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

Lecture 5

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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  - 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:

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

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

converges quadratically according to:

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

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

General comments of Newton's method

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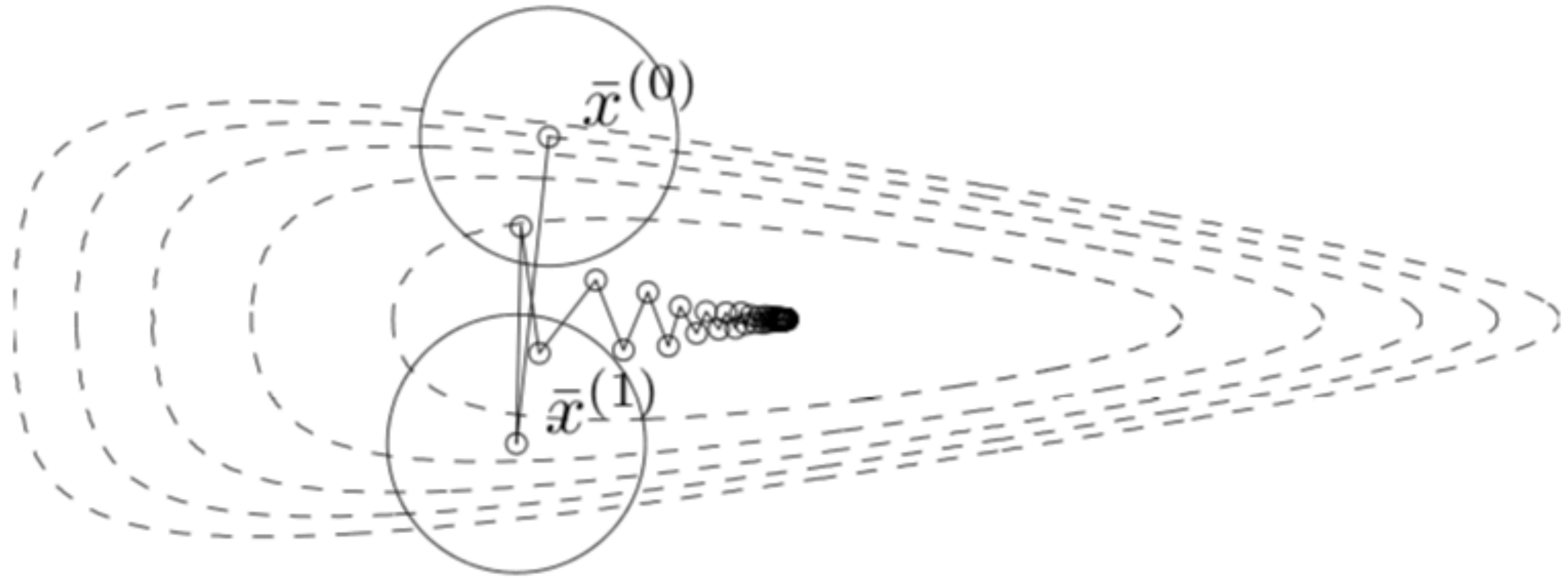
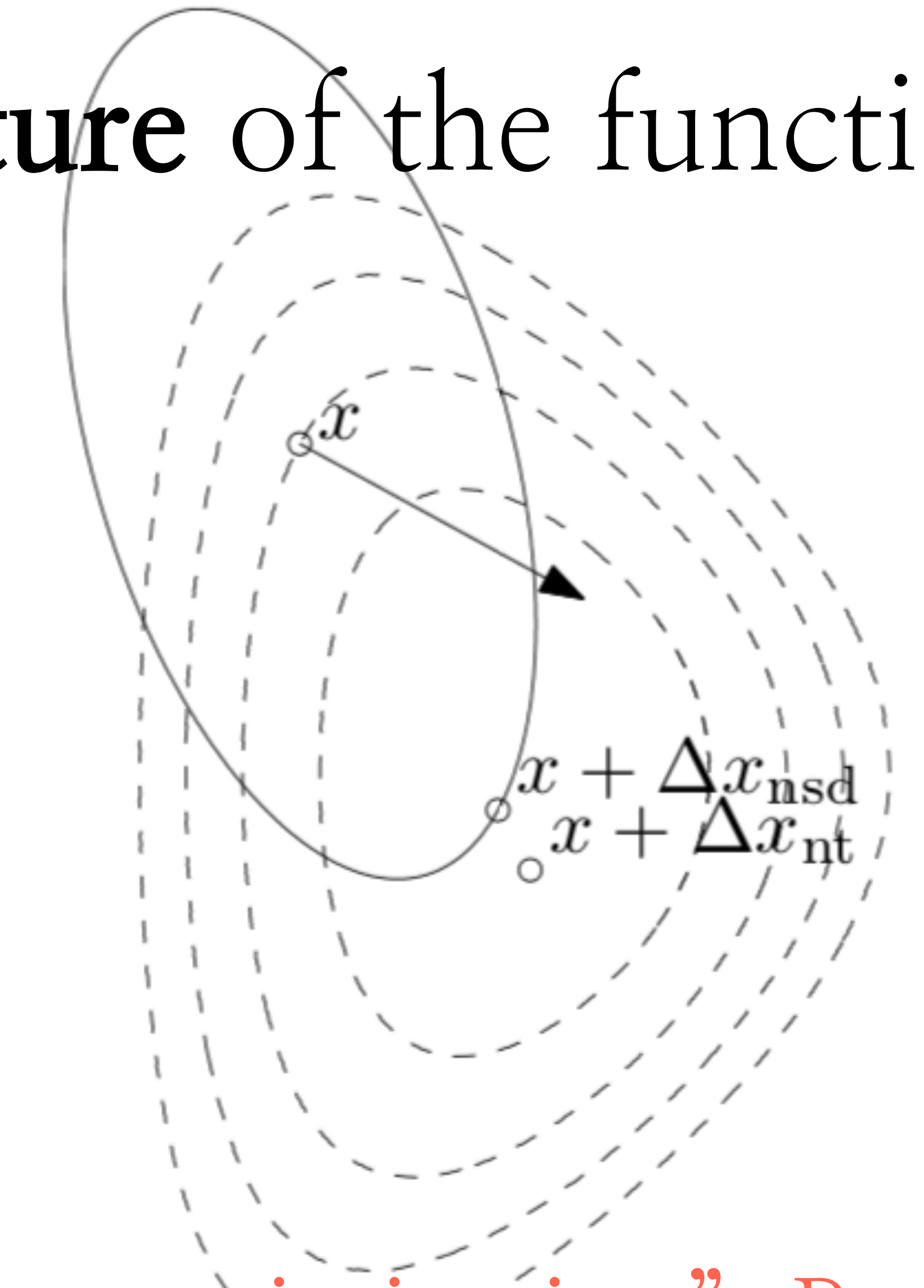
- Newton's method exploits the **local curvature** of the function





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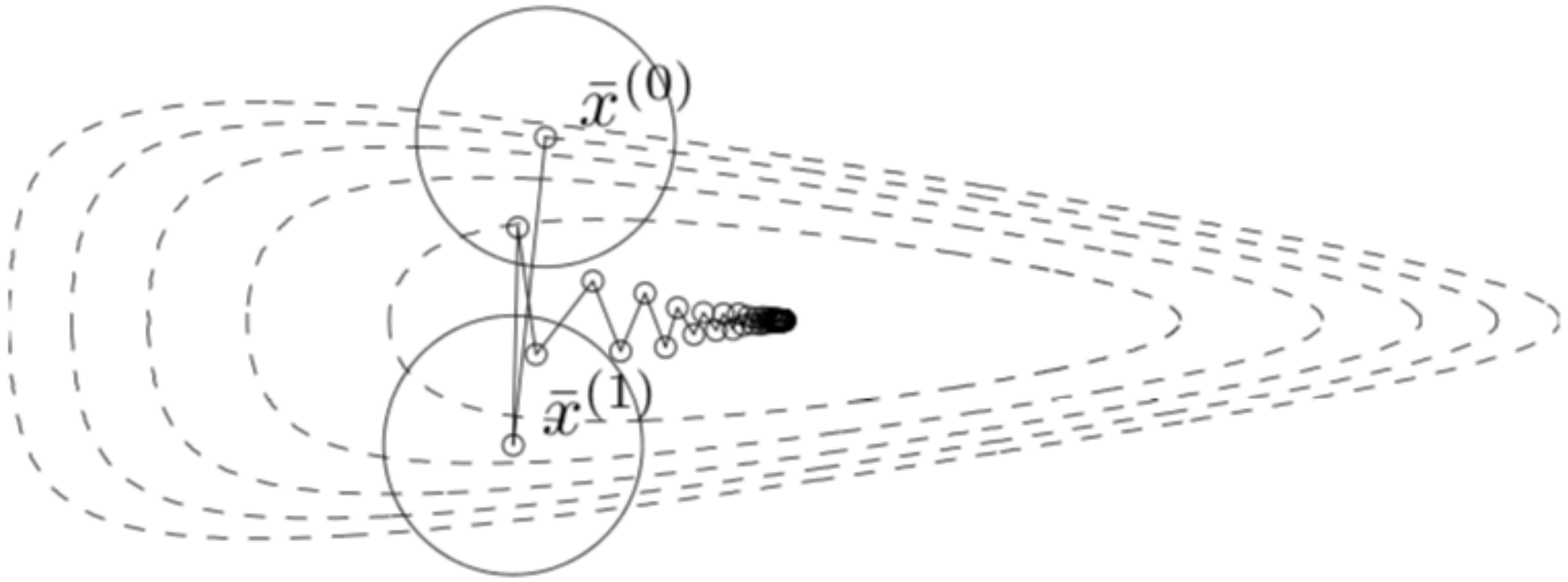

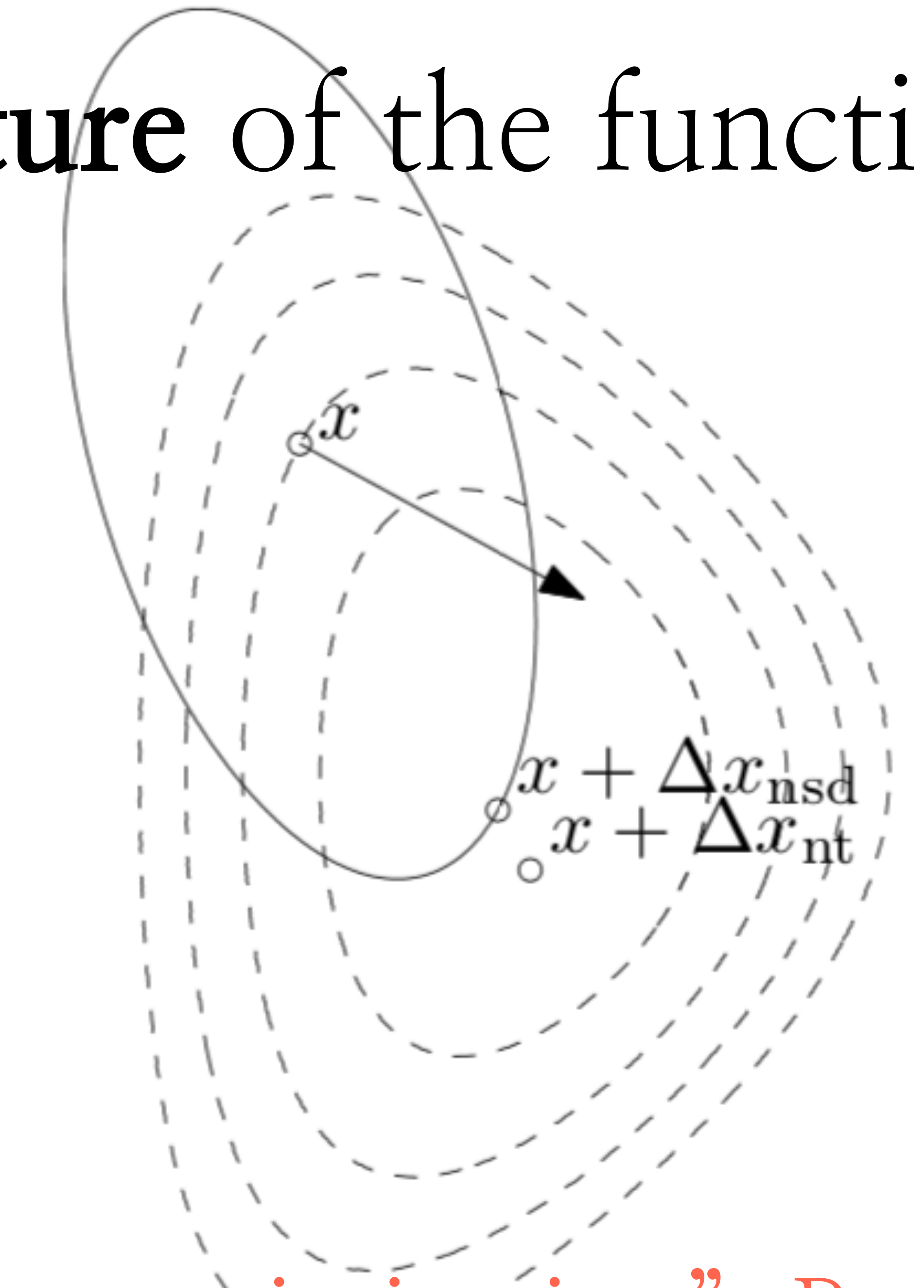

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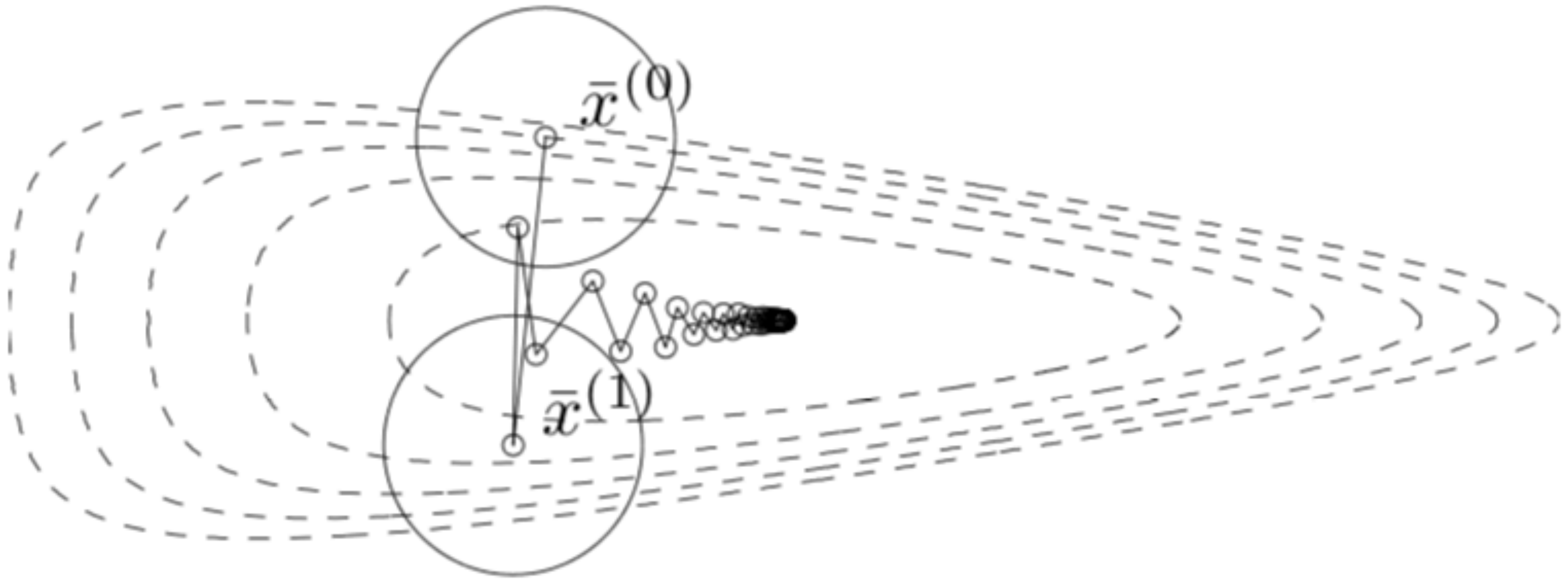

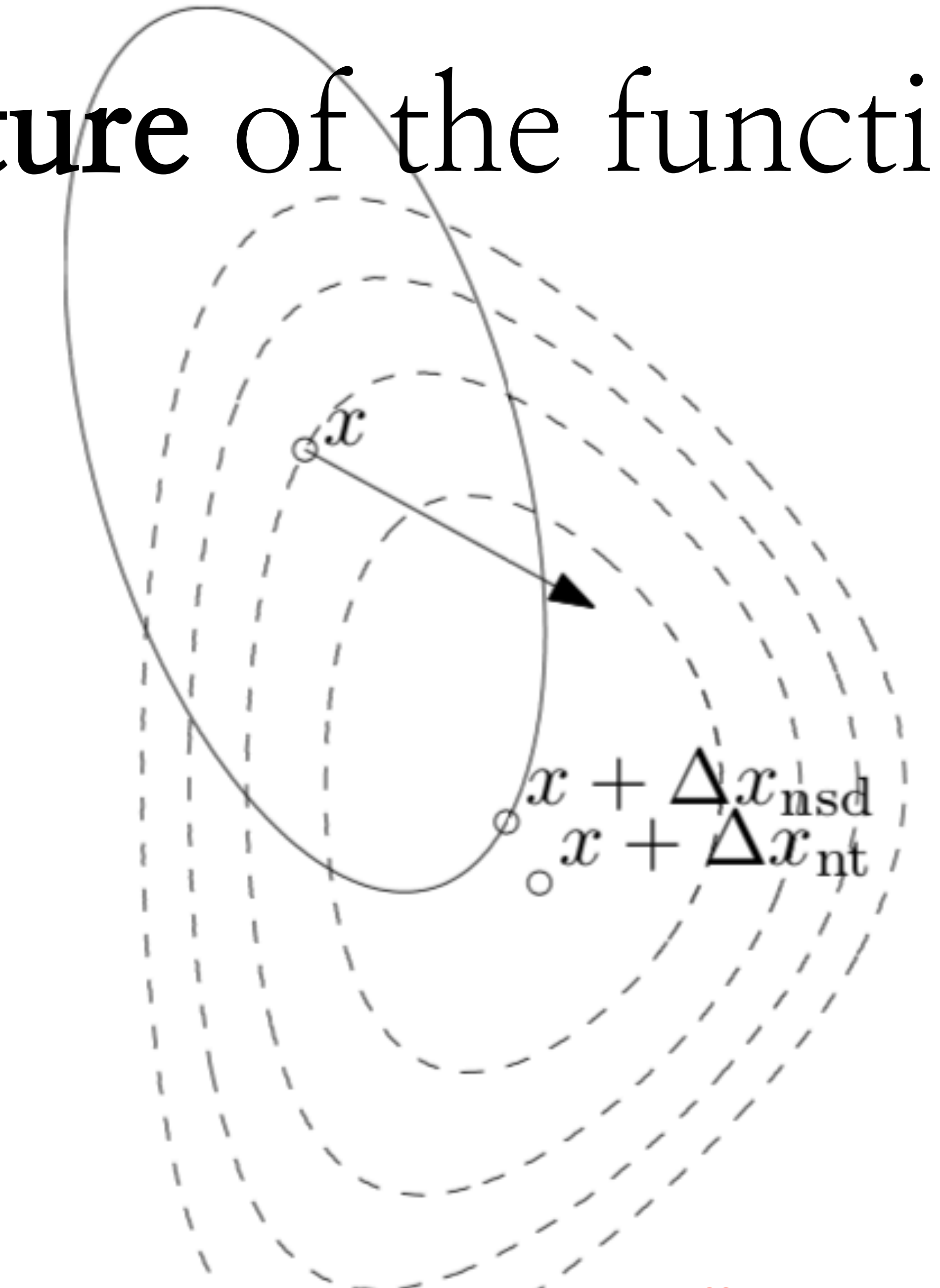

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(We often observe a two-phase behavior: A linear convergence at first, and then a quadratic one)

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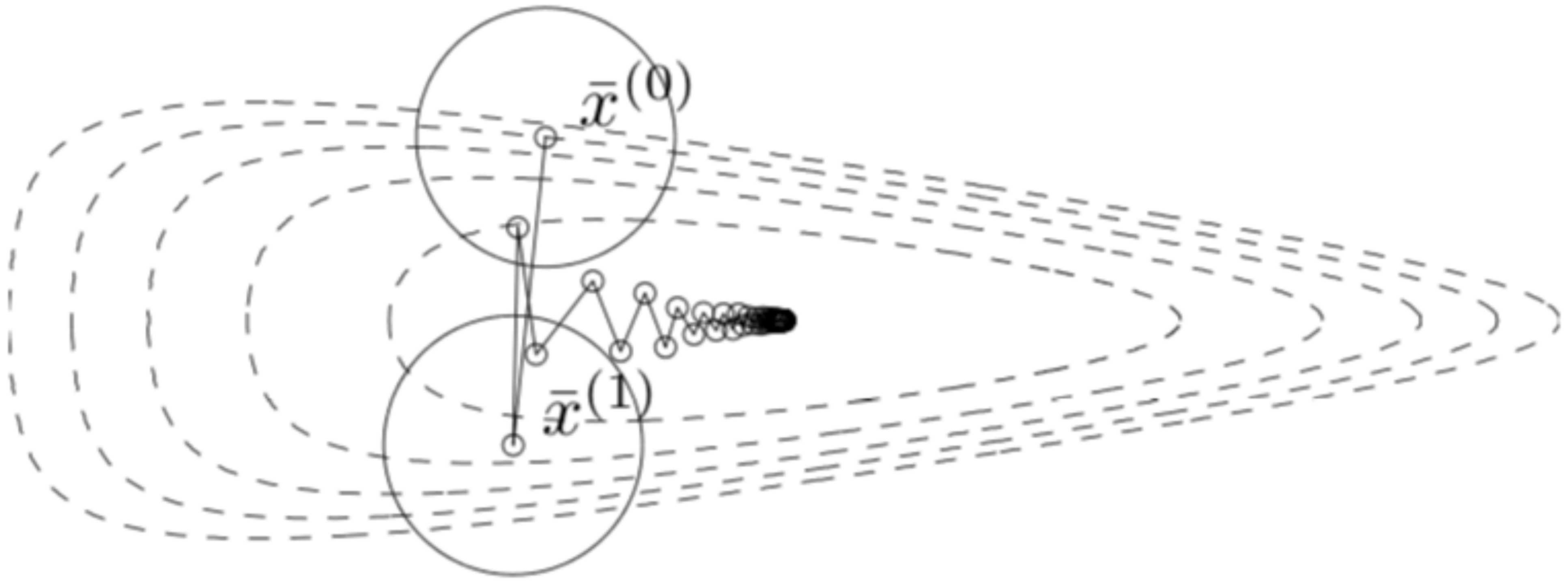

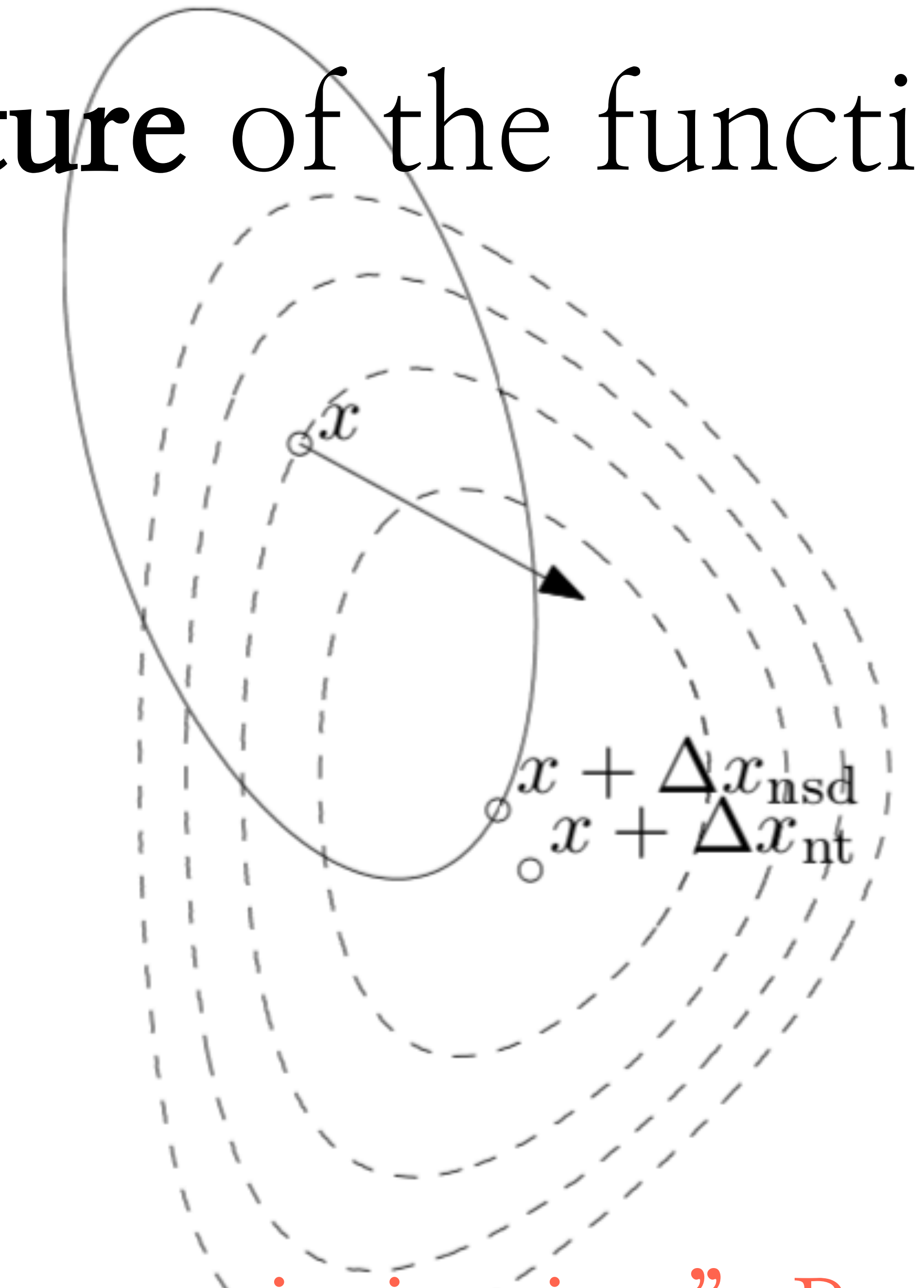

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  (We often observe a two-phase behavior: A linear convergence at first, and then a quadratic one)
- Useful for exact solutions; not often the situation in machine learning

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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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

Broyden, Fletcher, Goldfarb, Shanno

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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$$\nabla g_{t+1}(0) = \nabla f(x_{t+1})$$ (i.e., the new approximation should give back the gradient when no update step is performed)

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

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

(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 many H_{t+1} satisfy this? Infinite!

(How do we choose which one?)

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- By solving:

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

(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)

The SR1 method

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

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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..

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

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

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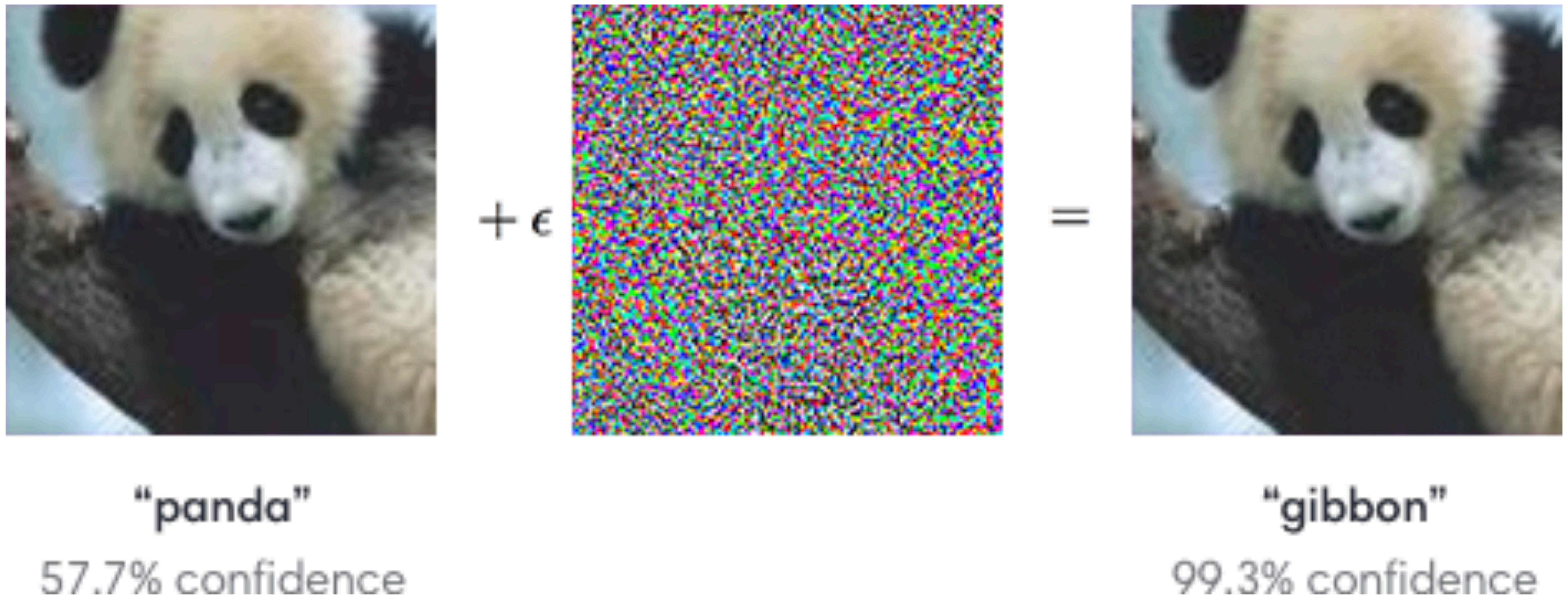
x $\quad + \epsilon \quad = \quad$ x_{adv}



y_{true}

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

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

Application: Adversarial examples in NN training

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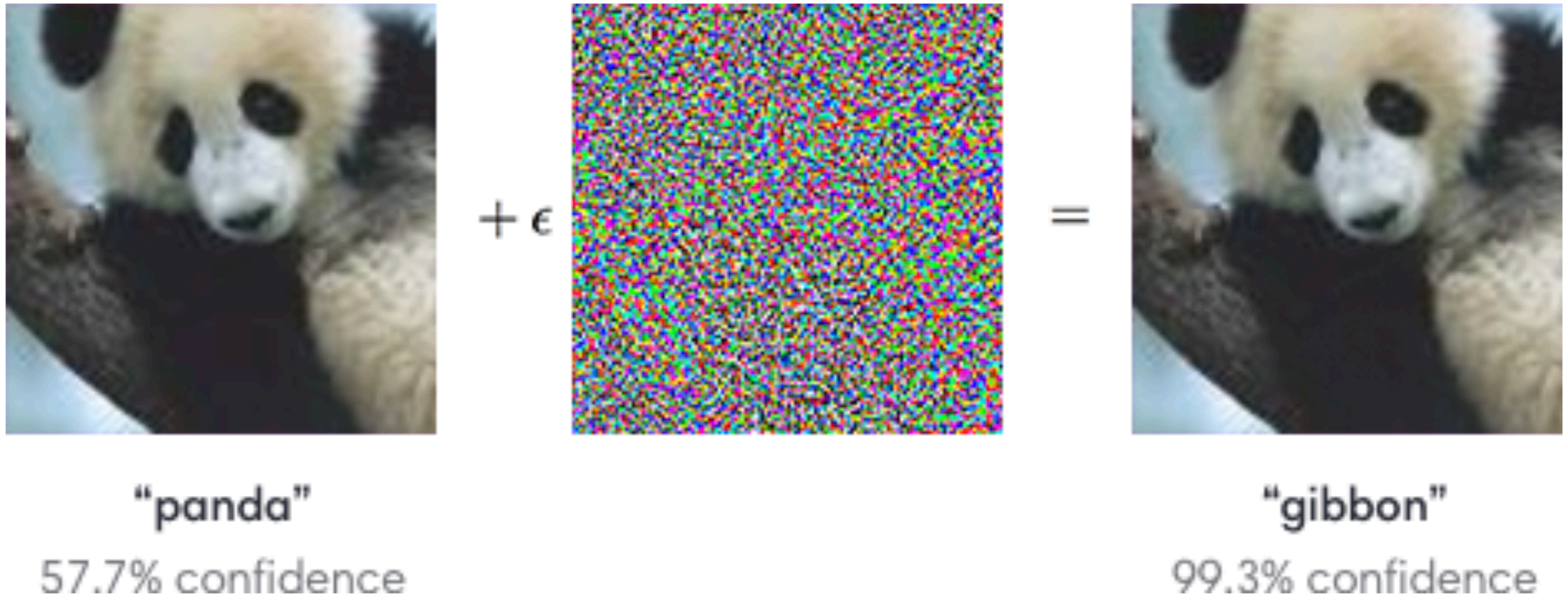
x



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

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

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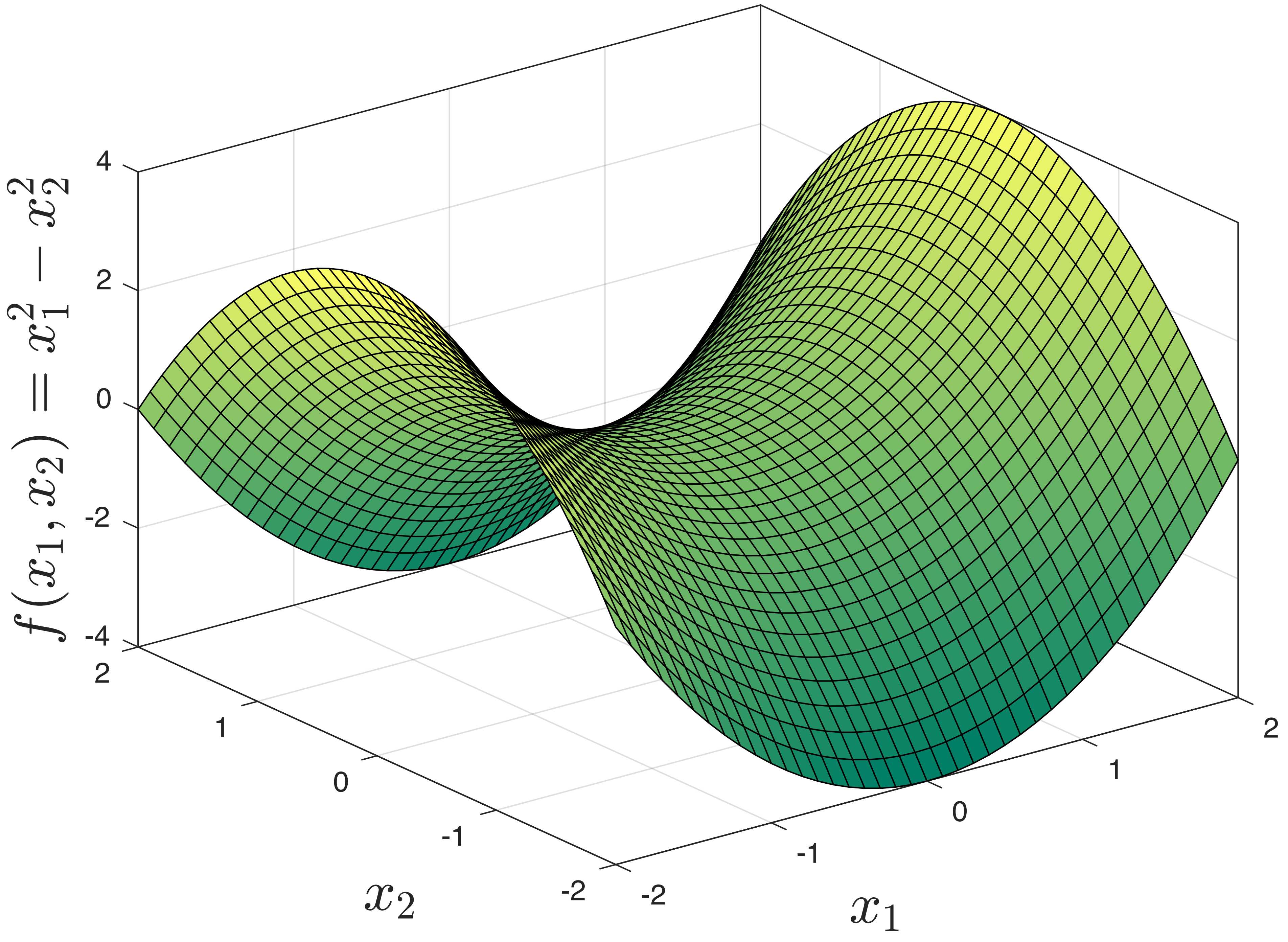

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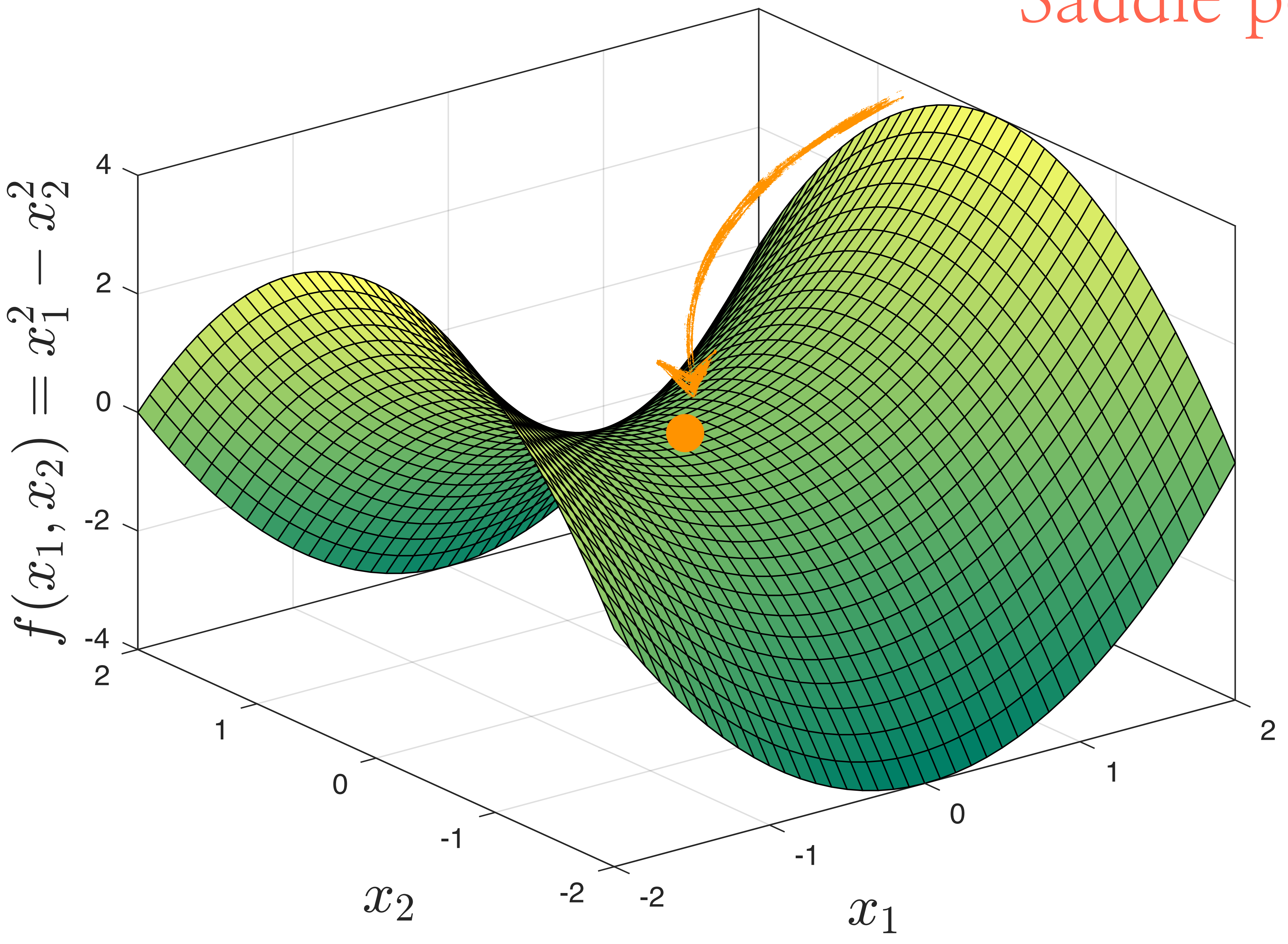

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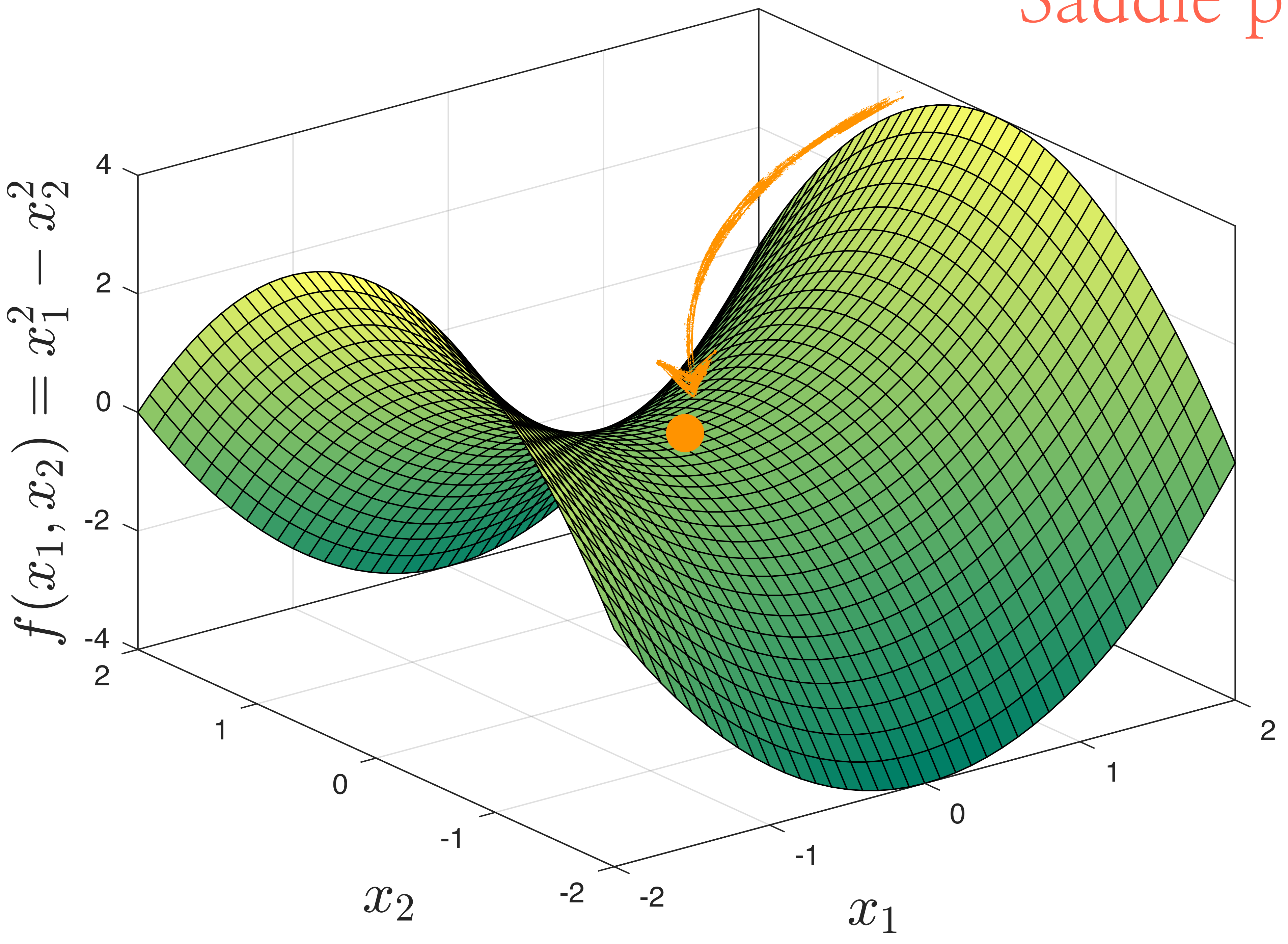

- Compute the Hessian:

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

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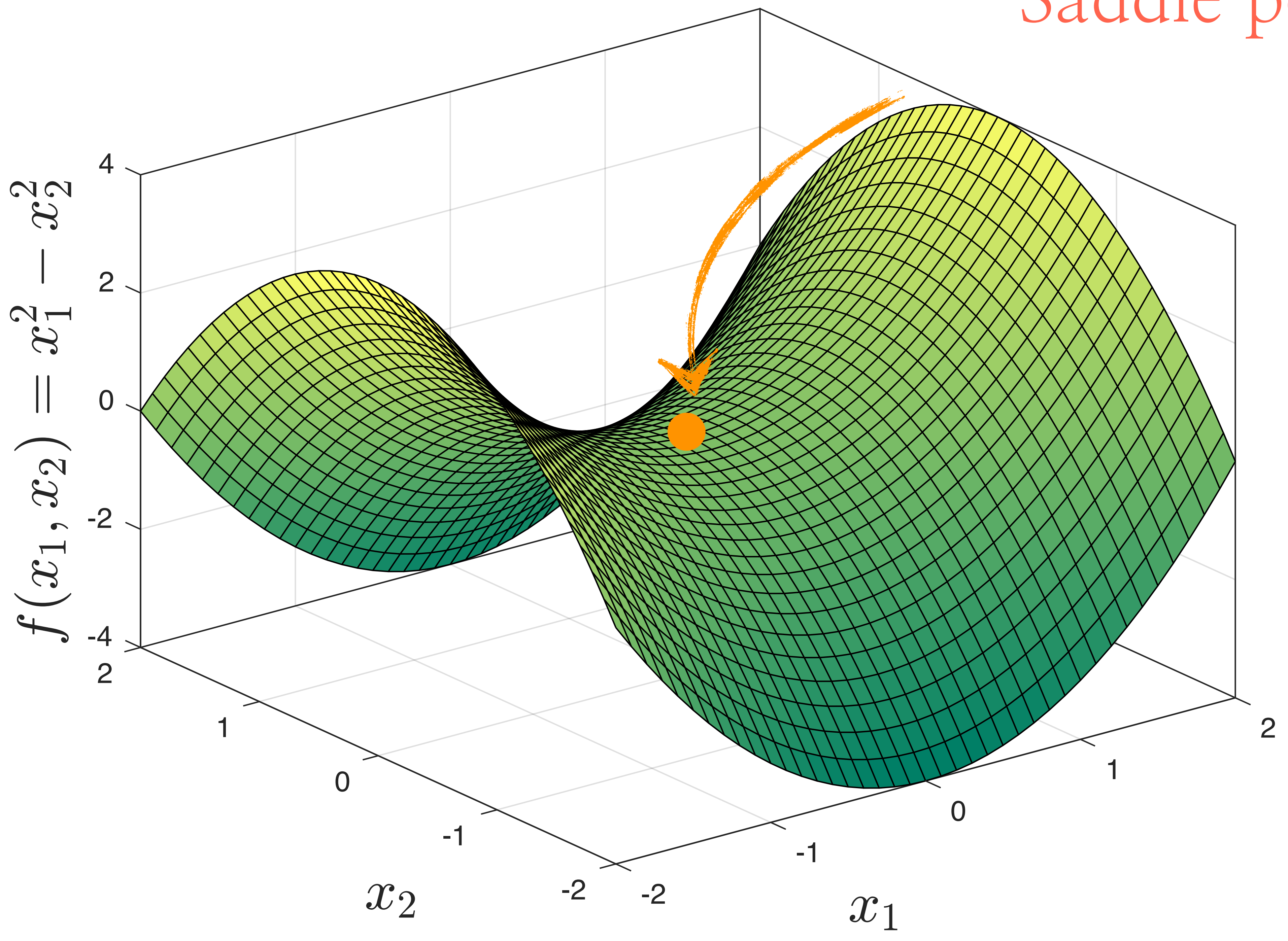

- Compute the Hessian:

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

- Compute the inverse Hessian:

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

Why using vanilla Newton's method might not be a good idea

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

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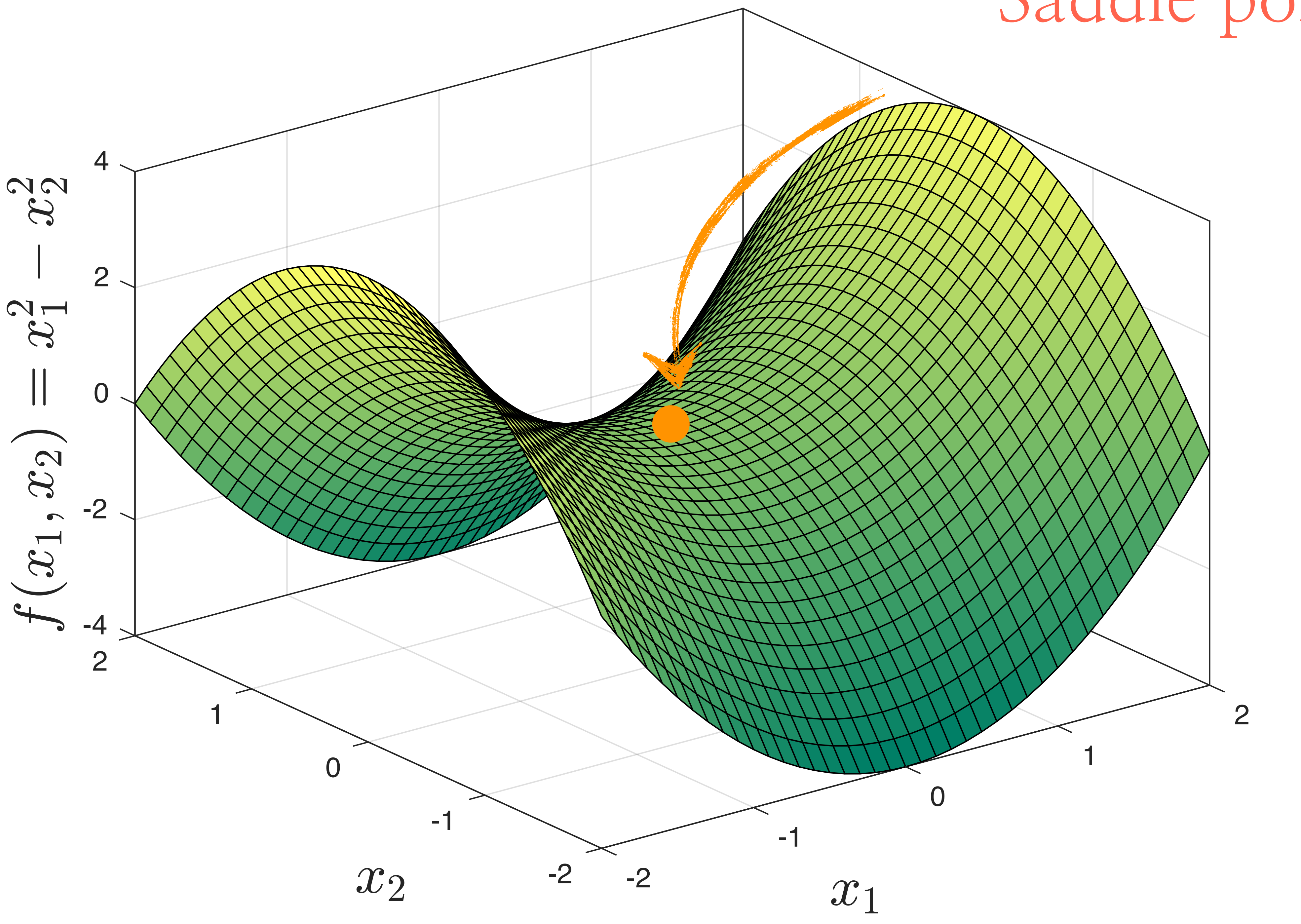

- Let's perform a single Newton iteration:

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

$$= \begin{bmatrix}(x_t)_1 \\ (x_t)_2\end{bmatrix} - \begin{bmatrix}1/2 & 0 \\ 0 & -1/2\end{bmatrix}\begin{bmatrix}2(x_t)_1 \\ 2(x_t)_2\end{bmatrix}$$

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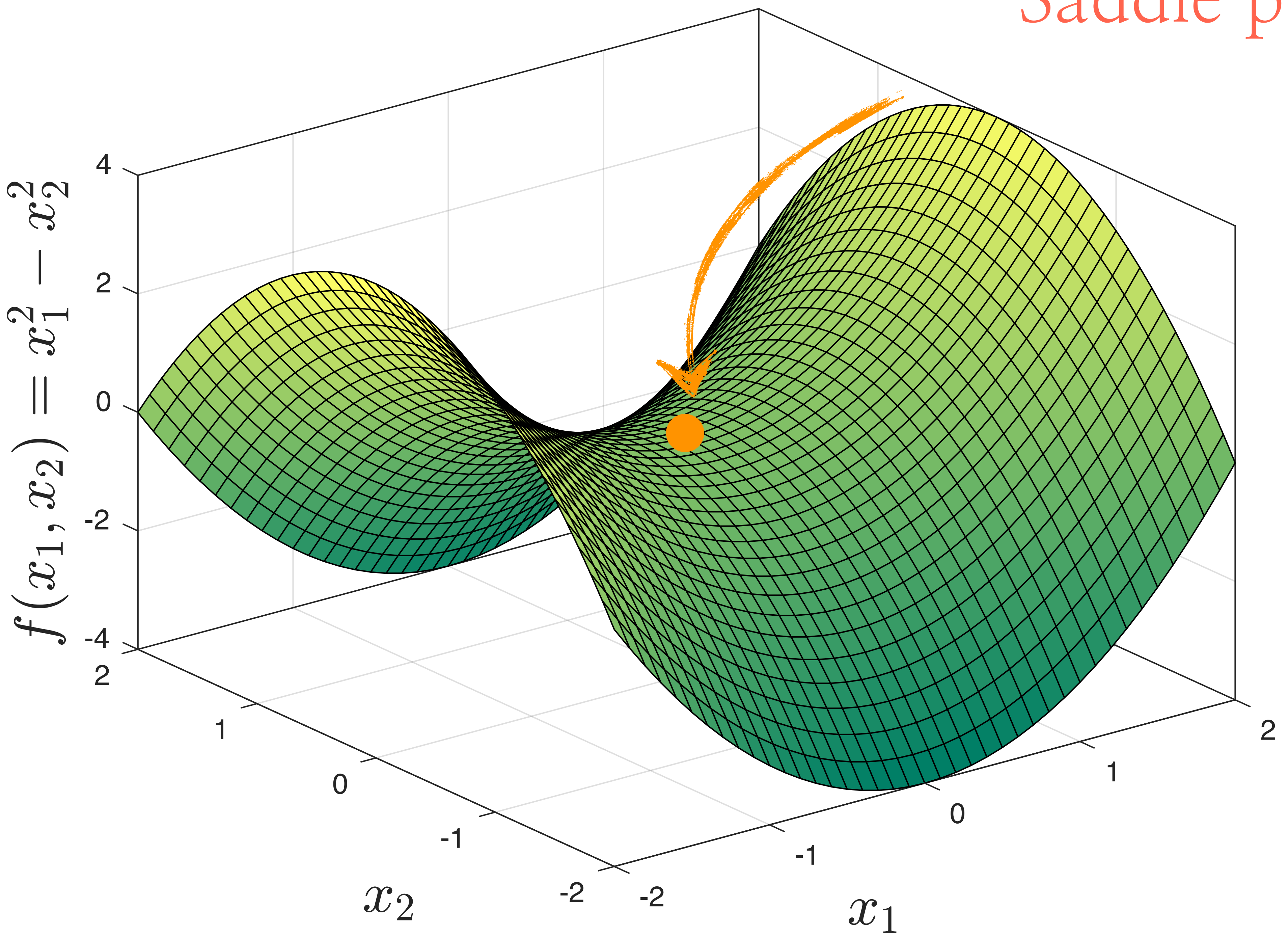

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$$= \begin{bmatrix}(x_t)_1\\(x_t)_2\end{bmatrix} - \begin{bmatrix}(x_t)_1\\(x_t)_2\end{bmatrix} = \begin{bmatrix}0\\0\end{bmatrix}$$

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

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