COMP 414/514: Optimization – Algorithms, Complexity and Approximations

Lecture 5

Overview

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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

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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)

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:

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

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

converges quadratically according to:

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

Guarantees of Newton's method

Local convergence guarantees

Assumes no convexity – but assumes good initialization

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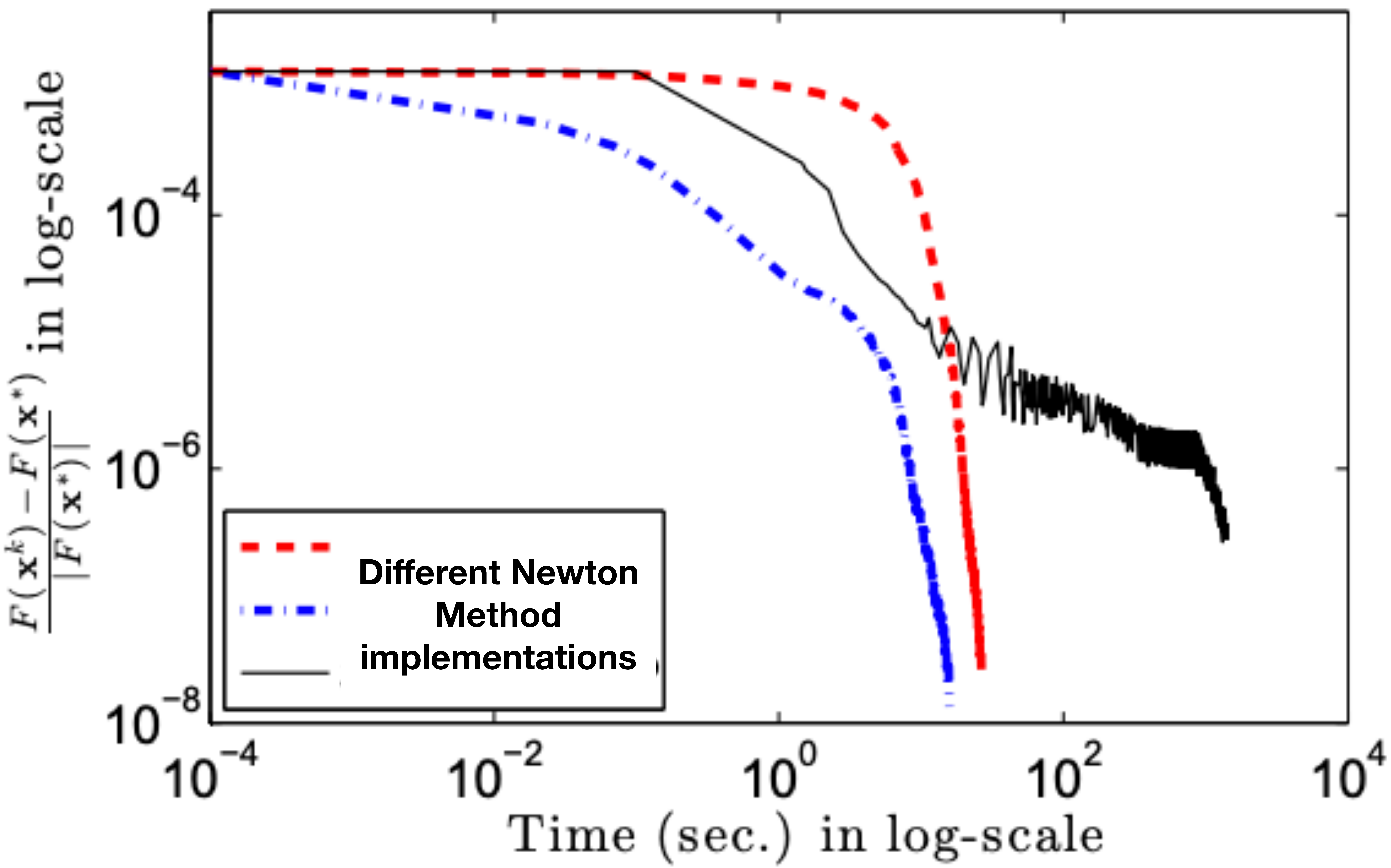
Guarantees of Newton's method

Whiteboard

Guarantees of Newton's method



The notorious Newton's method

Demo

General comments of Newton's method

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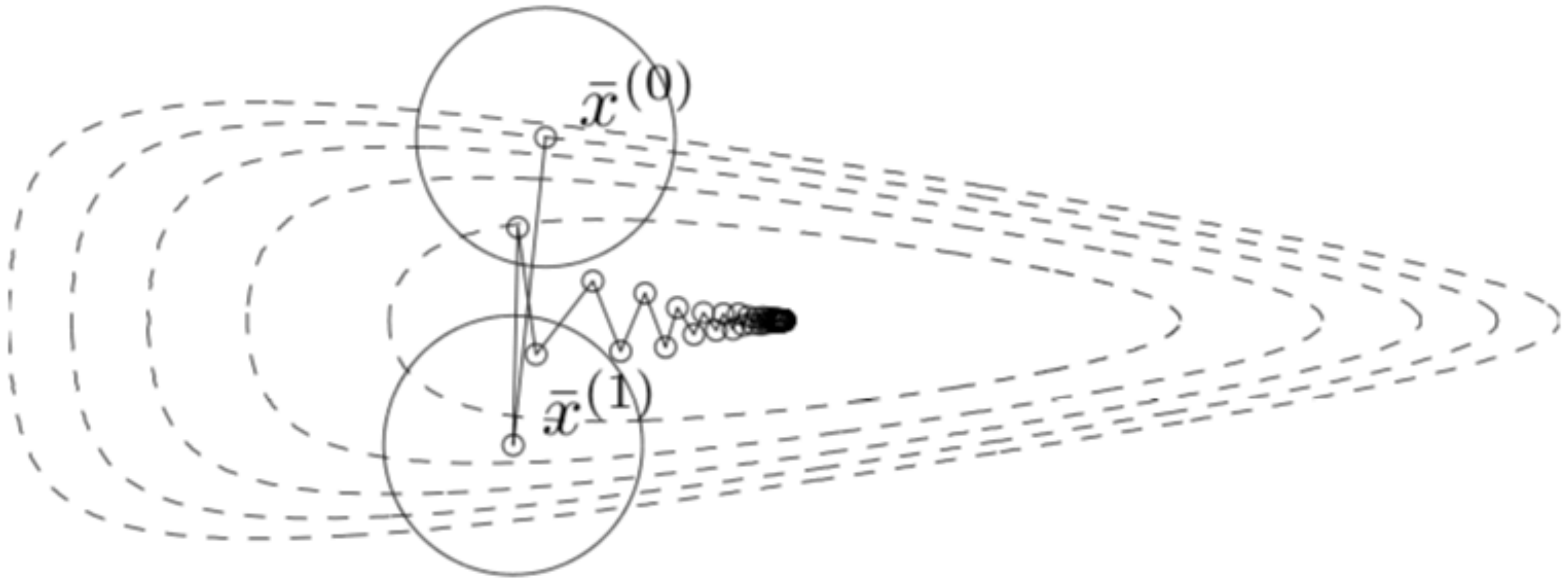
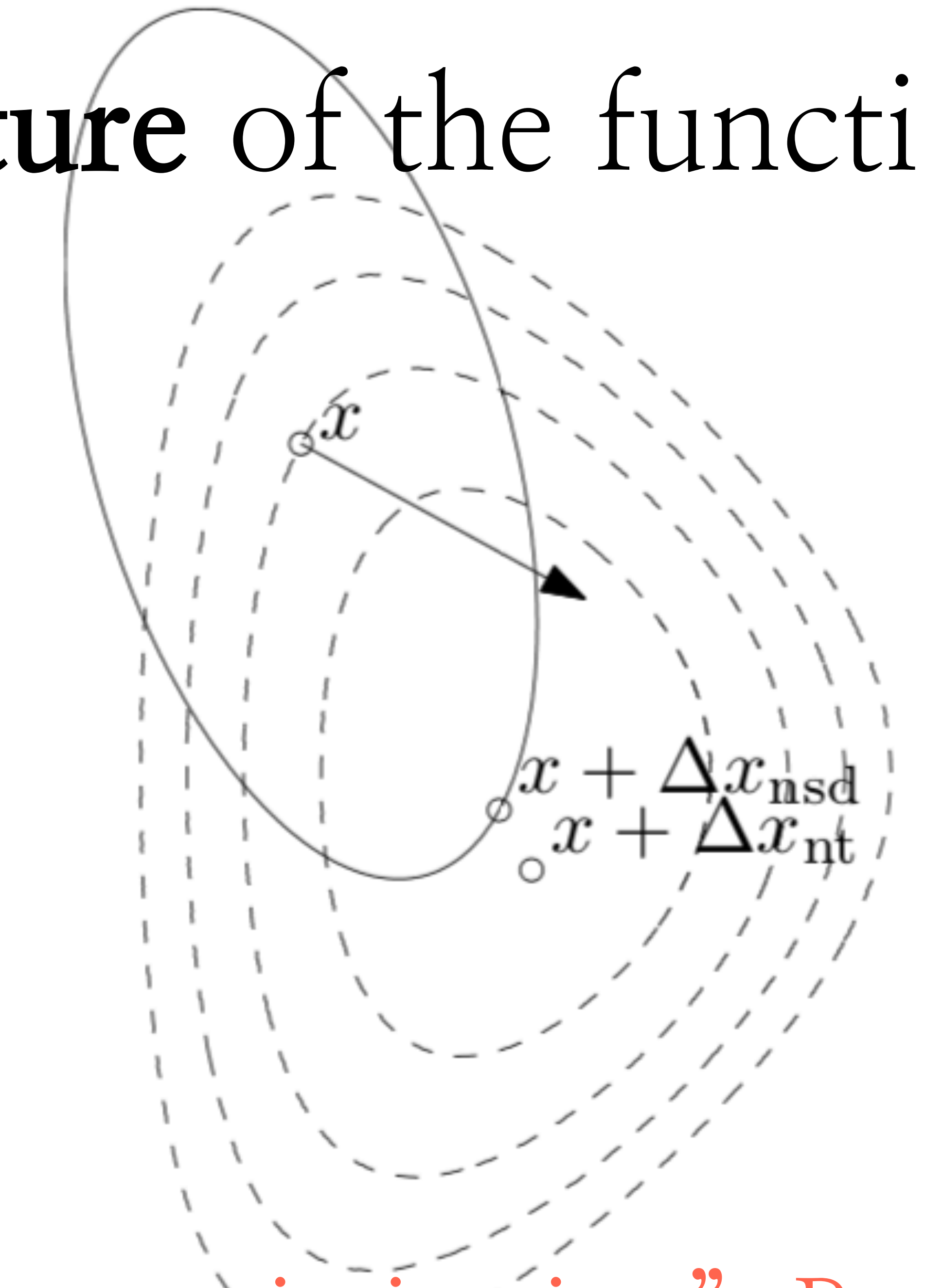
– Newton's method exploits the **local curvature** of the function





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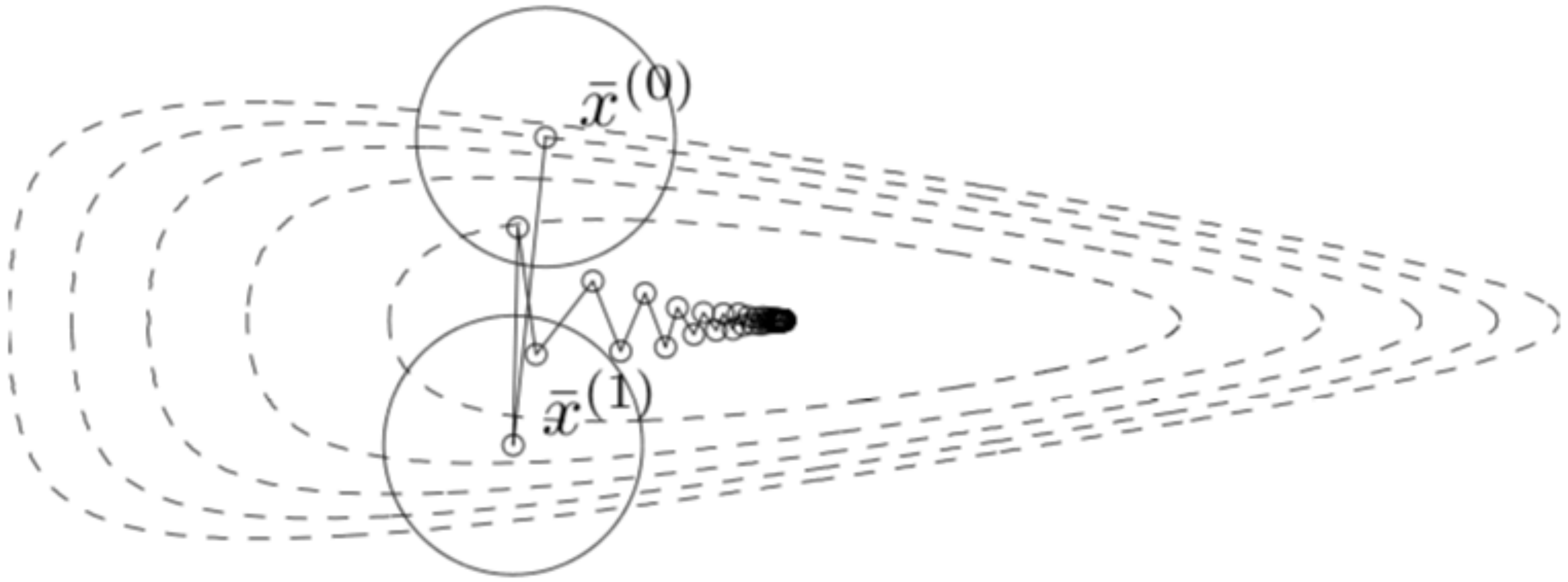

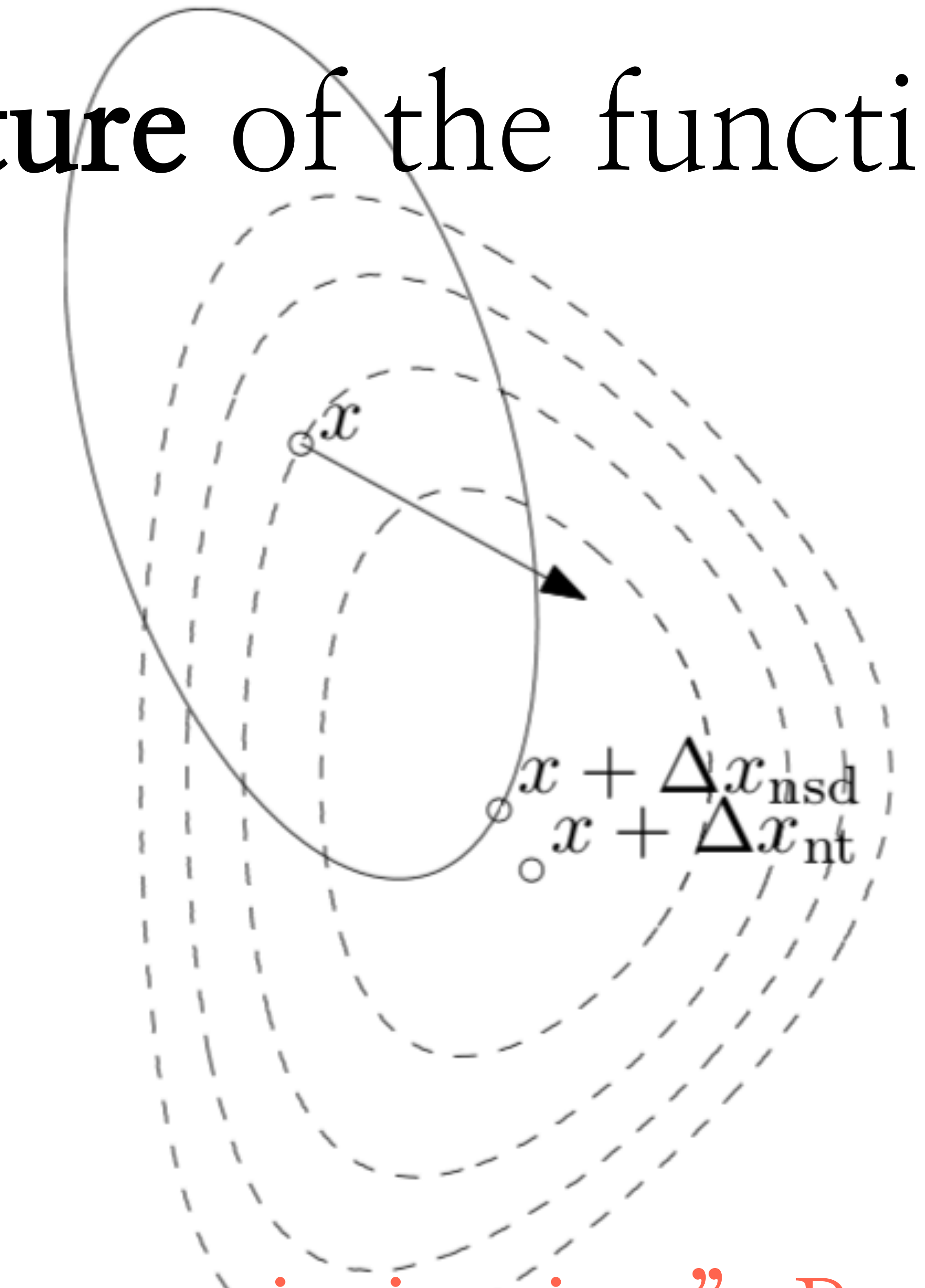

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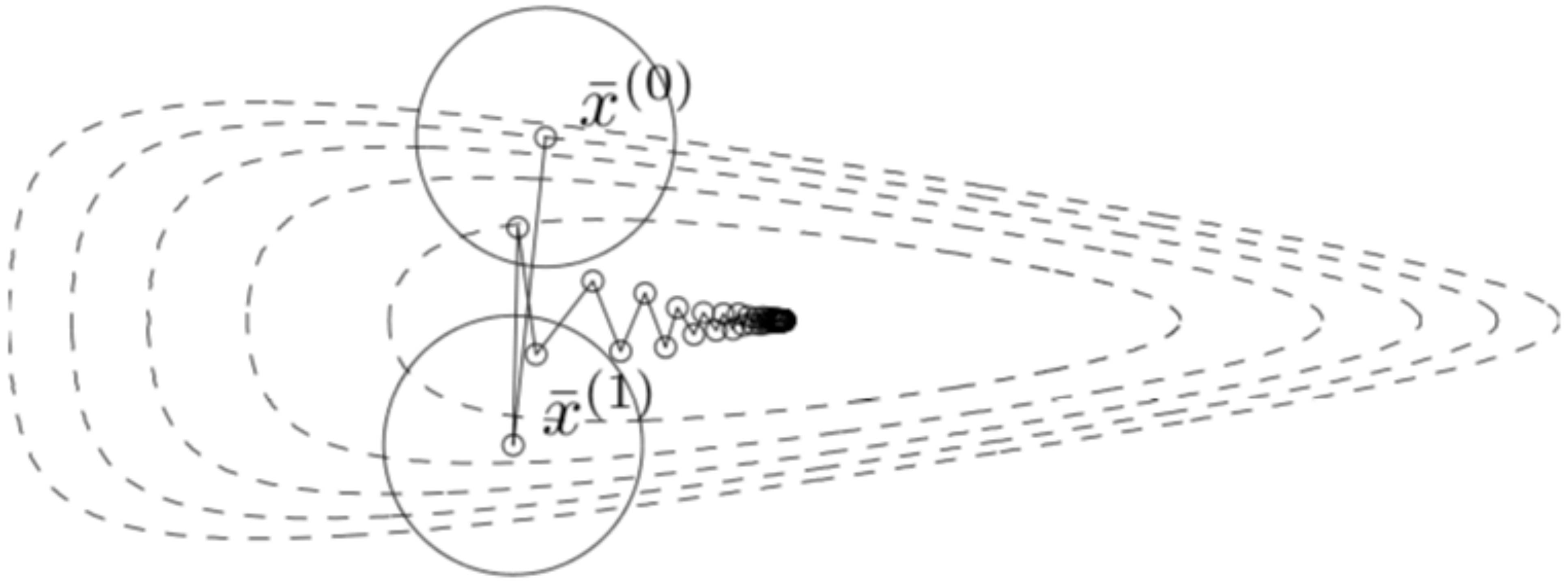

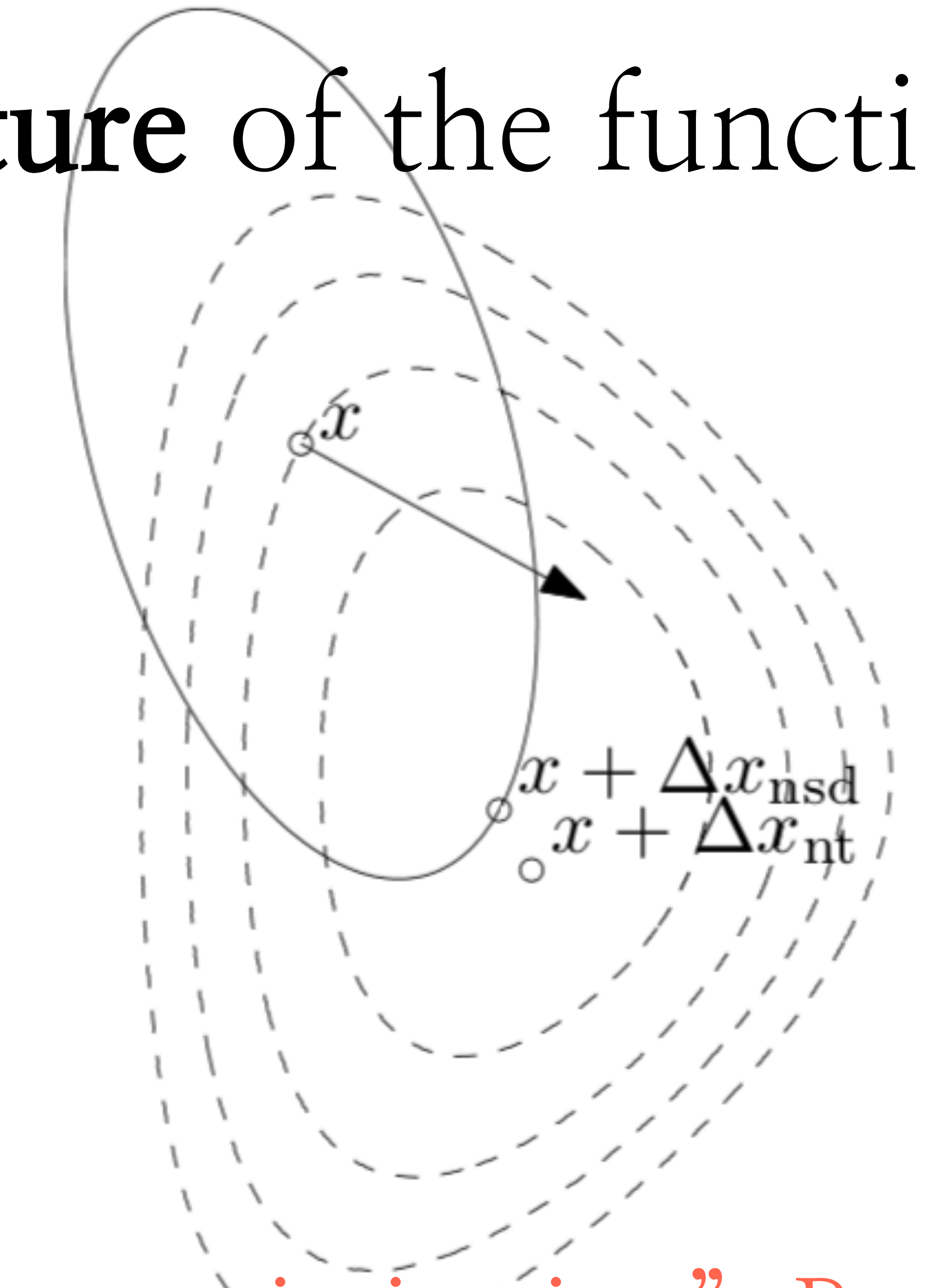

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(We often observe a two-phase behavior: A linear convergence at first, and then a quadratic one)

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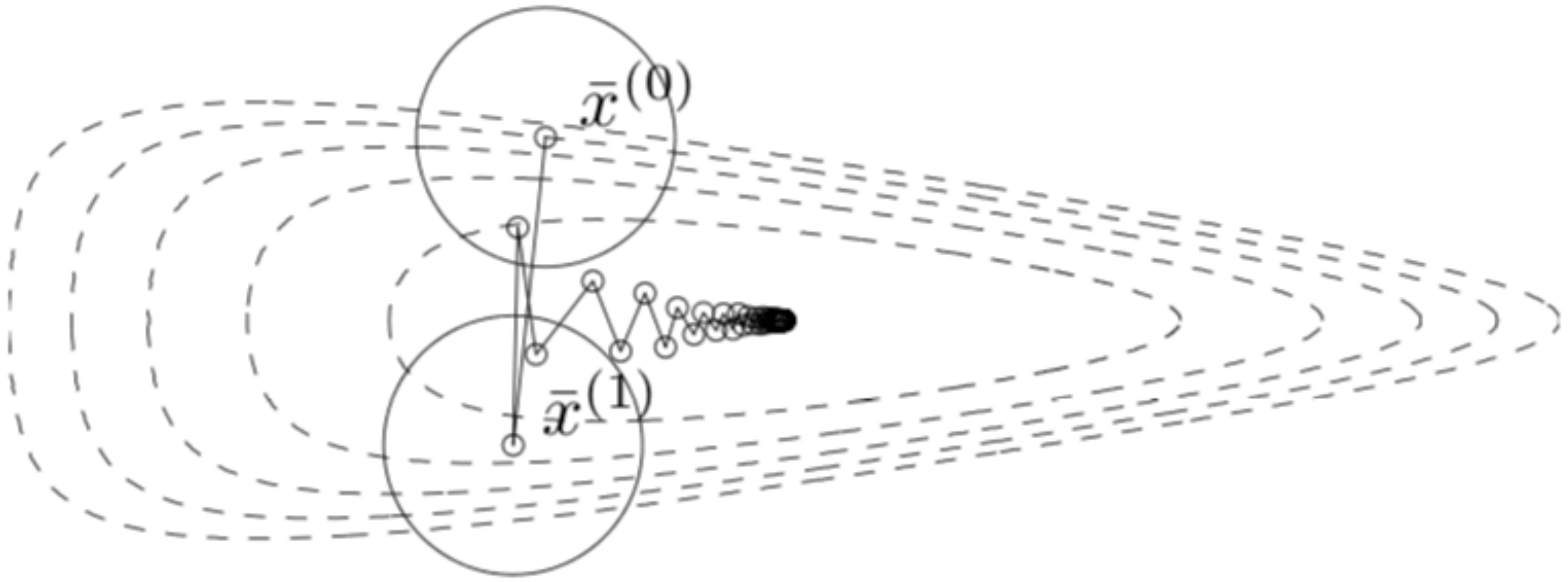

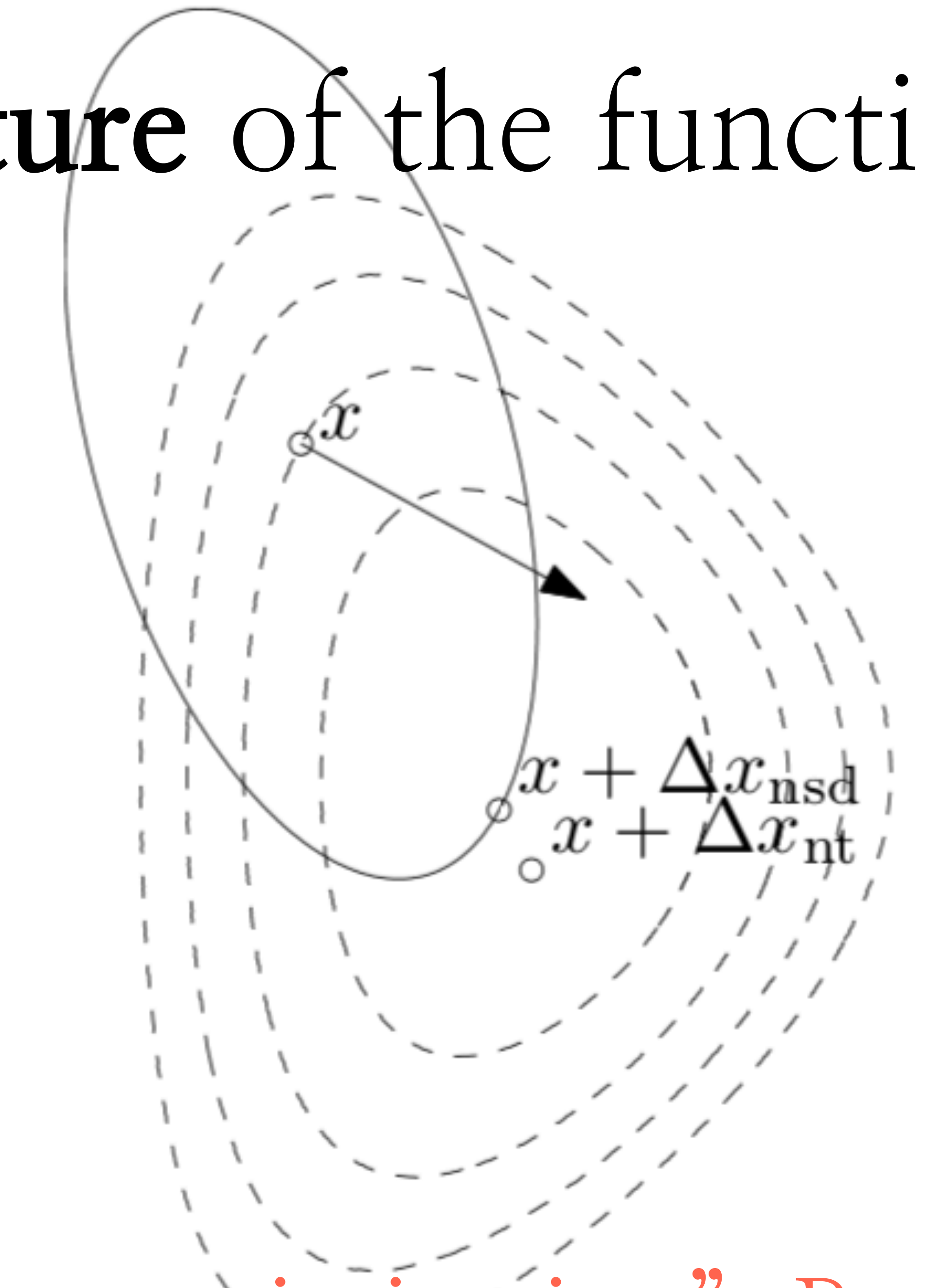

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– Useful for exact solutions; not often the situation in machine learning

Between gradient descent and Newton's method

- Quasi−Newton methods

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

Between gradient descent and Newton's method

– **Quasi-Newton methods**

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Approximation of the inverse Hessian

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– "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

Broyden, Fletcher, Goldfarb, Shanno

Paying tribute to these gentlemen

The BFGS method

– Quadratic approximations around current point

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

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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:

$$\nabla g_{t+1}(0) = \nabla f(x_{t+1})$$

(i.e., the new approximation should give back the gradient when no update step is performed)

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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:

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

(Intuition?)

The BFGS method

- The BFGS method goes a bit further:

Approximates directly the inverse!

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

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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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$$H_{t+1} = H_t + \sigma v v^\top \qquad \text{and secant equation is satisfied}$$

(Rank−1 update)

$\sigma \in \{\pm 1\}$

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- SR1 rule:

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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

$$\|x_{k+1} - x^\star\|_2 \leq c_k \|x_k - x^\star\|_2 \qquad \text{where} \qquad c_k \to 0$$

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(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..

0–th order optimization

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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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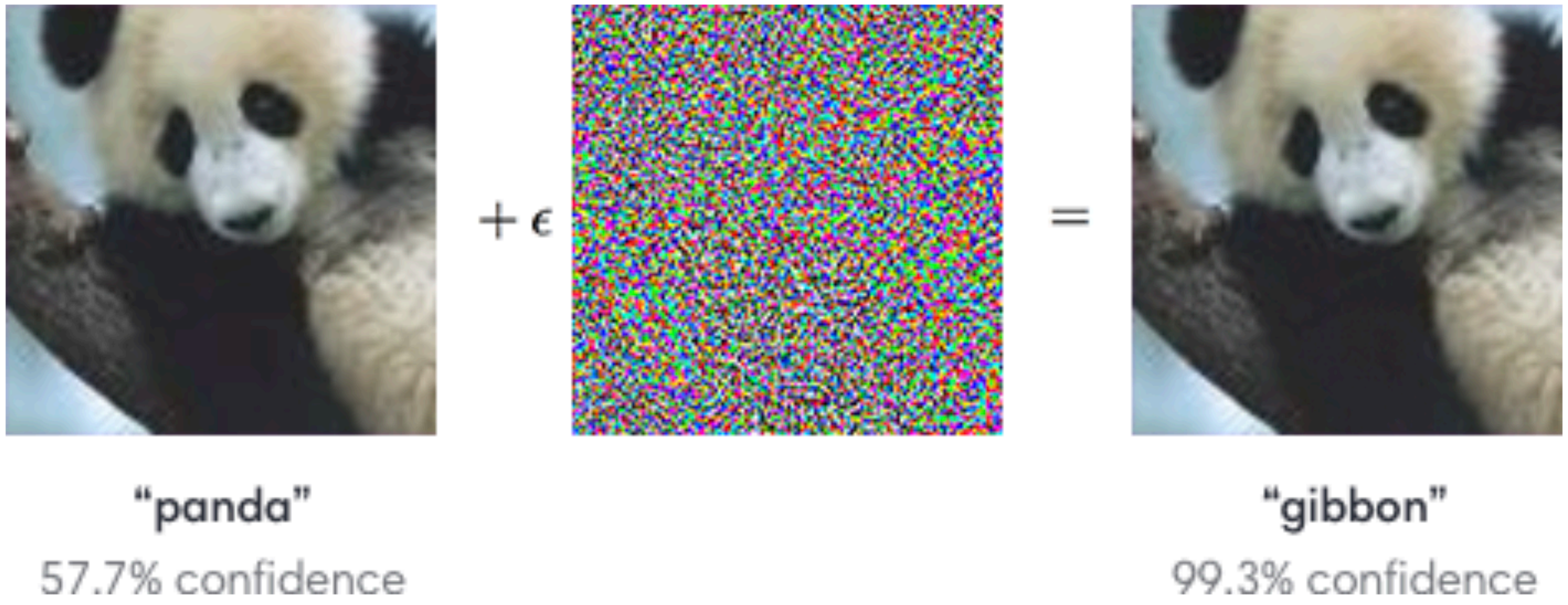
x $+\epsilon$ $=$ x_{adv}



y_{true}

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

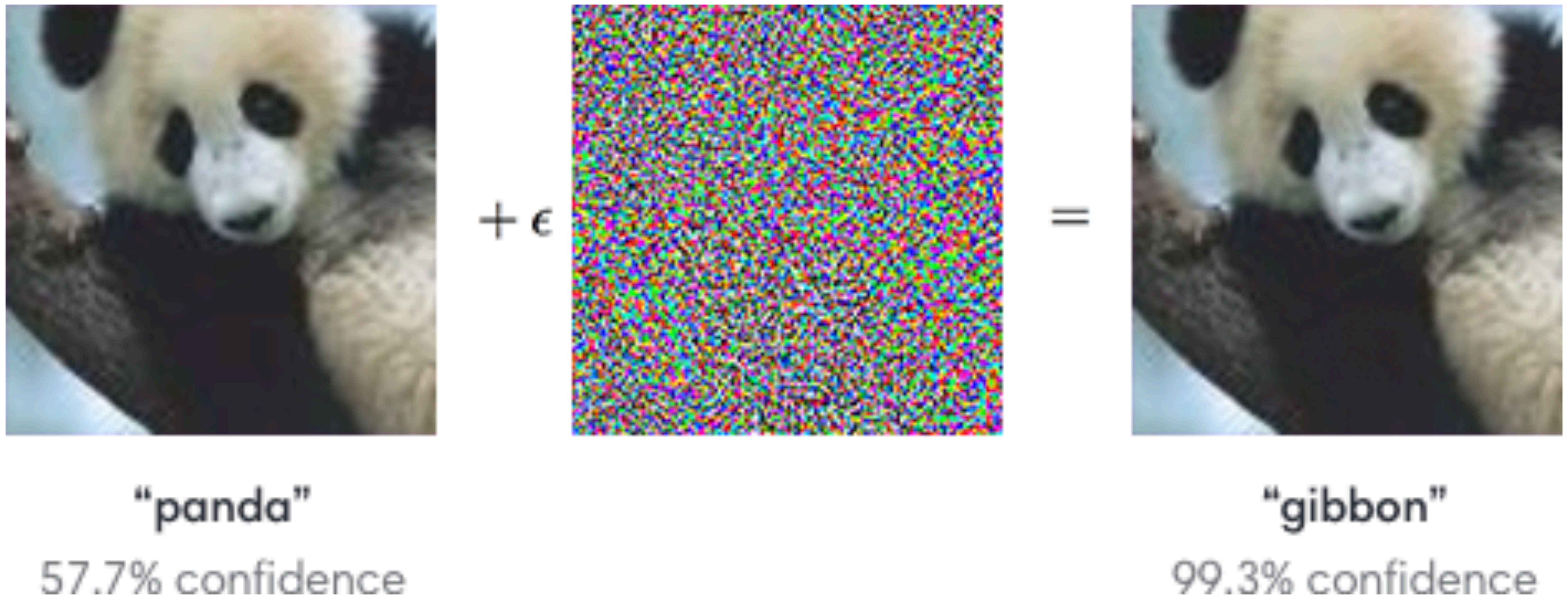
(The objective represents a complex model like a neural network)

Application: Adversarial examples in NN training

(A quick description)

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

x



x_{adv}

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We are looking into directions that move away from the minimum

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

Application: Adversarial examples in NN training

(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

Conclusion

- We studied algorithms beyond gradient descent: Newton's method, quasi-Newton algorithms, derivative-free optimization, and natural gradient descent method

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

- While thee methods match or even overcome the lower bounds, we have been "cheating" by exploiting exact or approximate second-order information

Next lecture

- We will discuss a bit about acceleration and stochasticity in optimization