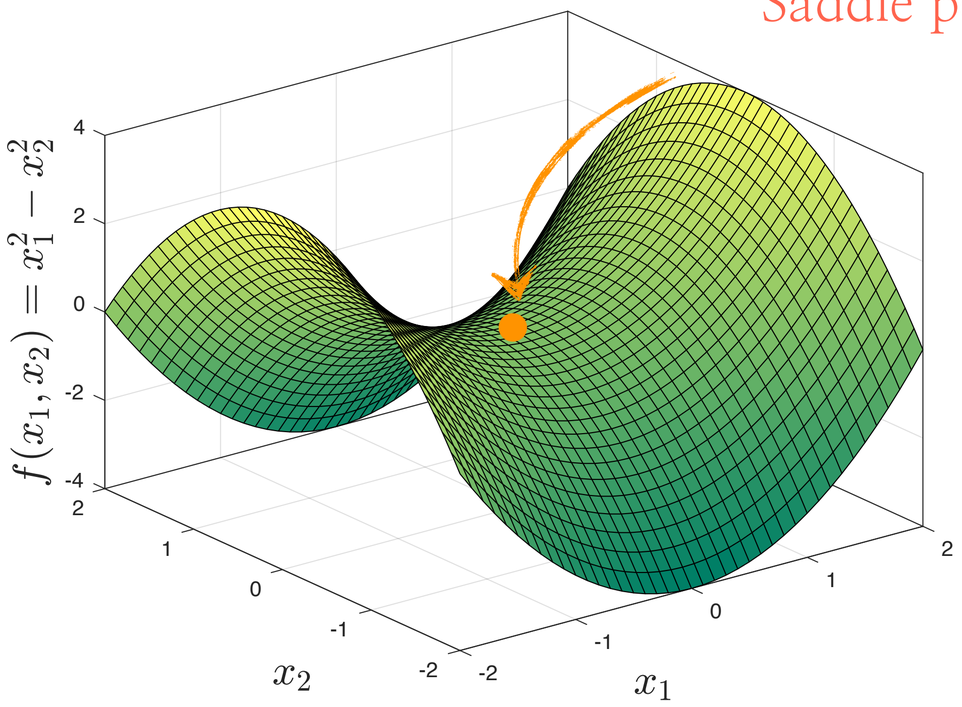

- Compute the Hessian:

$$H = \begin{bmatrix} \frac{\partial^2 f(x_1,x_2)}{\partial x_1^2} & \frac{\partial^2 f(x_1,x_2)}{\partial x_1 x_2} \\ \frac{\partial^2 f(x_1,x_2)}{\partial x_2 x_1} & \frac{\partial^2 f(x_1,x_2)}{\partial x_2^2} \end{bmatrix} = \begin{bmatrix} 2 & 0 \\ 0 & -2 \end{bmatrix}$$

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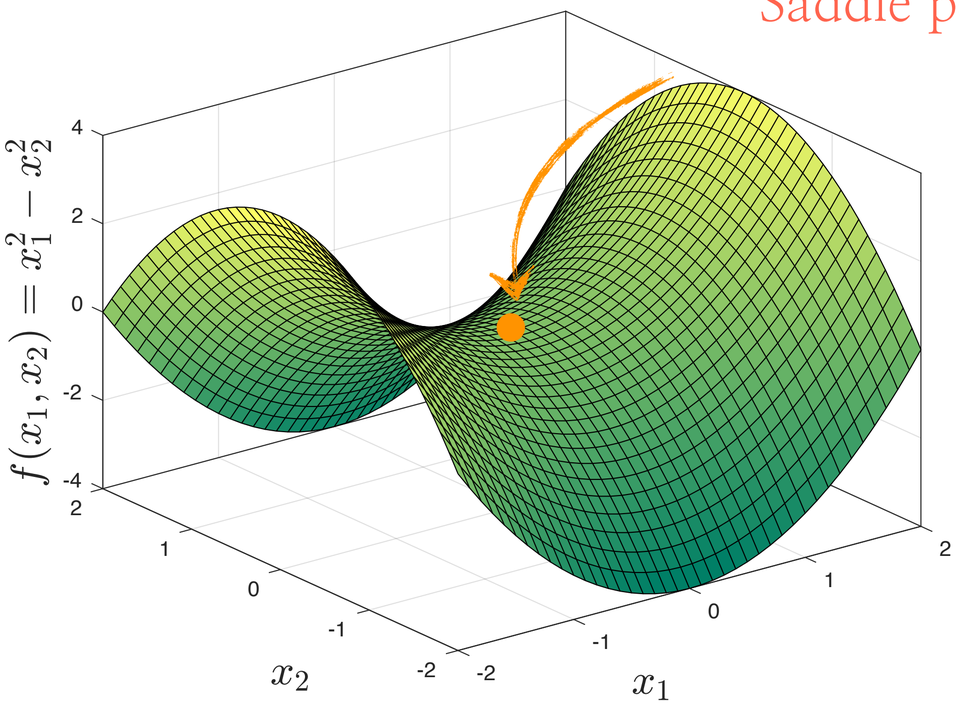

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- Compute the inverse Hessian:

$$H^{-1} = \begin{bmatrix} 1/2 & 0 \\ 0 & -1/2 \end{bmatrix}$$

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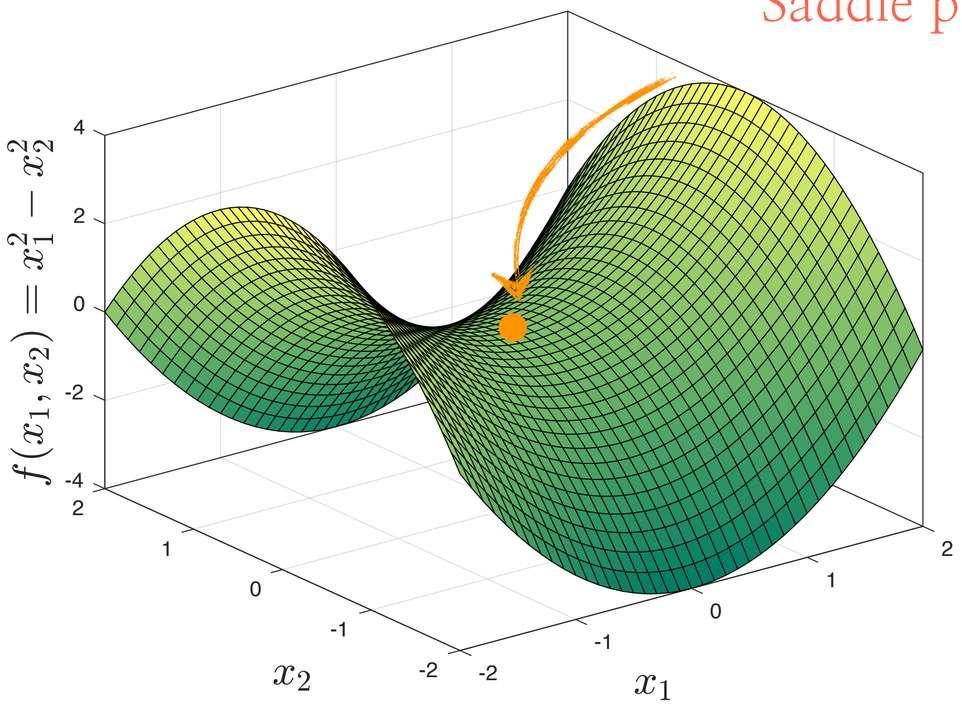

- Let's perform a single Newton iteration:

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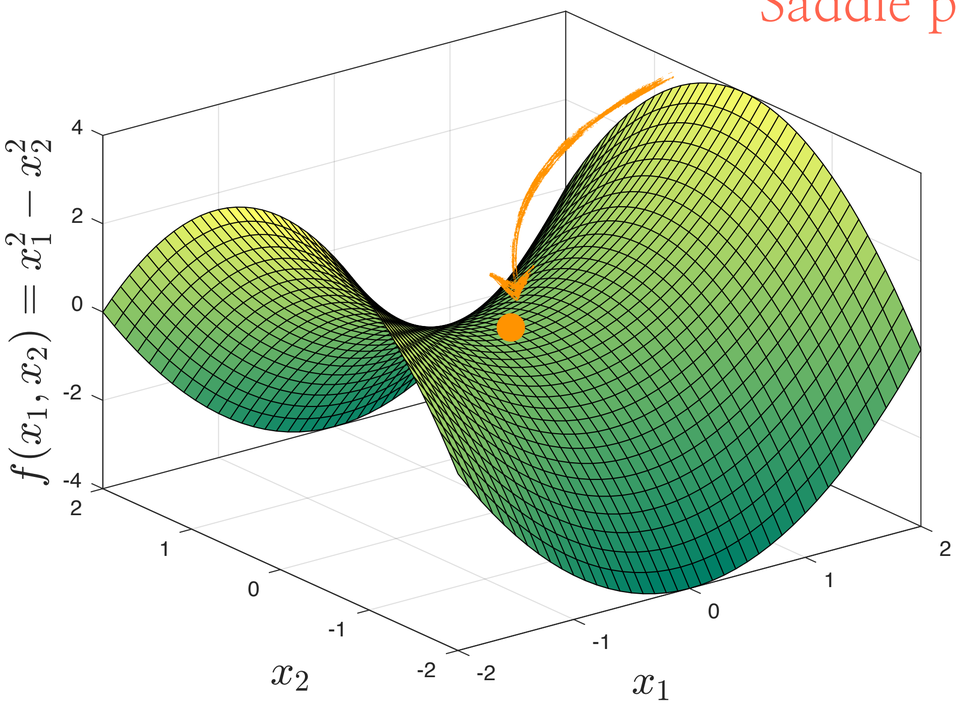

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\end{aligned}
$$

For this toy example, Newton seems to be attracted to the saddle point!

Acceleration #3: Coordinate descent methods

- Stochastic gradient descent (SGD) selects mini batches of training data; what if we subselect variables to update per iteration?

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(Assume least-squares objective)

- When is $n \ll p$? High-dimensional case
  - There is not enough data
  - We will see that it provides solutions to distributed systems

Papers to review – due next Tuesday

(Select one of the following papers)

- "Adaptive Restart for Accelerated Gradient Schemes", O'Dononghue and Candes, 2012.

- "Why momentum really works", Goh, 2017.

- "Solving large-scale linear prediction problems using SGD", Zhang, 2004.

- "Stochastic Gradient Descent, Weighted Sampling, and the Randomized Kaczmarz algorithm", Needell et al., 2015.

- "Coordinate descent algorithms", Wright, 2015.

(The first 20 pages)

Conclusion

- We studied algorithms beyond gradient descent: Newton's method, quasi-Newton algorithms, derivative-free optimization, acceleration methods, and stochastic variants

- Which one to use depends on the problem at hand (accuracy, complexity)

- There's a lot of tuning going on..

..which is probably the most crucial part, if we want to be fair in comparison!

Next lecture

- We will discuss a bit about **hyper-parameter tuning**