

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

Lecture 9

Overview

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 - Started talking about non-convex optimization, where non-convexity is introduced by the constraints
 - We consider the special case of sparsity
 - We provide conditions that lead to global convergence guarantees

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 - Started talking about non-convex optimization, where non-convexity is introduced by the constraints
 - We consider the special case of sparsity
 - We provide conditions that lead to global convergence guarantees
- For the next 2–3 lectures, we will consider (possibly) another case of non-convex constraints: **low-rank optimization**
 - We will provide motivation, background and alternative solutions
 - We will see that this structure provides **various ways** to be.. non-convex
 - We will focus on how we can **provably and efficiently solve** such problems

Overview

$$\begin{array}{ll} \min_{x} & f(x) \\ \text{s.t.} & x \in \mathcal{C} \end{array}$$

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s.t.

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$$x \in C$$

We will consider convex objectives..

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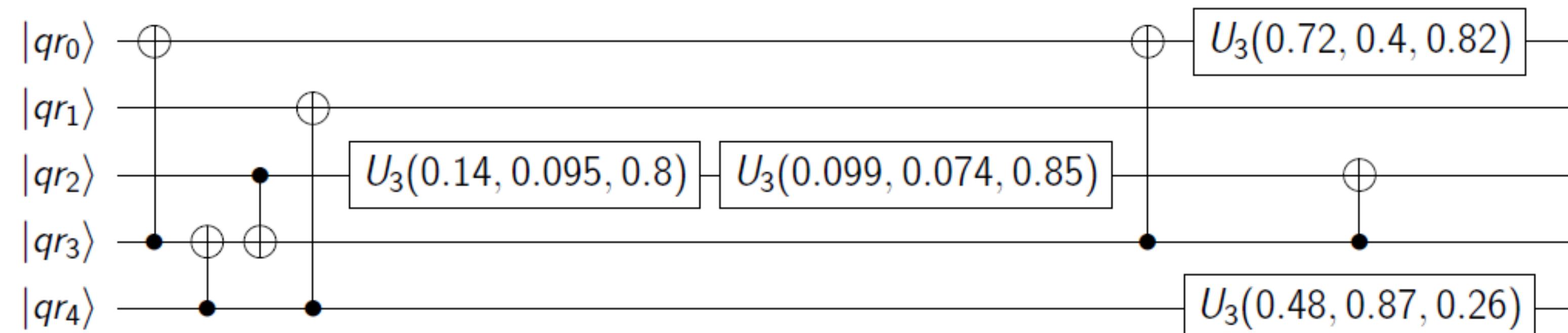
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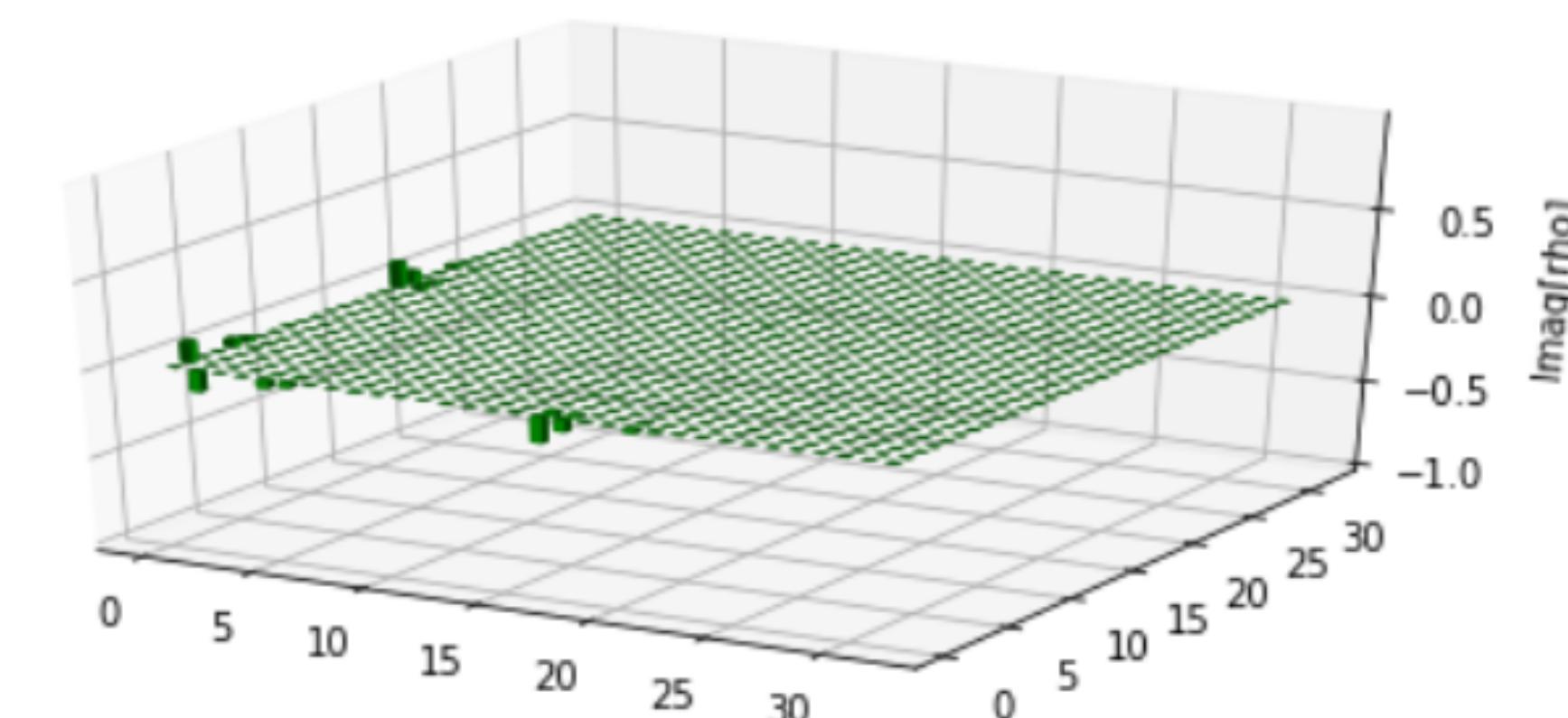
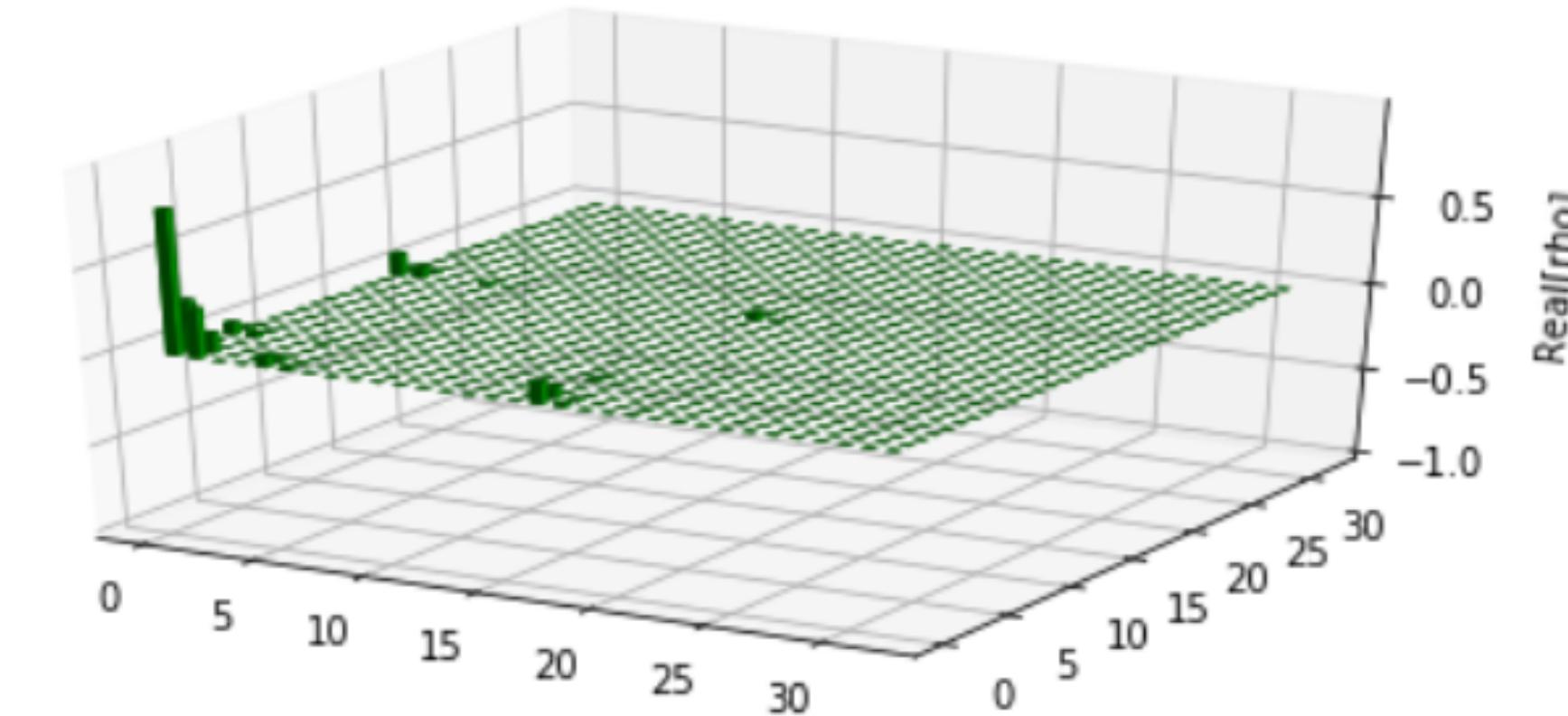
- We will focus on the cases of (structured) sparsity and **low-rankness**
(But I open to other alternatives as we proceed)

Problem setting via an application

IBM

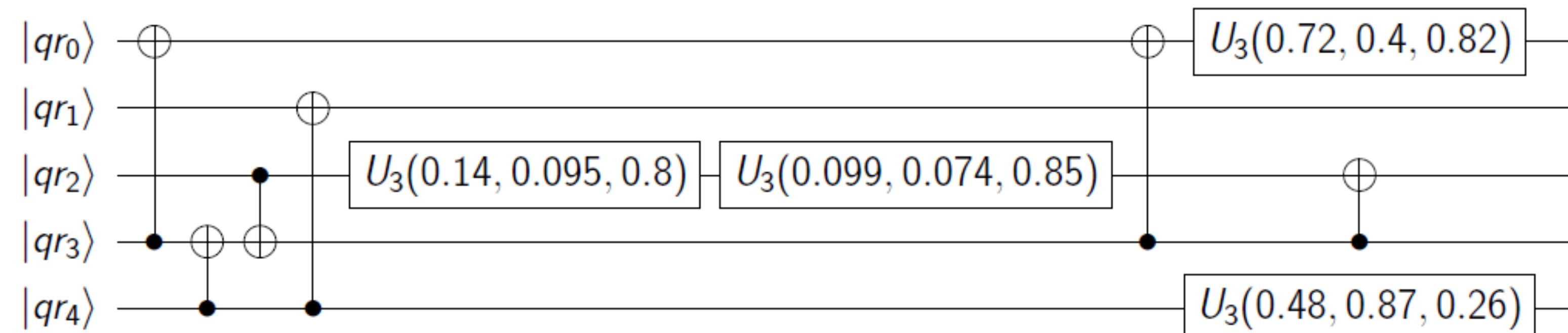


```
OPENQASM 2.0;
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qreg qr[5];
creg cr[5];
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cx qr[4],qr[3];
cx qr[2],qr[3];
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u3(0.139745784966679,0.0948307634768559,0.799402574081021) qr[2];
u3(0.0987633446591477,0.0737424336287251,0.850473826259255) qr[2];
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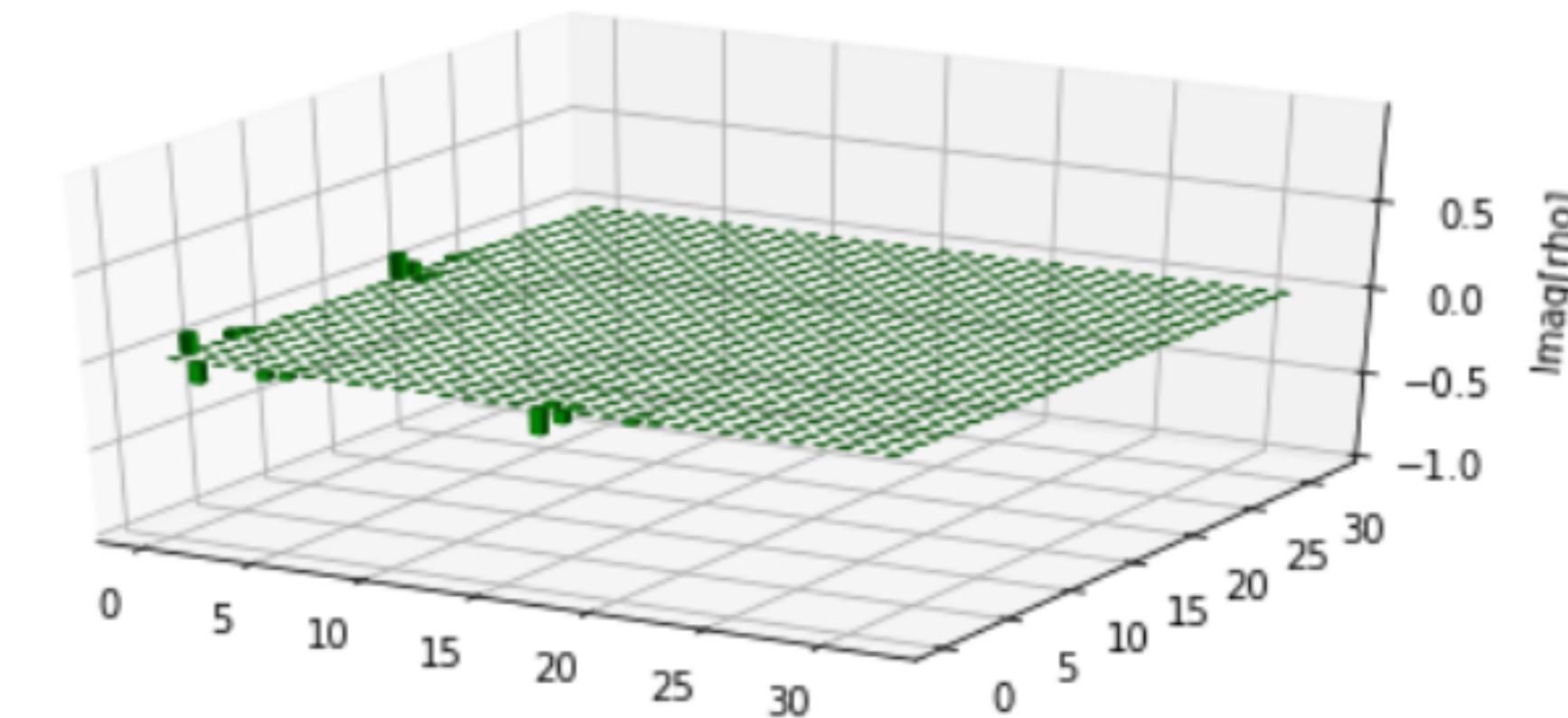
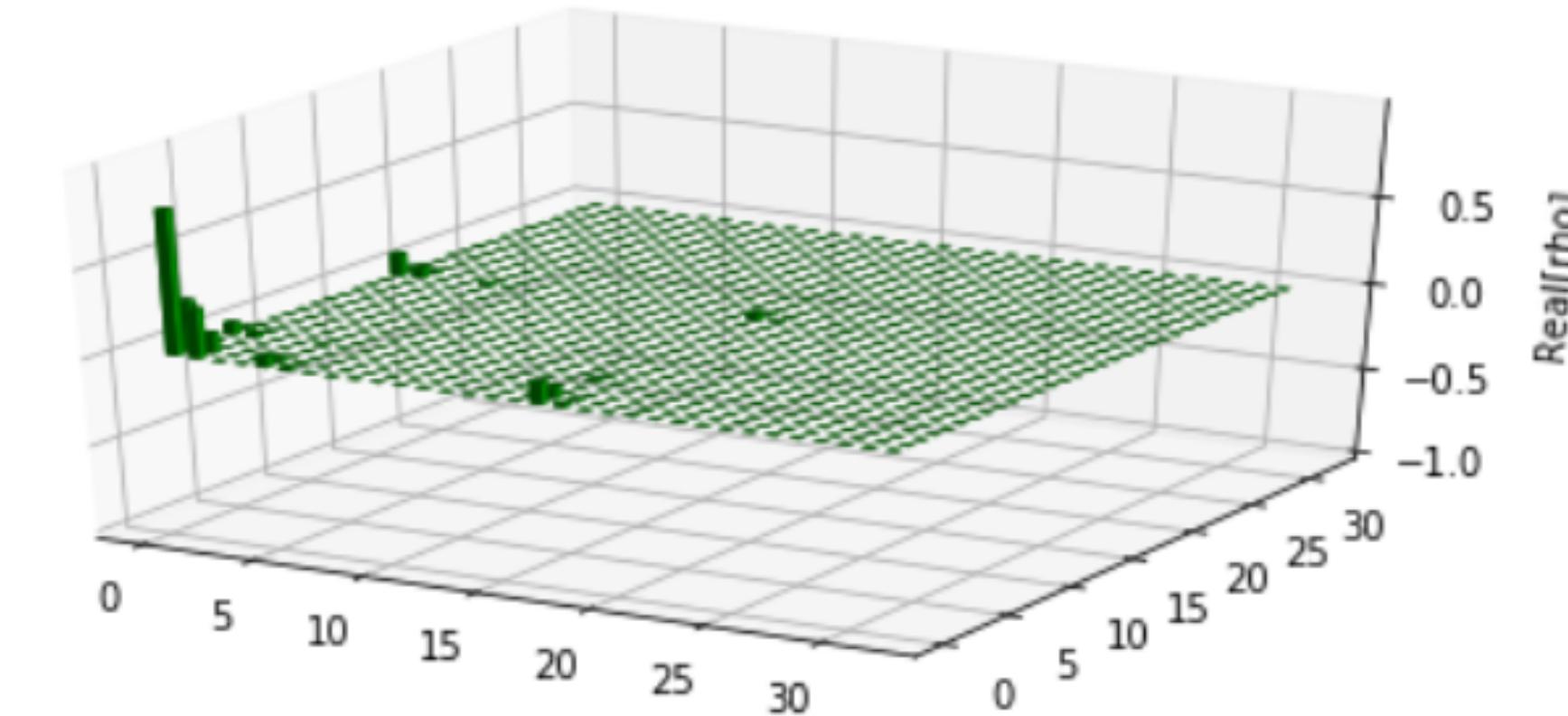
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- Goal: Validate the system is in the expected.. state,
the computations are completed ..as expected



Quantum state tomography

(Much easier than it sounds like..)

- Generative model: $y_i = \langle A_i, X^* \rangle + w_i = \text{Tr}(A_i X^*) + w_i$
 - $A_i \in \mathbb{R}^{p \times p}$: features
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 5. But if we perform the steps "correctly", w.h.p. we measure the anticipated state

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 10. When $q = 20$ or even 50, do the math

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 12. Theoretically, we can assume rank-1 constructed density matrices; noise + other Phenomena increases the rank in practice

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- How do we measure?

1. Select: $A_i = \sigma_{i_1} \otimes \sigma_{i_2} \otimes \cdots \otimes \sigma_{i_q}$, where

$$\sigma_I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

(Pauli operators)

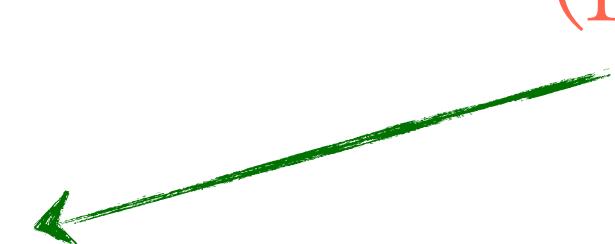


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(Pauli operators)


 2. Applying it to the system is equivalent (for the moment) with

$$y_i = \langle A_i, X^* \rangle + w_i = \text{Tr}(A_i X^*) + w_i$$

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$$\min_{X \in \mathbb{R}^{p \times p}} \frac{1}{2} \sum_{i=1}^n (y_i - \langle A_i, X \rangle)^2$$

s.t.

$$X \succeq 0, \quad \text{Tr}(X) \leq 1$$

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- X has $O(4^q)$ parameters
- This means that we need that many measurements

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s.t. $X \succeq 0, \text{Tr}(X) \leq 1, \text{rank}(X) \leq r$

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s.t.

$$X \succeq 0, \text{Tr}(X) \leq 1, \text{rank}(X) \leq r$$

- X has $O(2^q r)$ parameters
- If rank is small compared to ambient dimension, then there is hope

Quantum state tomography

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$$\begin{aligned} \min_{X \in \mathbb{R}^{p \times p}} \quad & \frac{1}{2} \sum_{i=1}^n (y_i - \langle A_i, X \rangle)^2 \\ \text{s.t.} \quad & X \succeq 0, \text{Tr}(X) \leq 1, \text{rank}(X) \leq r \end{aligned}$$

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- Can we recover $X^* \in \mathbb{R}^{p \times p}$ from limited set of measurements?

RIP for Pauli operators

$$(1 - \delta) \|X\|_F^2 \leq \|\mathcal{A}(X)\|_2^2 \leq (1 + \delta) \|X\|_F^2, \quad \forall \text{ rank-}r X \in \mathbb{R}^{p \times p}$$
$$[\mathcal{A}(X)]_i = \text{Tr}(A_i, X)$$

(RIP also holds for (sub-)Gaussian matrices,
Fourier, etc.)

- Similar to the sparsity case, RIP leads to convergence for various algos

Matrix sensing

(without the trace and PSD constraints)

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(Pros & Cons?)

- Definition of the **nuclear norm**: $\|X\|_* = \sum_{i=1}^p \sigma_i(X)$

(Requires full SVD for its calculation)

Matrix sensing

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Hard-thresholding

- Definition of the projection onto low-rank matrices

$$\begin{aligned} \widehat{X} \in \min_X \quad & \frac{1}{2} \|X - Y\|_F^2 \\ \text{s.t.} \quad & \text{rank}(X) \leq r \end{aligned}$$

(Requires truncated SVD
for its calculation)

But before we proceed..

- Some questions:

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- Q: "Why then do we have hopes solving this problem?"
- A: "Similar to sparsity, under assumptions on average this problem can be solved in polynomial time"

Iterative hard thresholding (IHT)

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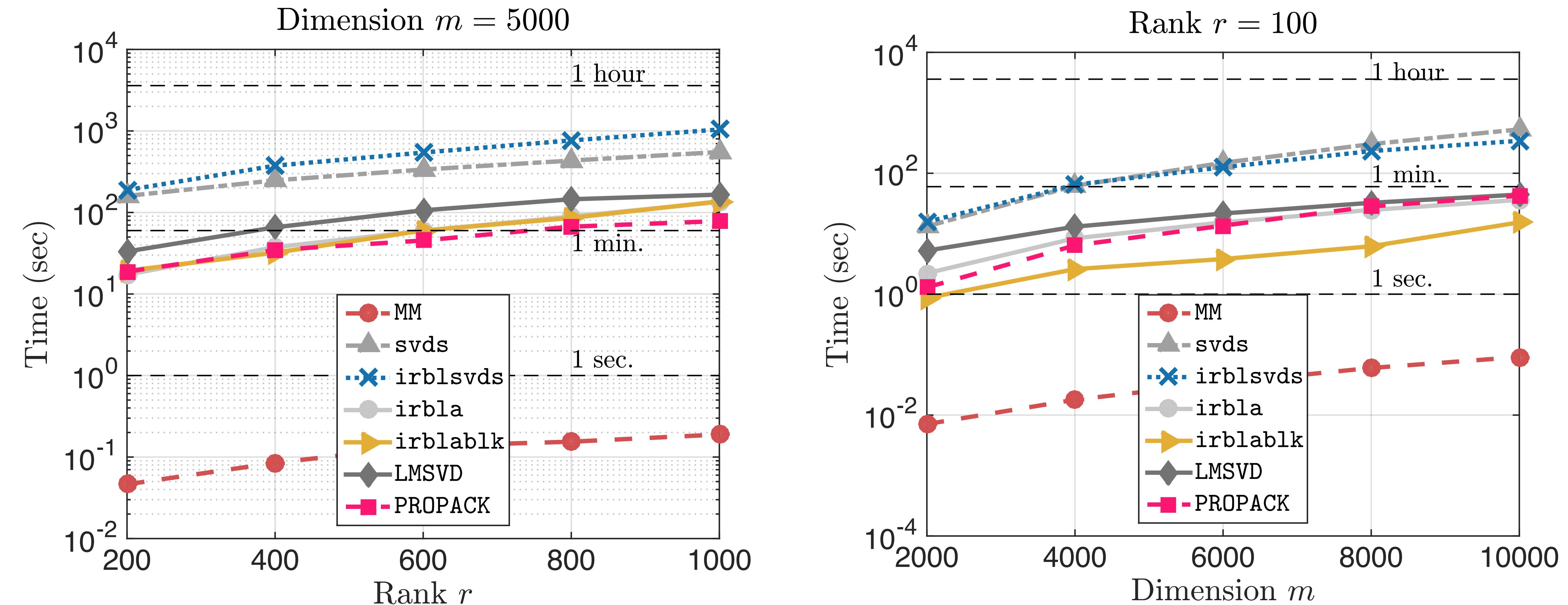
where $H_r(Z) \in \min_{X \in \mathbb{R}^{p \times p}} \|X - Z\|_F^2$ (Have we seen this before?)
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Convexification vs. hard-thresholding in practice

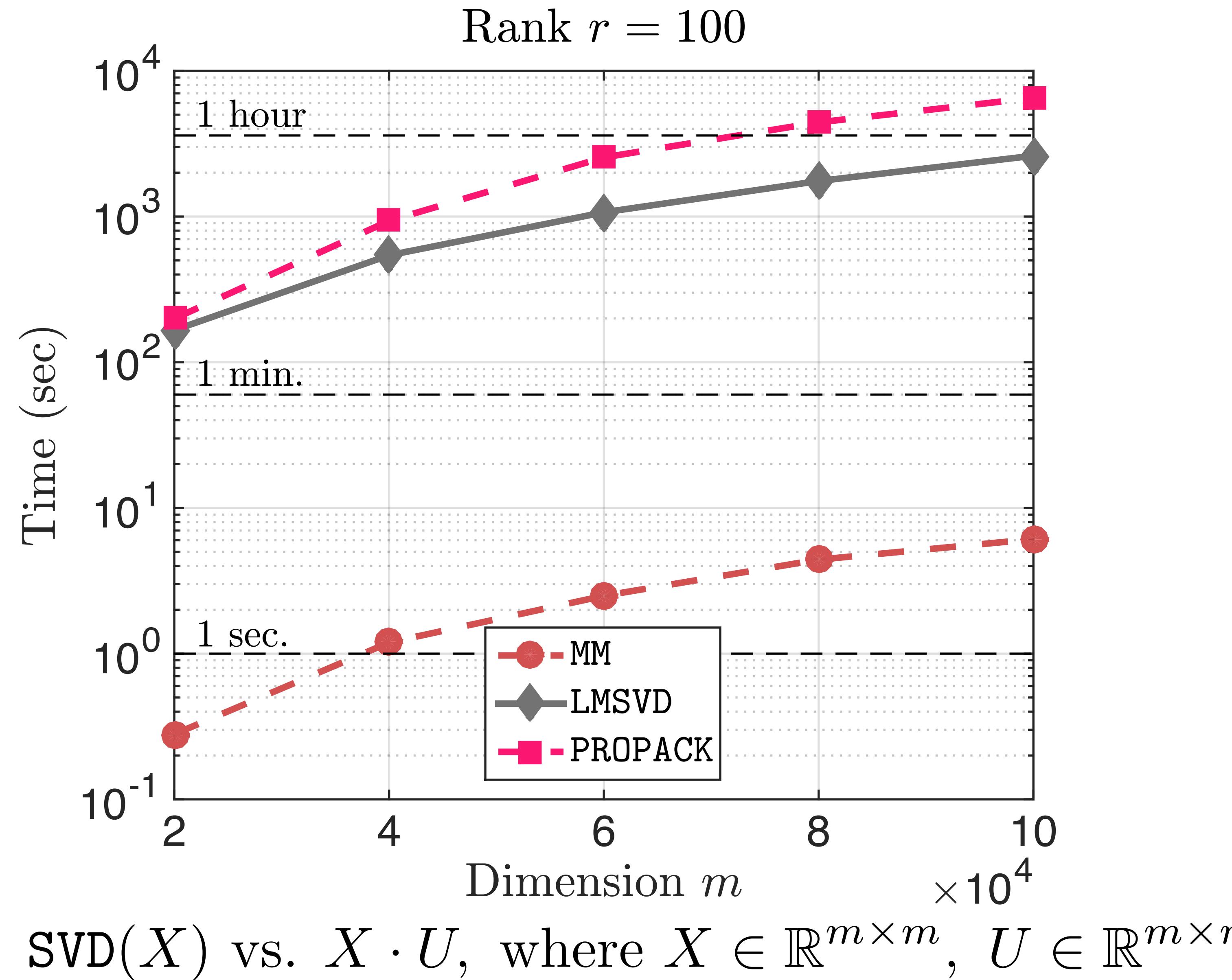
Demo

The price of SVD



$\text{SVD}(X)$ vs. $X \cdot U$, where $X \in \mathbb{R}^{m \times m}$, $U \in \mathbb{R}^{m \times r}$

The price of SVD



$$X = UV^\top$$

Non-PSD

$$X \in \mathbb{R}^{n \times p}$$

$$U \in \mathbb{R}^{n \times r}$$

$$V \in \mathbb{R}^{p \times r}$$

PSD

$$X \in \mathbb{R}^{n \times n}$$

$$U = V \in \mathbb{R}^{n \times r}$$

First consider a simpler objective: Rank-1 PCA

Whiteboard

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Despite this, such convergence results are called **local convergence guarantees**

First consider a simpler objective: Rank-1 PCA

- Some properties of the proof:
 - Initialization does matter: e.g., for PCA there are initializations that do not lead to convergence
(More to come later on)
 - After proper initialization, one can prove convergence to global minimum. Despite this, such convergence results are called **local convergence guarantees**
 - Often the theory dictates how to set the step size, in order to obtain convergence. For some cases it is a range of values, in other cases we just rely on a specific step size.

Back to matrix sensing

$$\begin{aligned} \min_{X \in \mathbb{R}^{p \times p}} \quad & \frac{1}{2} \sum_{i=1}^n (y_i - \langle A_i, X \rangle)^2 \\ \text{s.t.} \quad & \text{rank}(X) \leq r \end{aligned}$$

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s.t.

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Non-convex!

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- Key differences with PCA:
 - Number of observations less than number of parameters
 - Mapping is identity, but satisfies a restricted isometry property

The same story holds for more general functions

$$\min_{\begin{array}{l} X \in \mathbb{R}^{m \times n} \\ \text{rank}(X) \leq r \end{array}} f(X)$$

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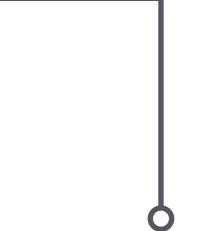
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- Key differences with matrix sensing:
 - Restricted isometry might be substituted by restricted strong cvx/smoothness
 - Restricted strong convexity might not hold

How would we solve this problem?

$$U_{i+1} = U_i - \eta \nabla f(U_i V_i^\top) \cdot V_i$$

$$V_{i+1} = V_i - \eta \nabla f(U_i V_i^\top)^\top \cdot U_i$$

How would we solve this problem?

$$U_{i+1} = U_i - \underbrace{\eta \nabla f(U_i V_i^\top)}_{\text{Gradient of } f \text{ w.r.t. } U} \cdot V_i$$

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Gradient of f w.r.t. V

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Select initial point

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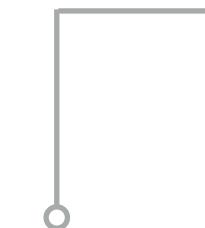
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Select step size

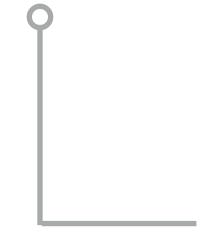
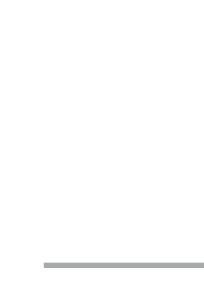


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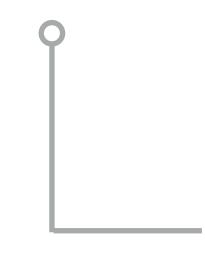
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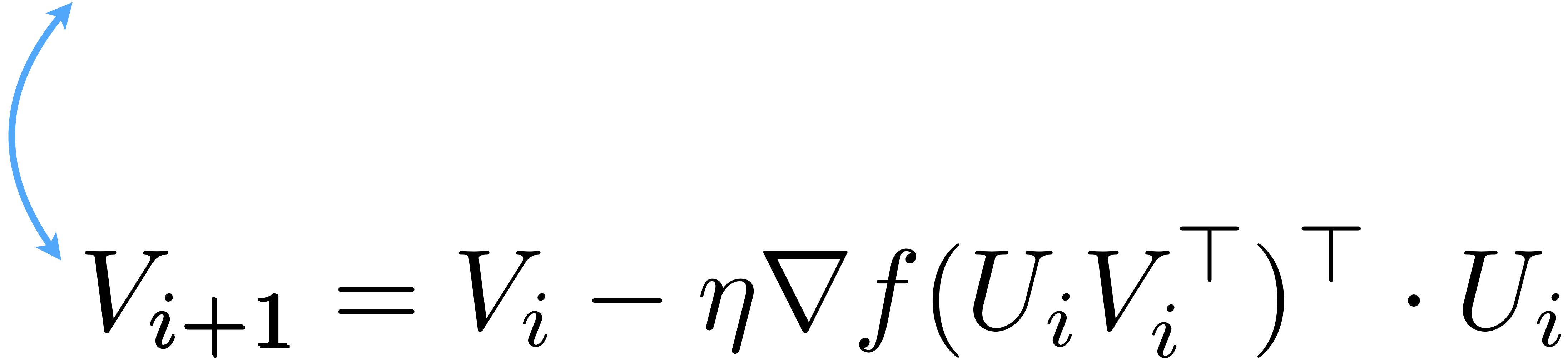
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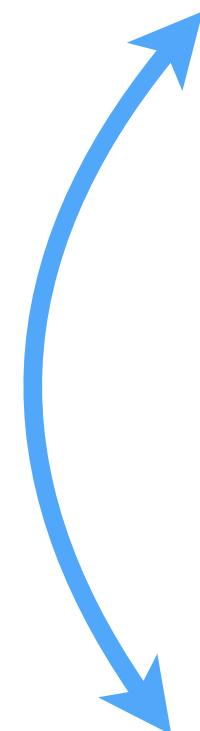
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How to initialize in practice (U_0, V_0) ?

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for all R such that $RR^\top = I$

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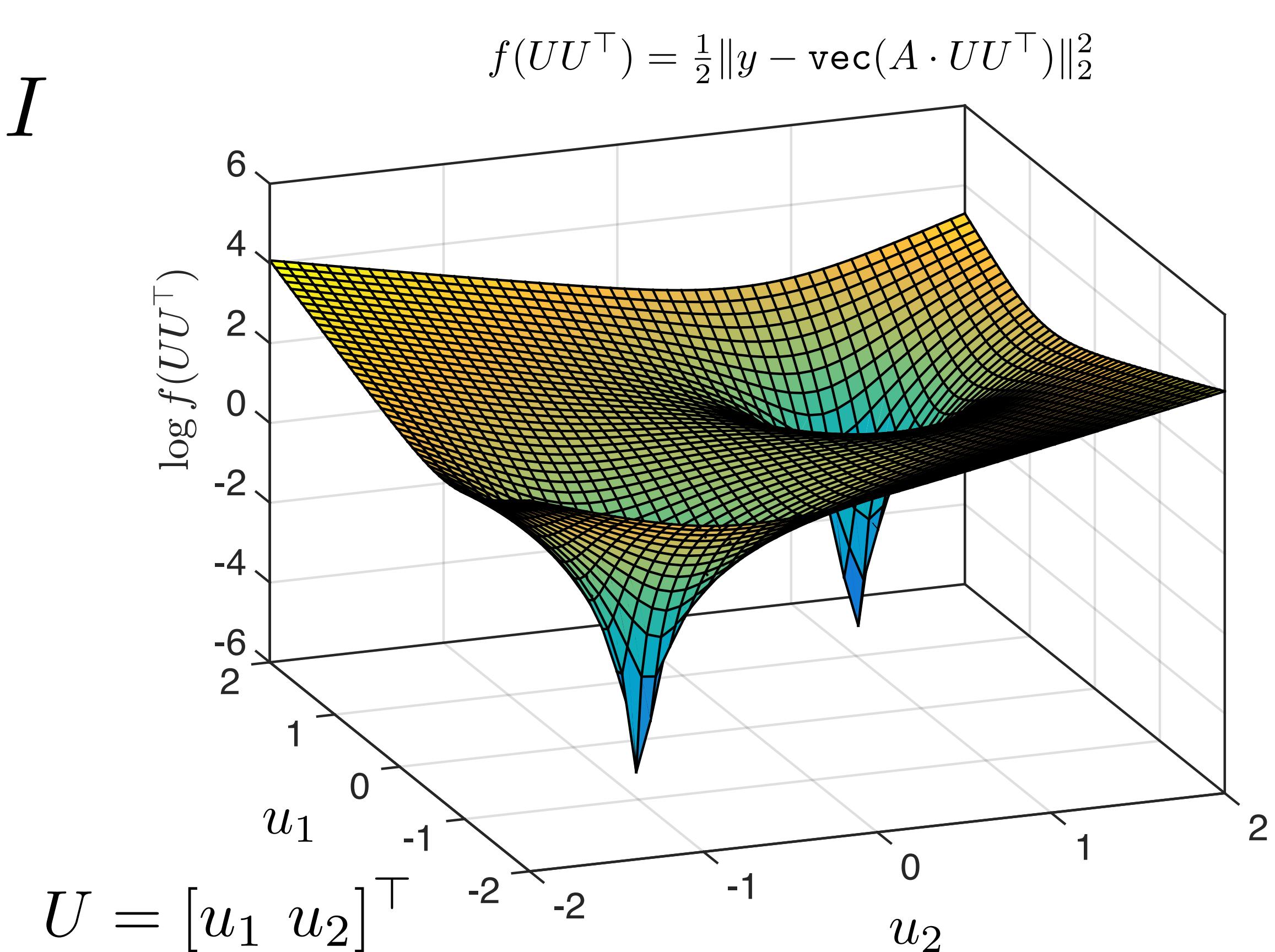
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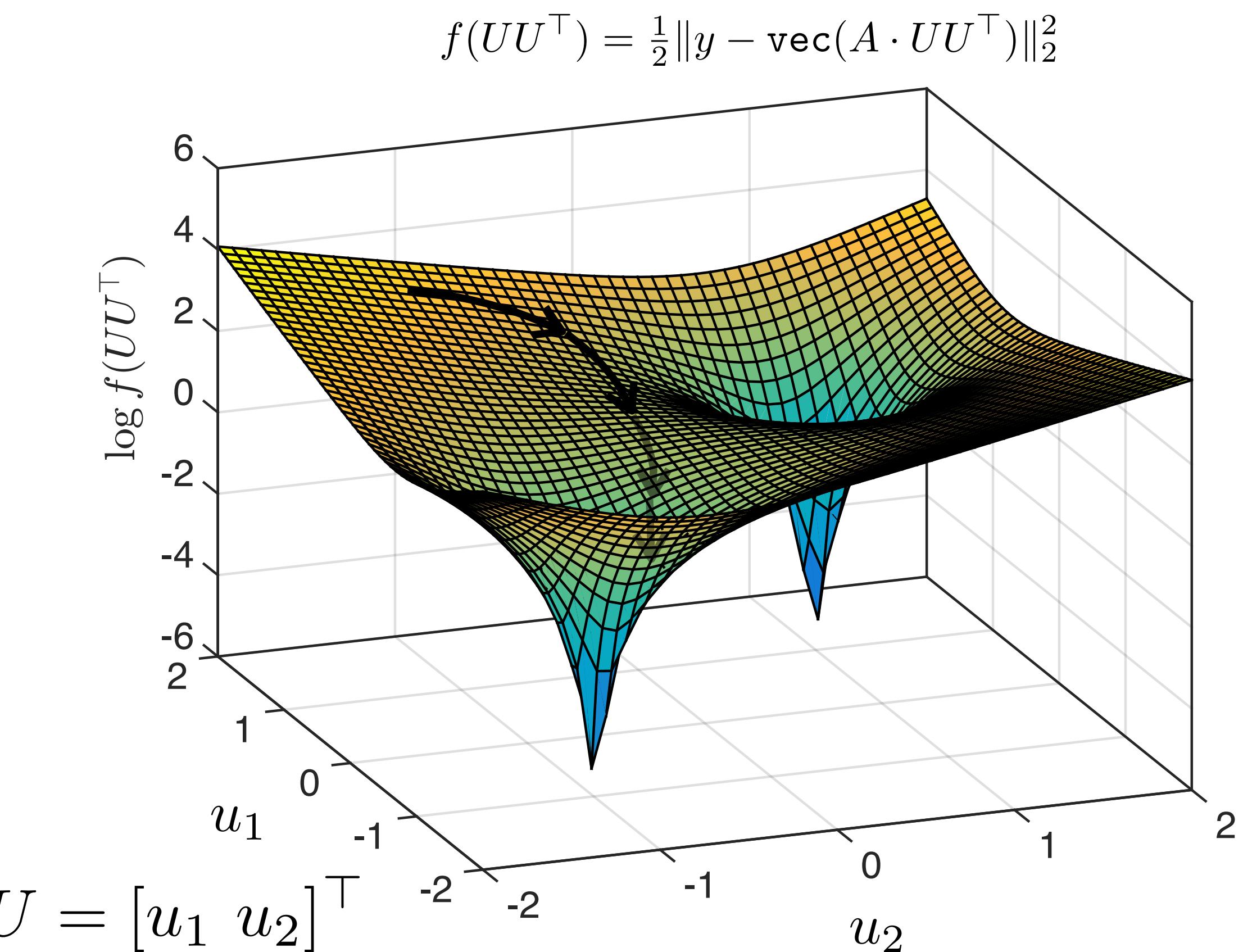
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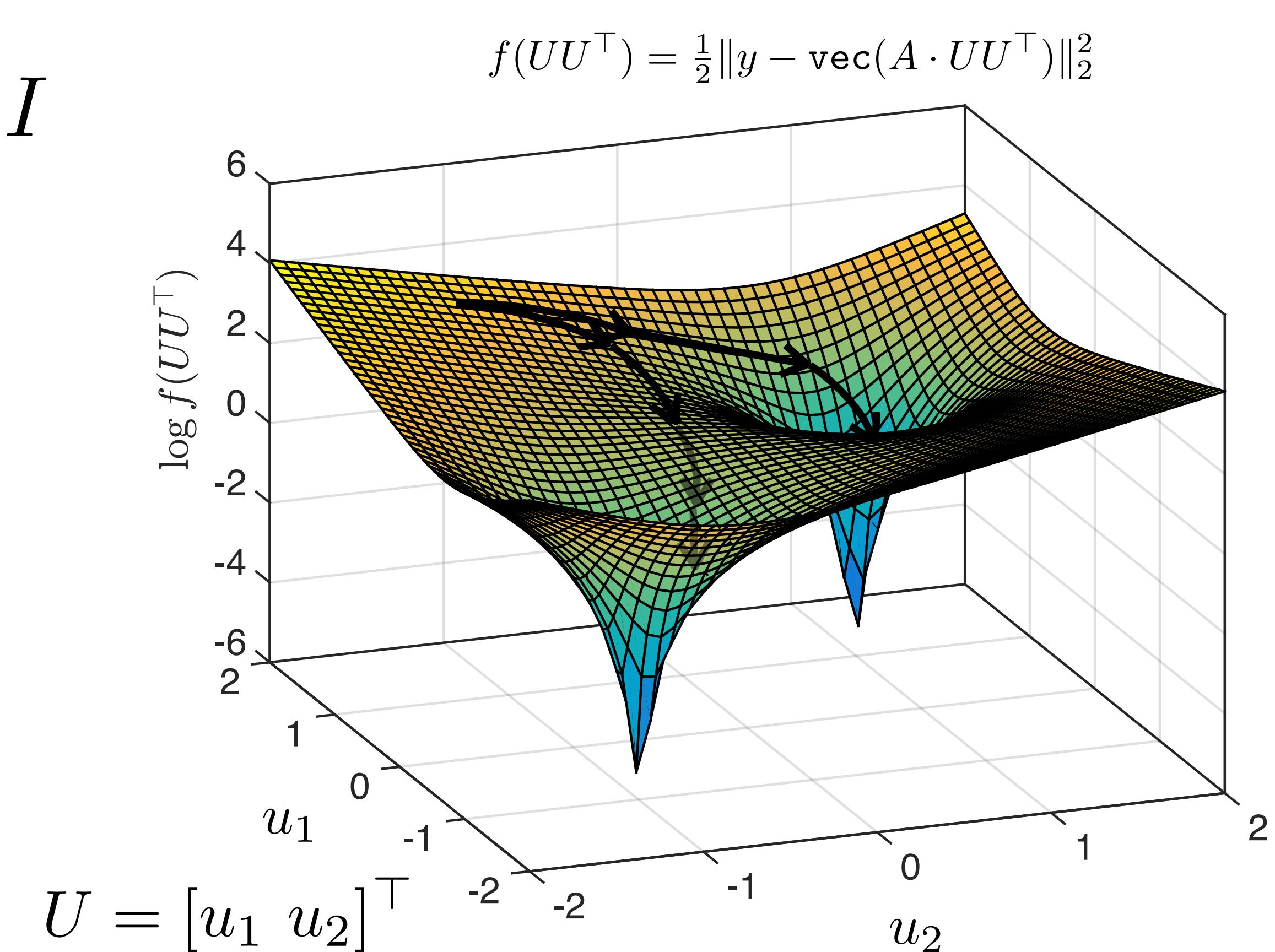
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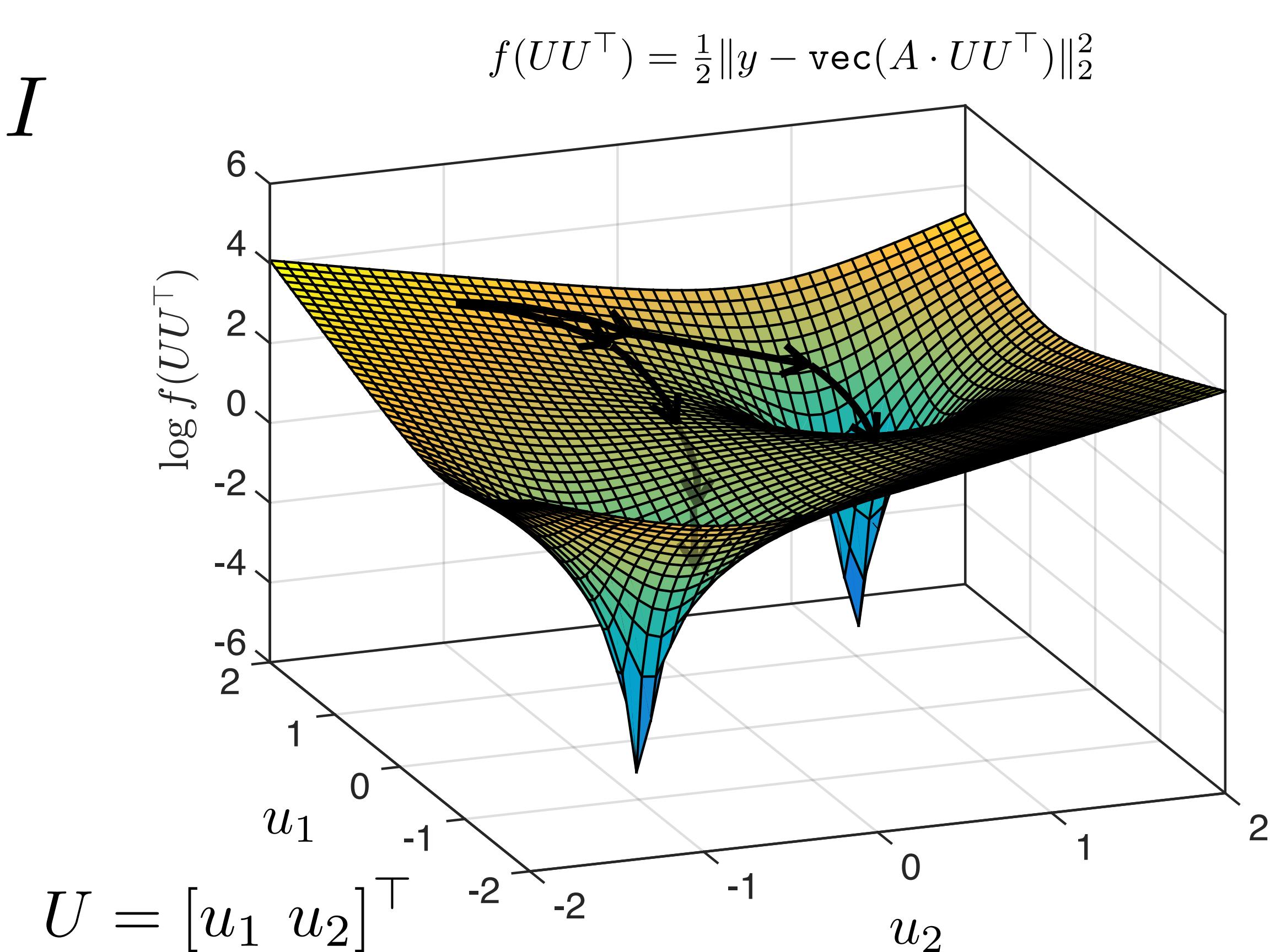
- Example:

- $X \mapsto UV^\top$ “ruins” convexity

where $X^* = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$ Unique!
 $(r=1)$

- Even local convergence results are important
In this case

$$U^* = [1 \ 1]^\top \text{ or } [-1 \ -1]^\top$$



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- Example: **Weighted low-rank approximation**

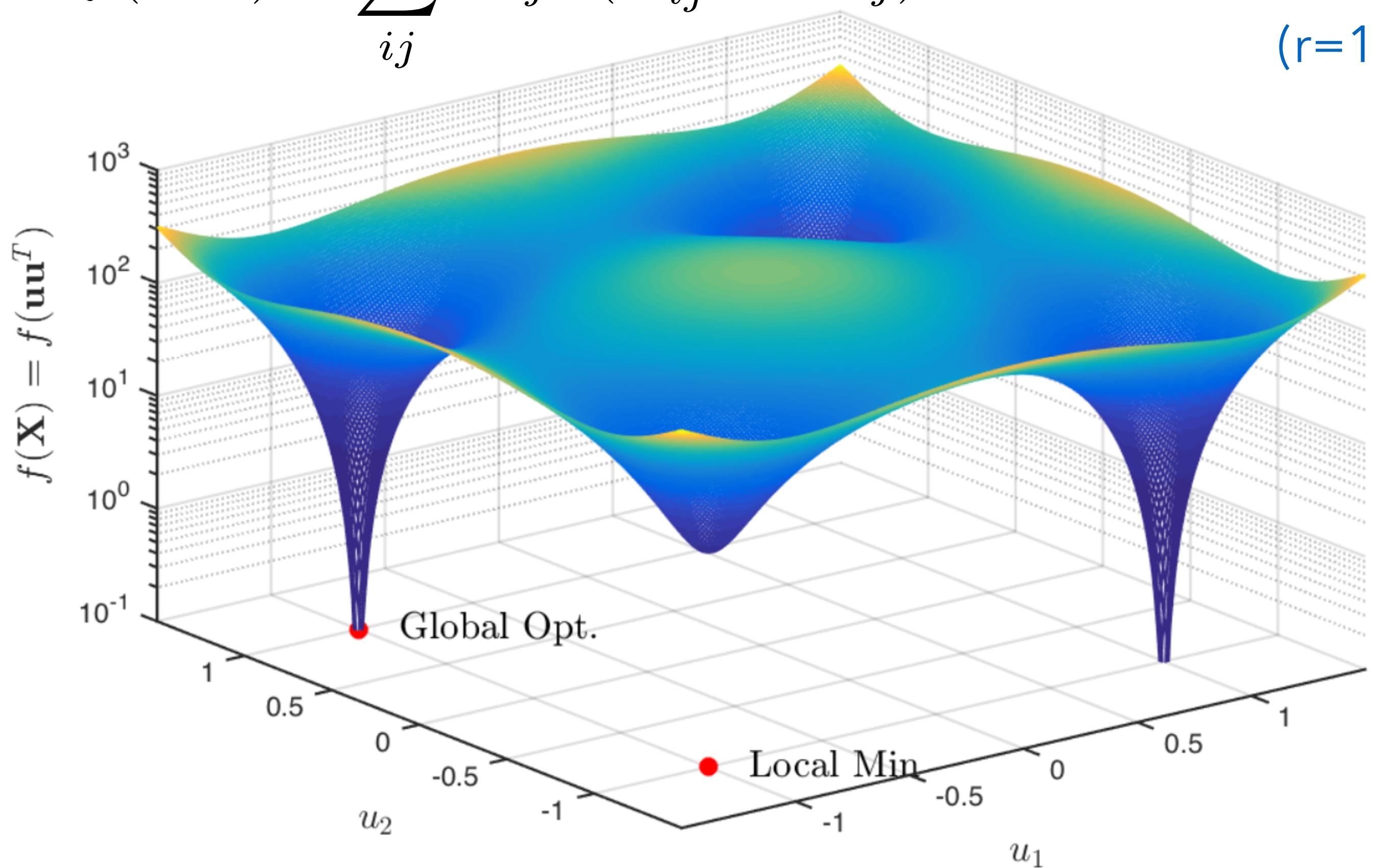
$$f(uu^\top) = \sum_{ij} W_{ij} \cdot (X_{ij}^* - u_i u_j) \quad \text{where} \quad X^* = \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \quad \text{and} \quad W = \begin{bmatrix} 100 & 1 \\ 1 & 100 \end{bmatrix}$$

$(r=1)$

What about local minima?

- Factorization might also introduce local minima
- Example: **Weighted low-rank approximation**

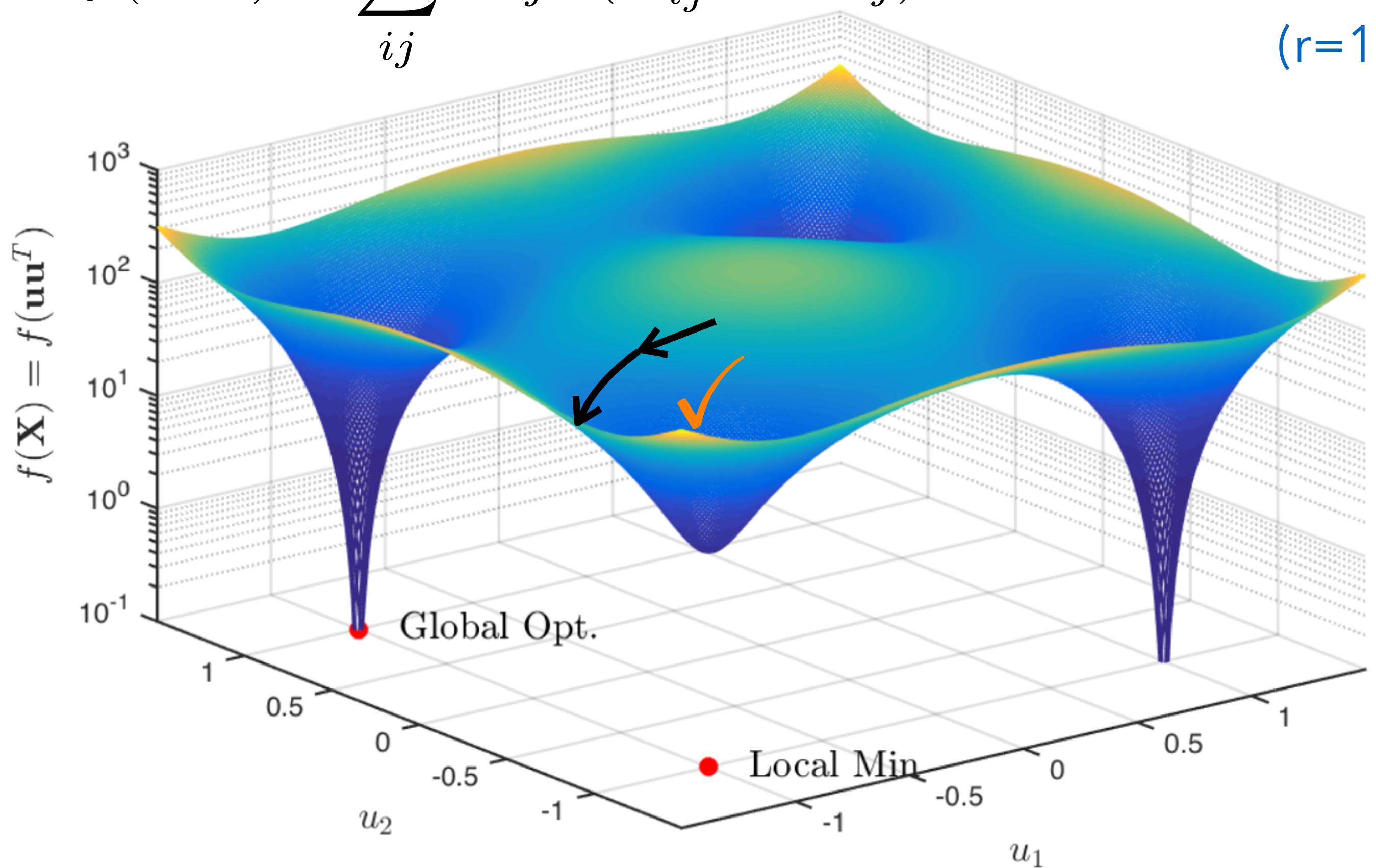
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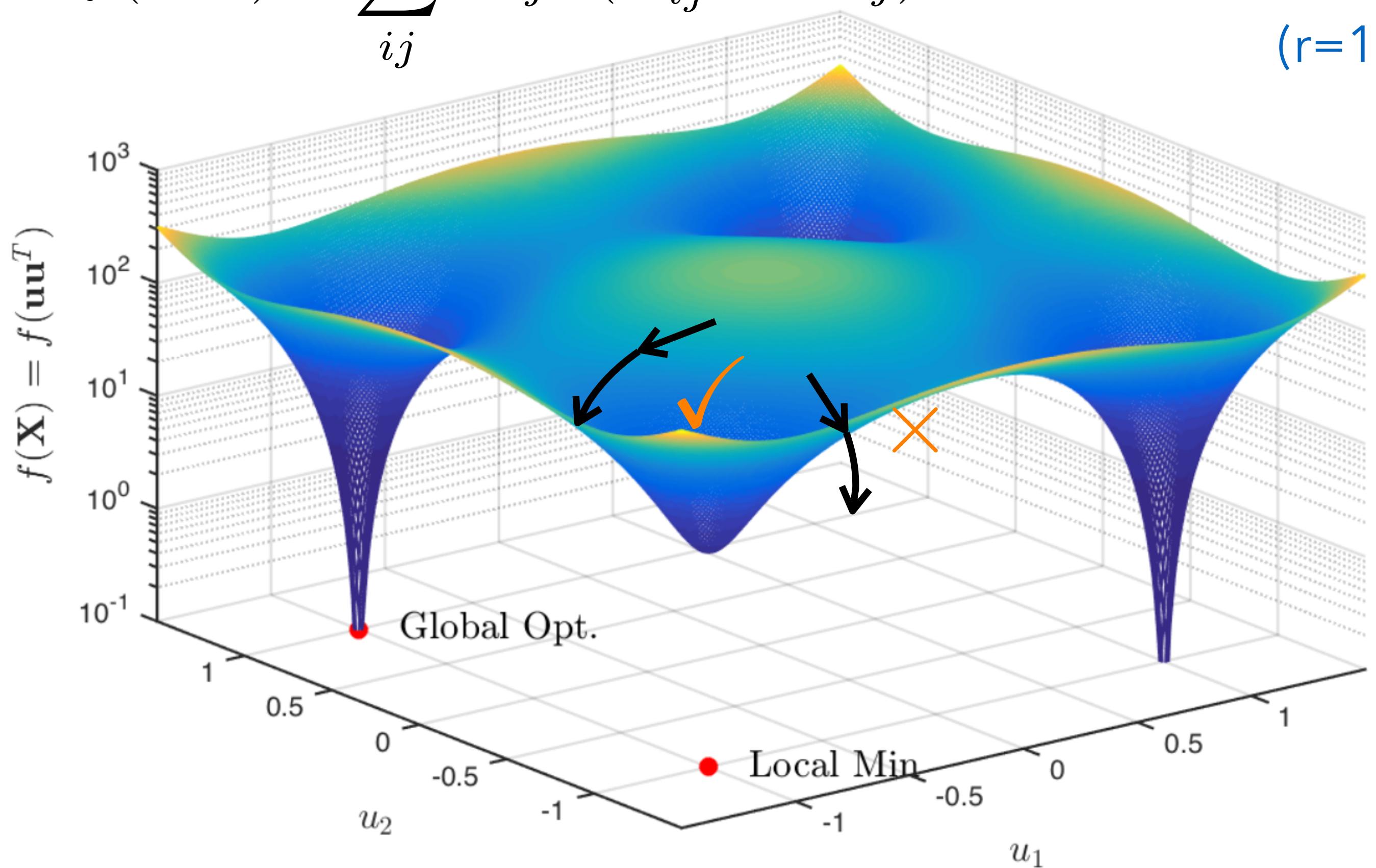
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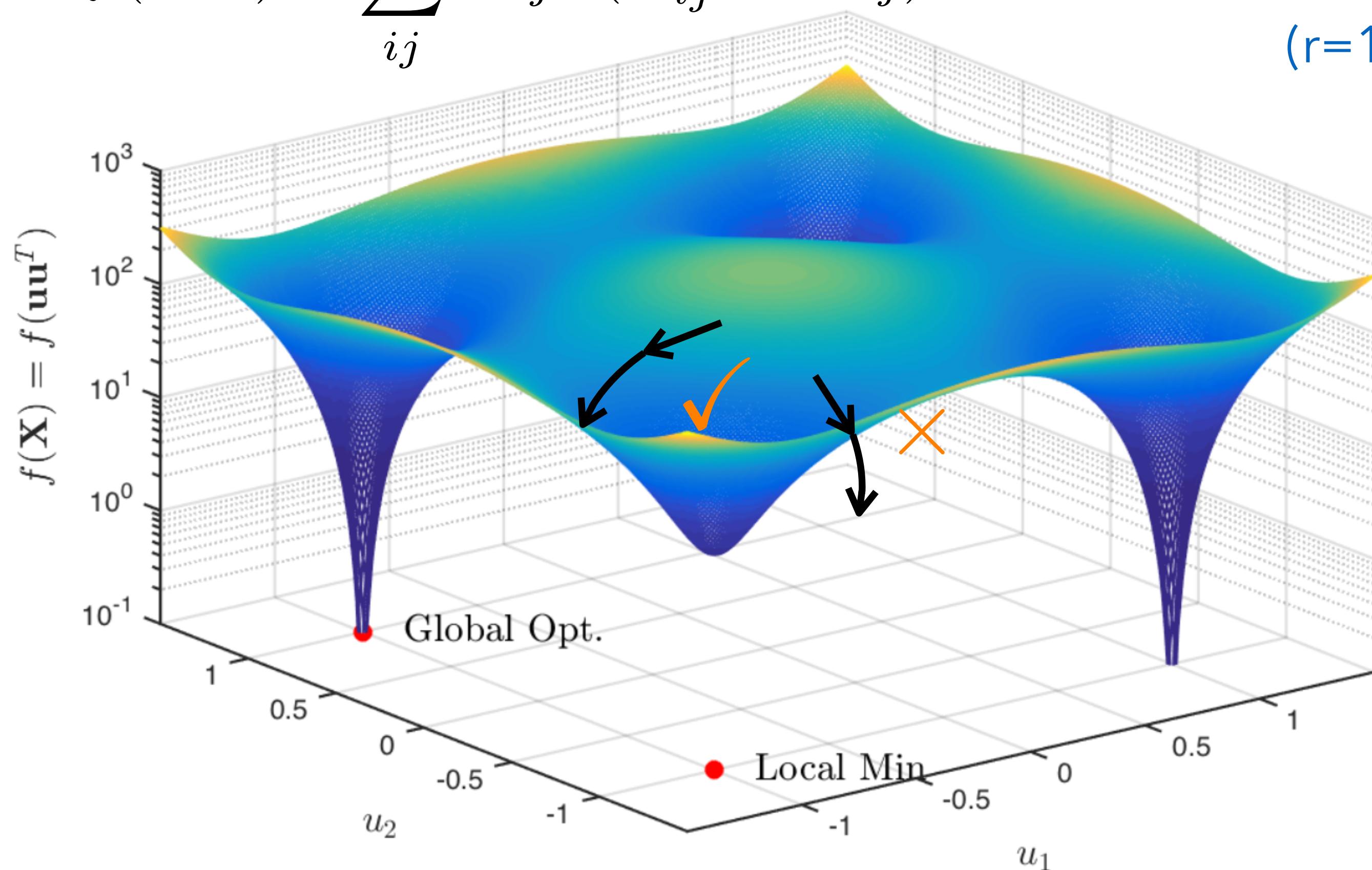
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- ⦿ Even simple objectives can be hard to handle
- ⦿ Proper initialization is key

Nevertheless, can we hope for some guarantees?

- General recipe

norm: abuse of notation to indicate a general class of distance functions

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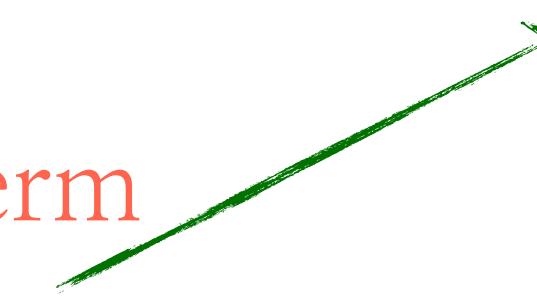
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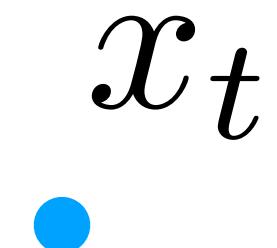
- Where can we actively intervene? By choosing appropriate step size!

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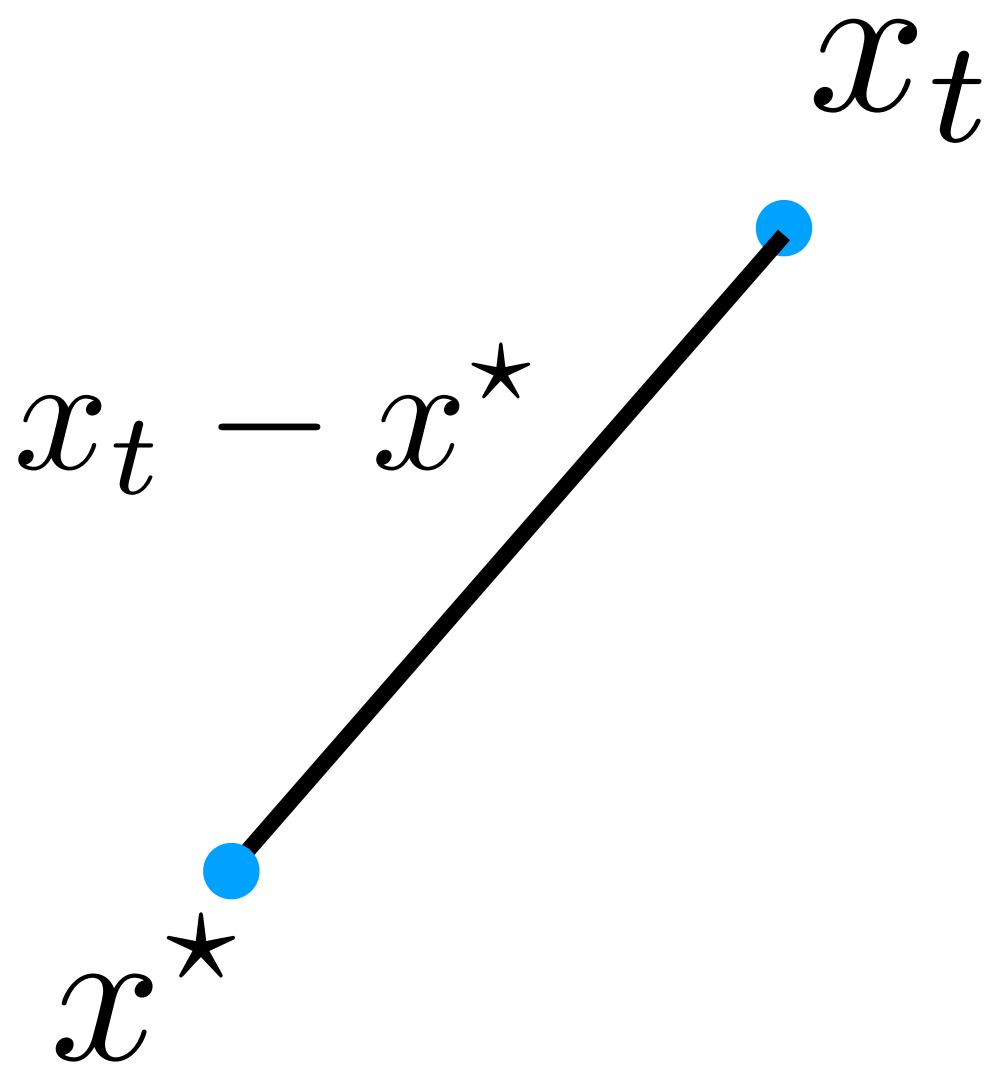
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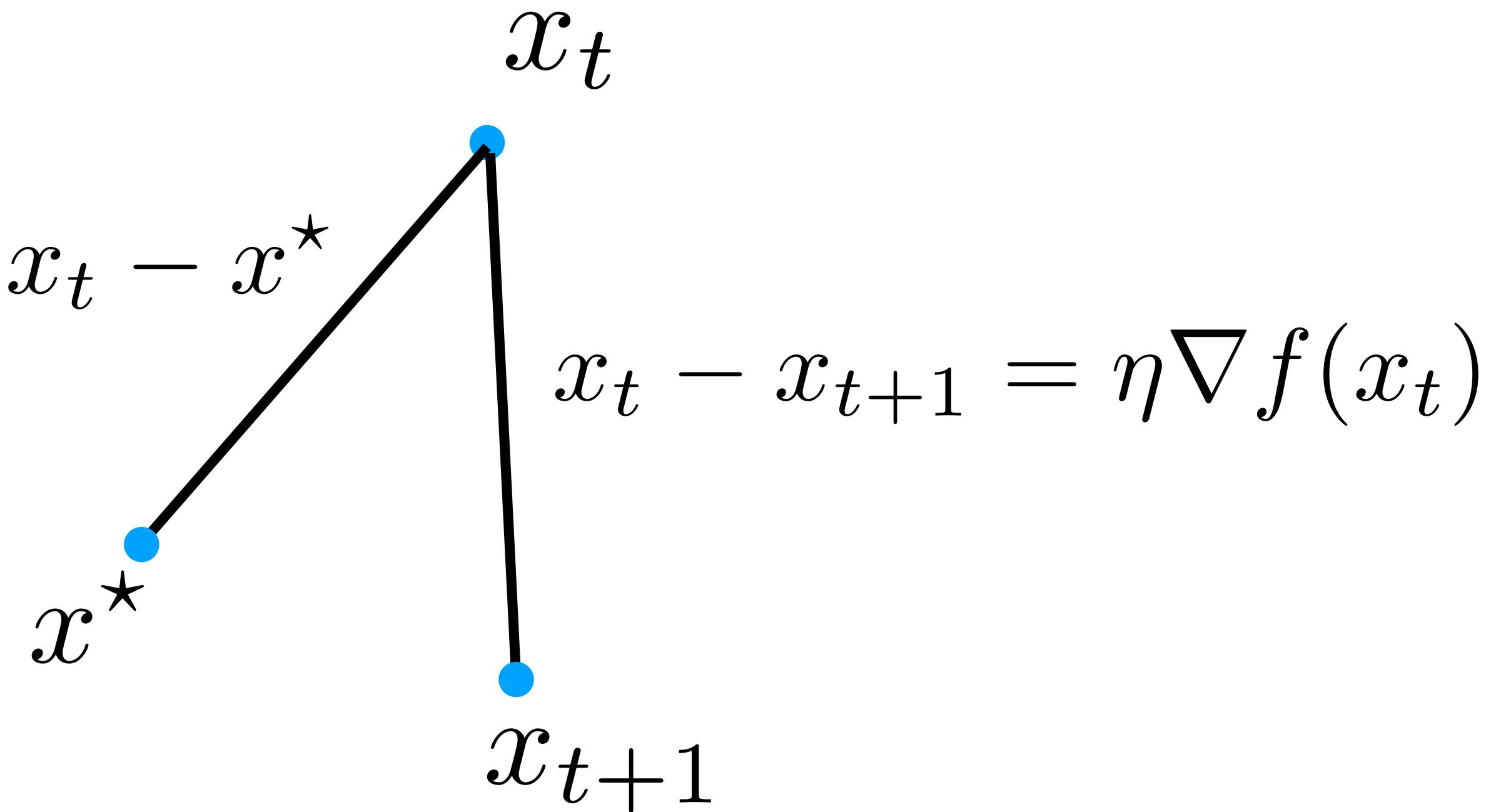
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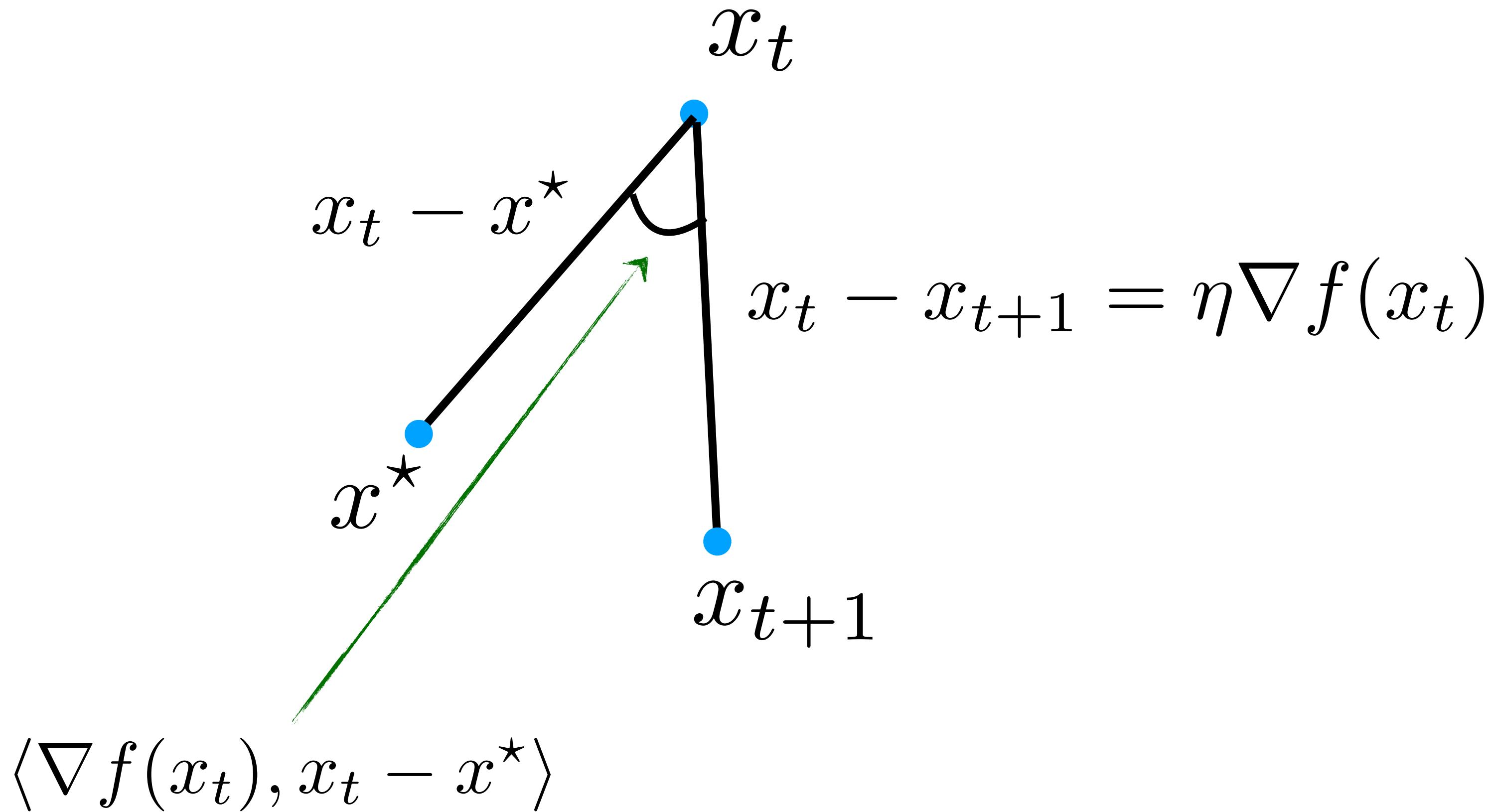
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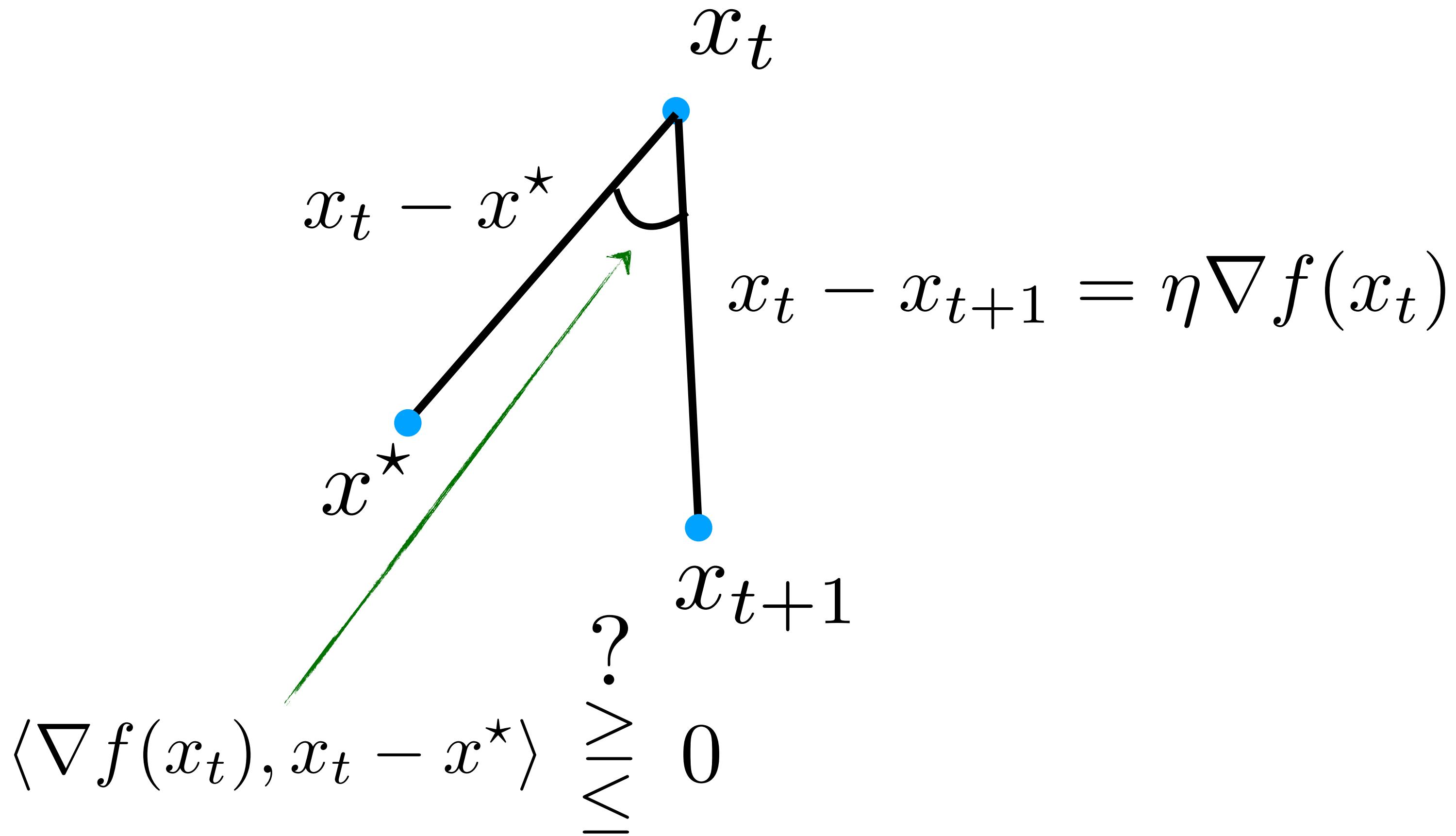
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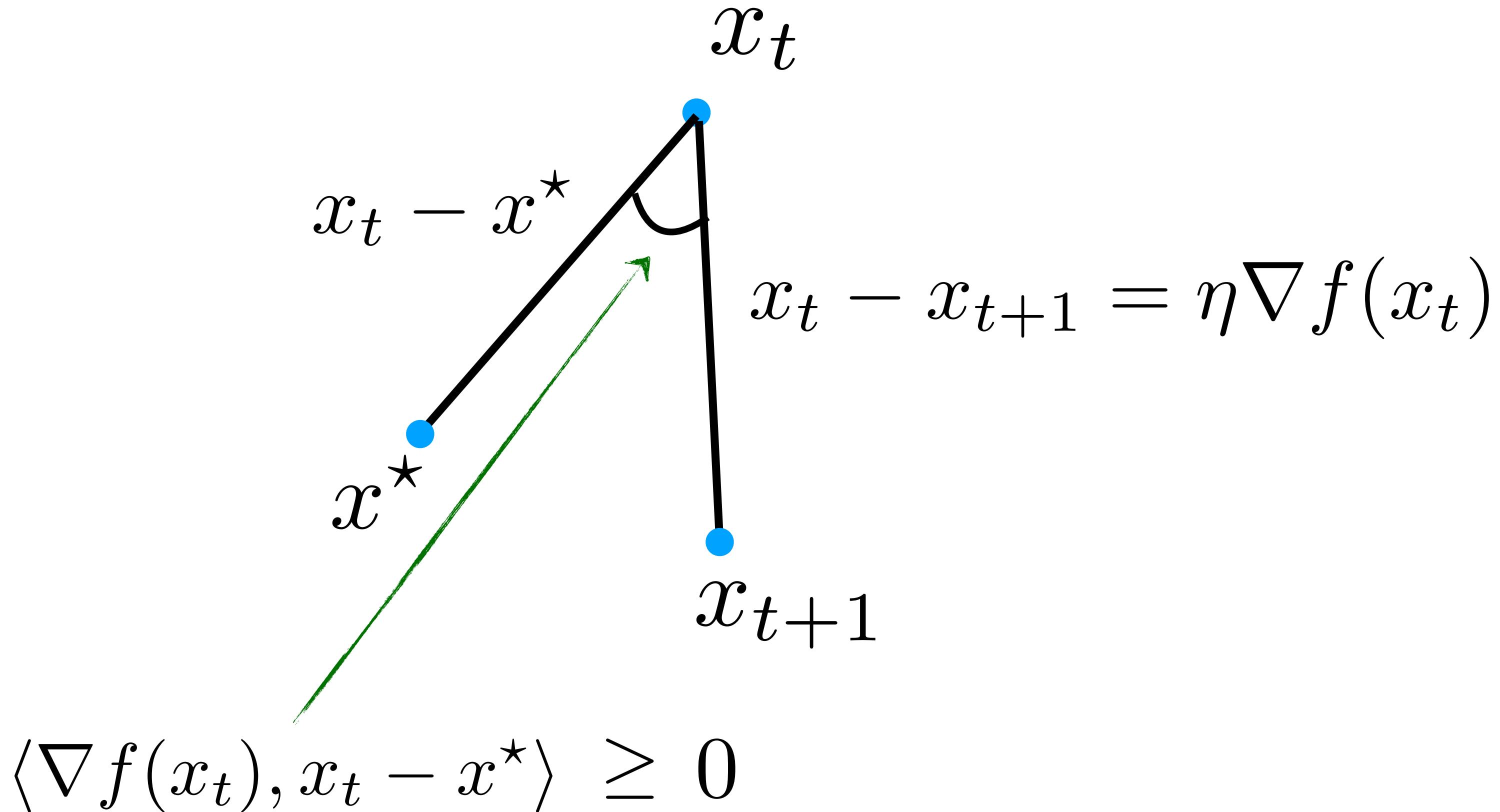
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for sufficient $\alpha, \beta \geq 0$ such that

$$\begin{aligned}\|x_t - x^*\|_\sharp^2 - 2\eta \langle \nabla f(x_t), x_t - x^* \rangle + \eta^2 \|\nabla f(x_t)\|_\sharp^2 \\ \leq \|x_t - x^*\|_\sharp^2 - c\alpha\eta \|x_t - x^*\|_\sharp^2 - (c\eta\beta - \eta^2) \|\nabla f(x_t)\|_\sharp^2\end{aligned}$$

c is problem dependent

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- Set $y = x^*$ and since $\nabla f(x^*) = 0$

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and compare with

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Local convergence guarantees for UU^\top

(The UV' case is left for you to study and explore)

- Define **distance function**:

$$\text{DIST}(U, U^*R) := \min_R \|U - U^*R\|_F$$

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- **Local convergence**: we assume we start from a sufficiently good initial point

Whiteboard

Main result: Local convergence guarantees

• f is convex and differentiable

$$U_{i+1} = U_i - \eta \nabla f(U_i V_i^\top) \cdot V_i^\top$$

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THEOREM: LOCAL CONVERGENCE

If f is a “nice” function and (U_i, V_i) are **sufficiently** close to (U^*, V^*) , then **non-convex** alternating gradient descent **i)** converges to (U^*, V^*) , and **ii)** achieves the same convergence guarantees with convex optimization:

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Impact in practice: Theory...

- ...provides insights for step size selection, proper initialization,
- ...covers cases where we do not know the rank parameter a priori,
- ...provides statistical guarantees for specific f .

Our proof strategy

Show how the algorithm behaves *locally*

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Convergence to global minimum for non-convex optimization!

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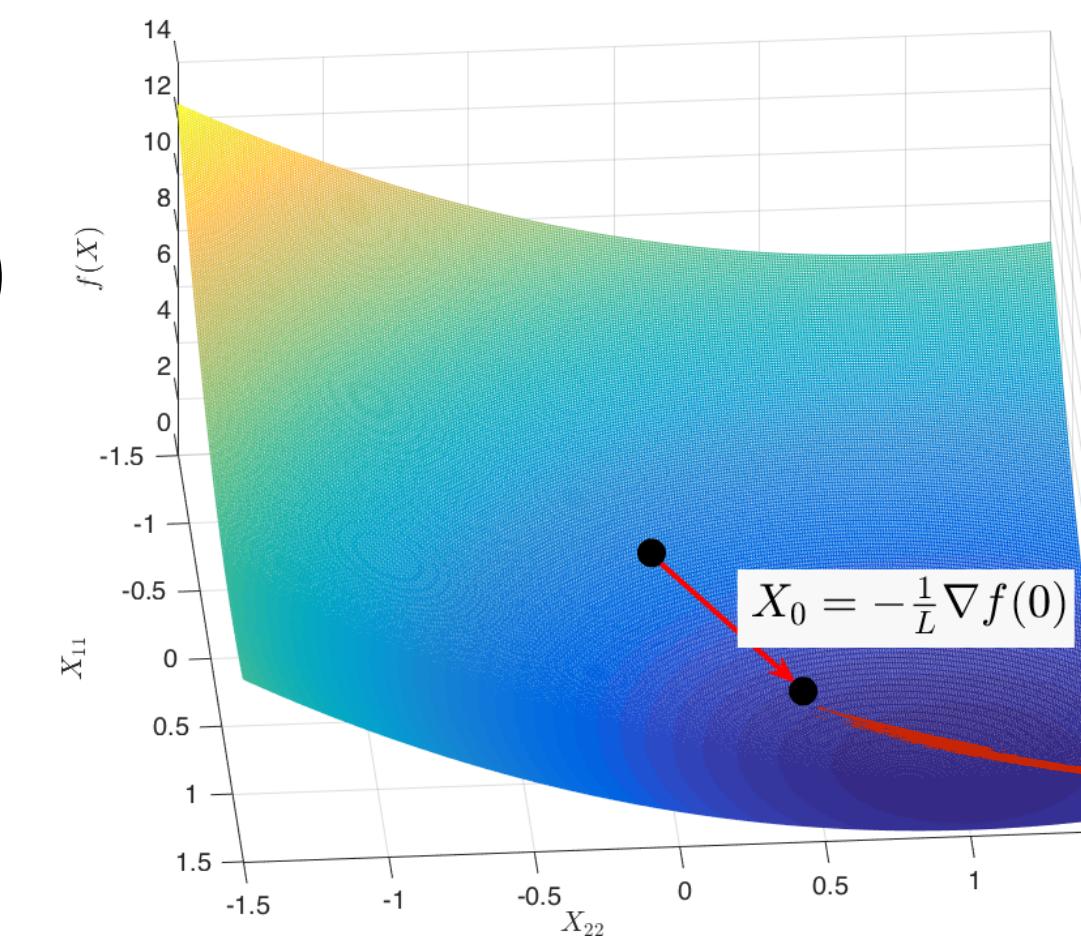
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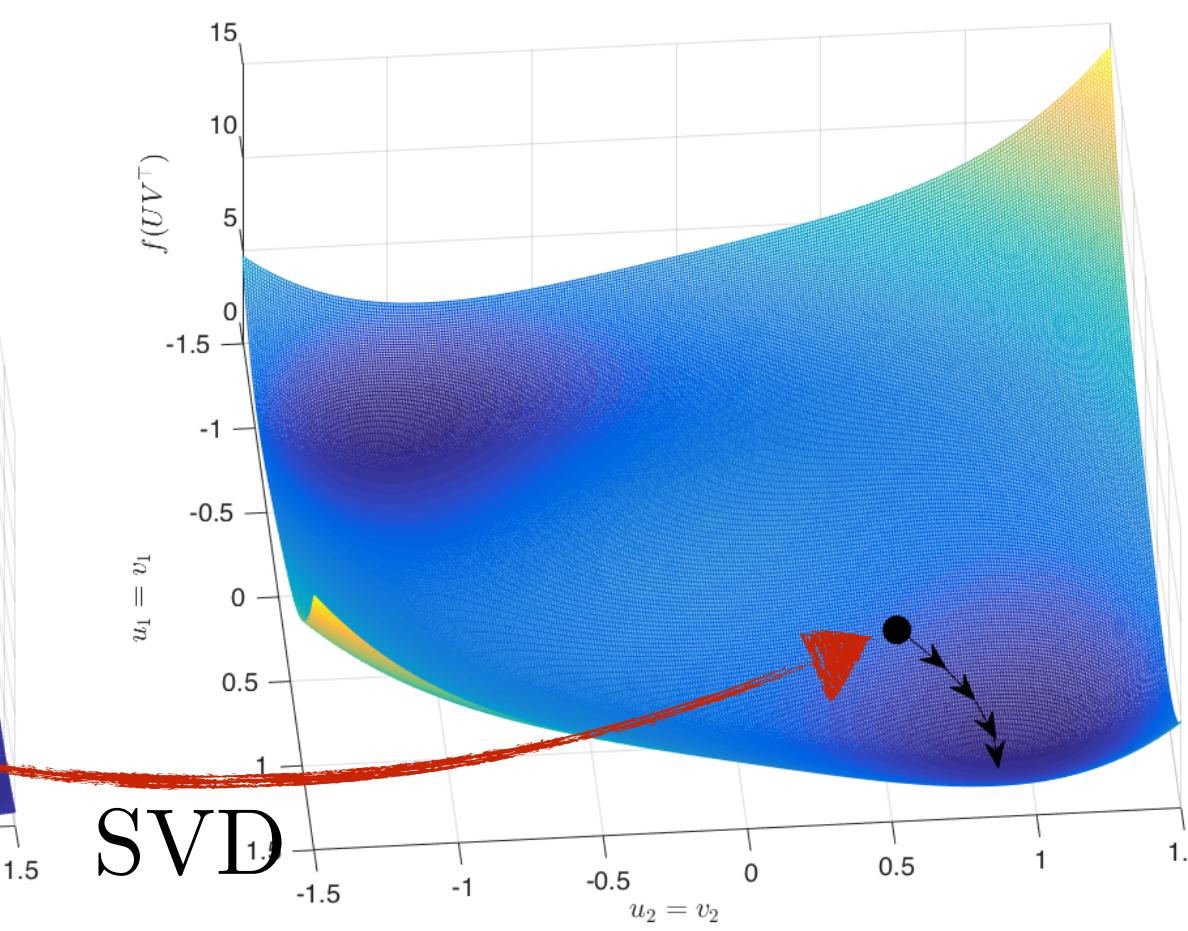
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- Compute $X_0 \propto -\nabla f(0)$
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$$X_0 = U_0 V_0^\top$$



Original space of X



Factored space

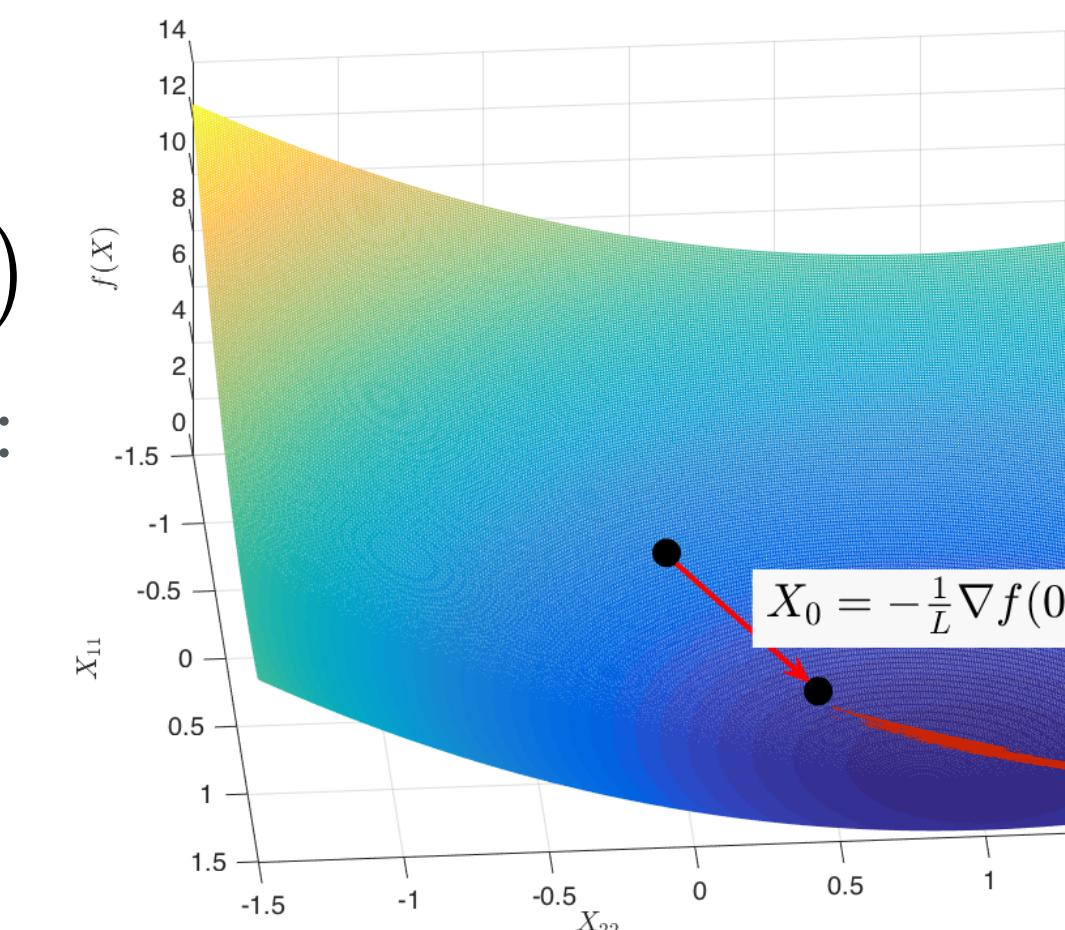
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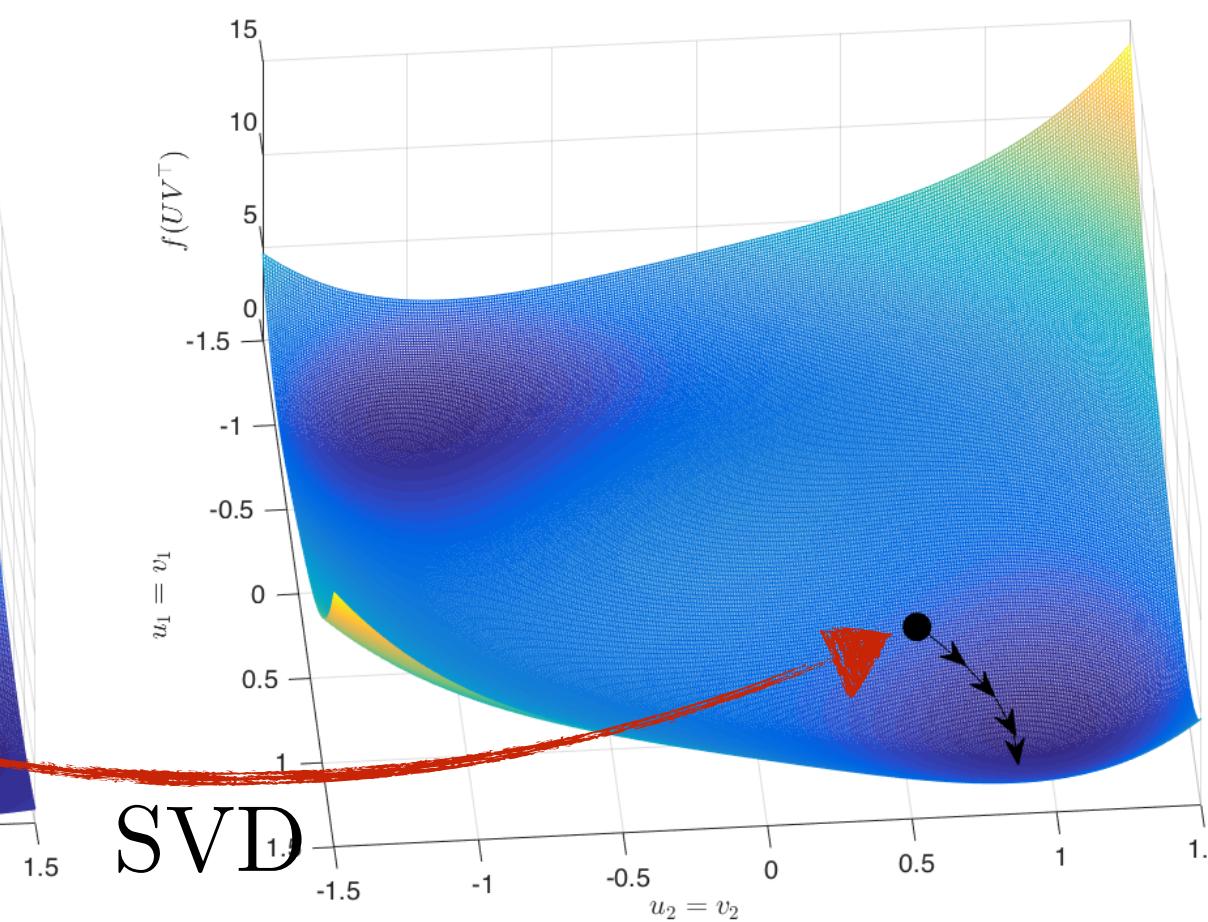
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THEOREM: GLOBAL CONVERGENCE

If the function f is “well-conditioned”, then non-convex alternating gradient descent converges to the global optimum / optima.

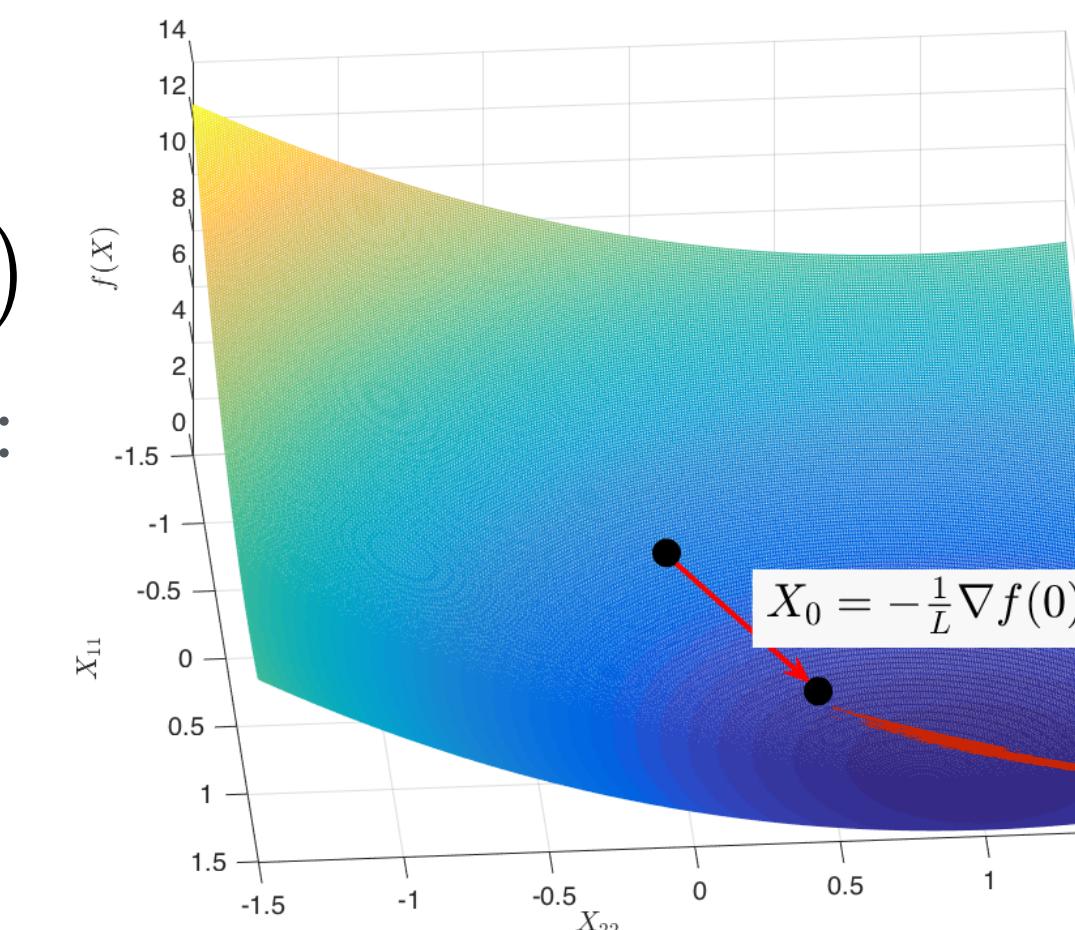
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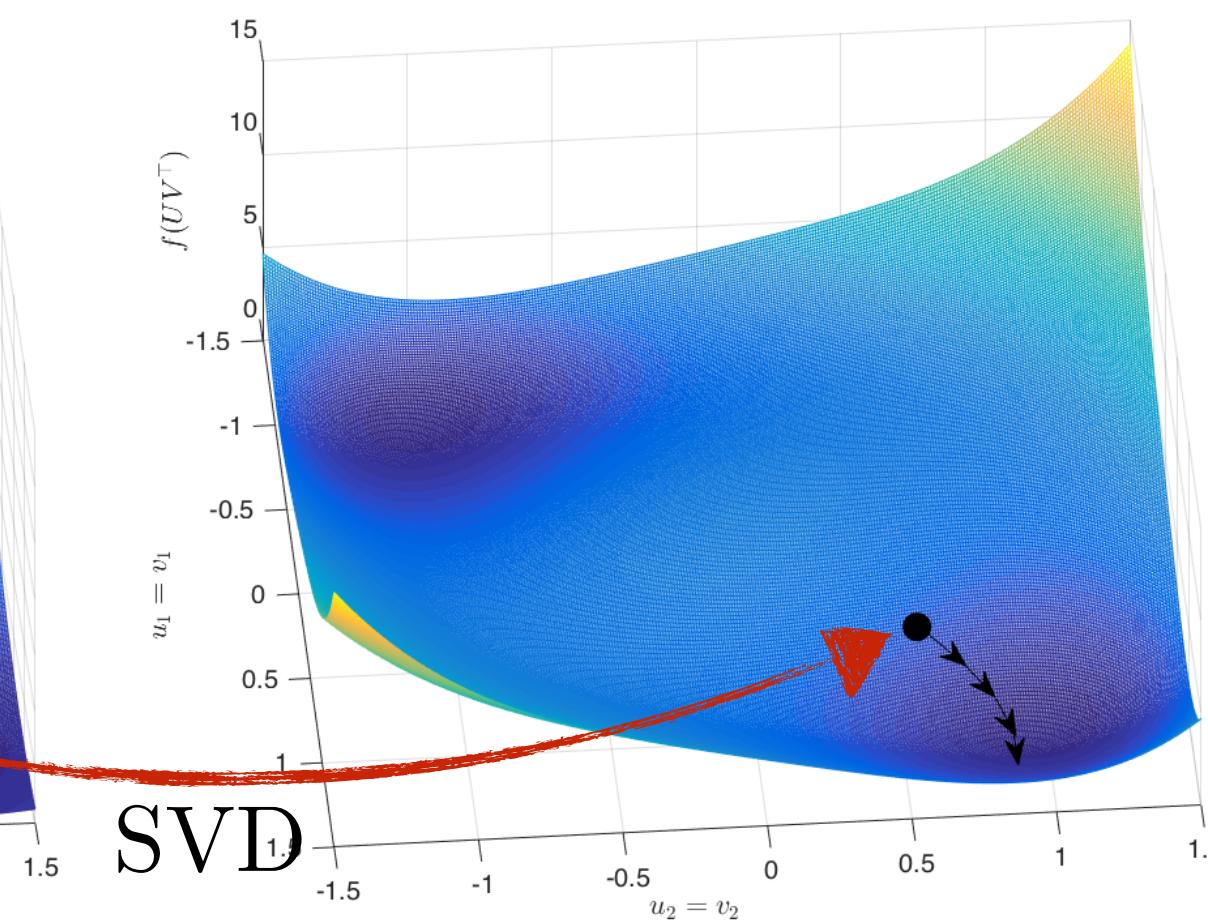
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PRACTICAL IMPACT

Practical aspects of optimizing $\min_{U \in \mathbb{R}^{m \times r}, V \in \mathbb{R}^{n \times r}} f(UV^\top)$

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$$(U_0, V_0) = \text{SVD}(-\nabla f(0_{n \times p}))$$

(Often called spectral method for initialization)

..the guarantees are weak, but often it works in practice!

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- Constant step size vs. adaptive step size (Open question for specific f)

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Demo

Conclusion

- This lecture considers **low-rank model selection** in Data Science applications
- While there are rigorous and efficient methods also in the convex domain we followed the **non-convex path**, beyond hard thresholding methods
- We discussed some global convergence guarantees (under proper initialization assumptions) and discussed about some open questions

Next lecture

- We will focus on the landscape of non-convex functions, starting from simple cases (such as low-rankness), and moving towards more generic scenarios