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

Lecture 9

Overview

- In the previous lecture, we:
  - 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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  - We consider the special case of sparsity
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- 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

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

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We will consider convex objectives..

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

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

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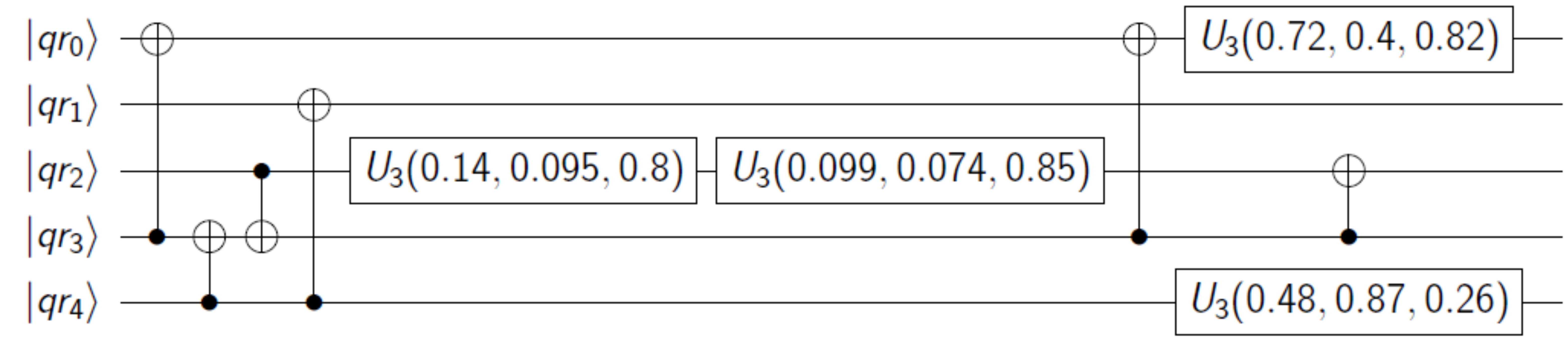
..over non−convex constraints

– 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




```
OPENQASM 2.0;
include "qelib1.inc";
qreg qr[5];
creg cr[5];
cx qr[3],qr[0];
cx qr[4],qr[3];
cx qr[2],qr[3];
cx qr[4],qr[1];
u3(0.139745784966679,0.0948307634768559,0.799402574081021) qr[2];
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fidelity: 0.997607
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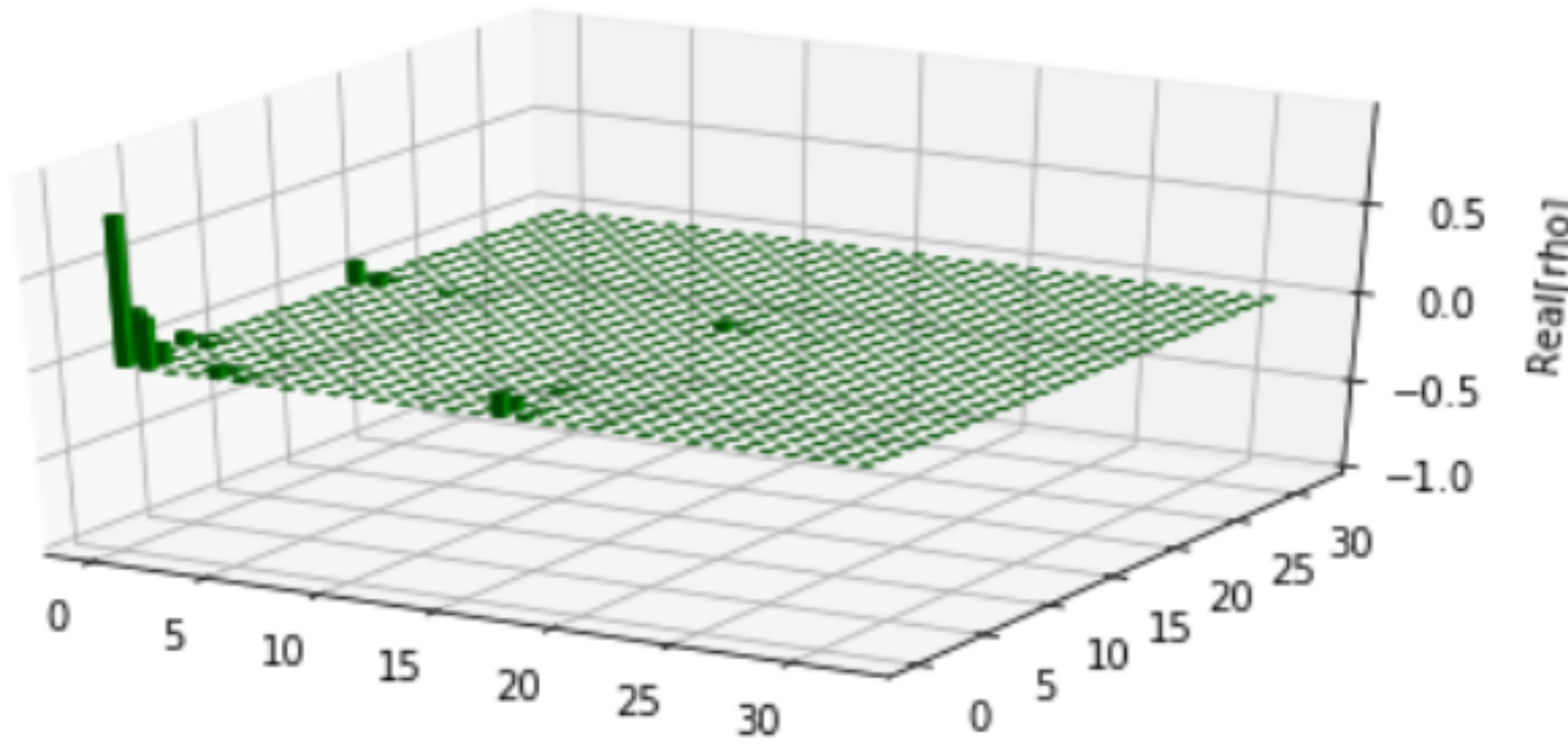

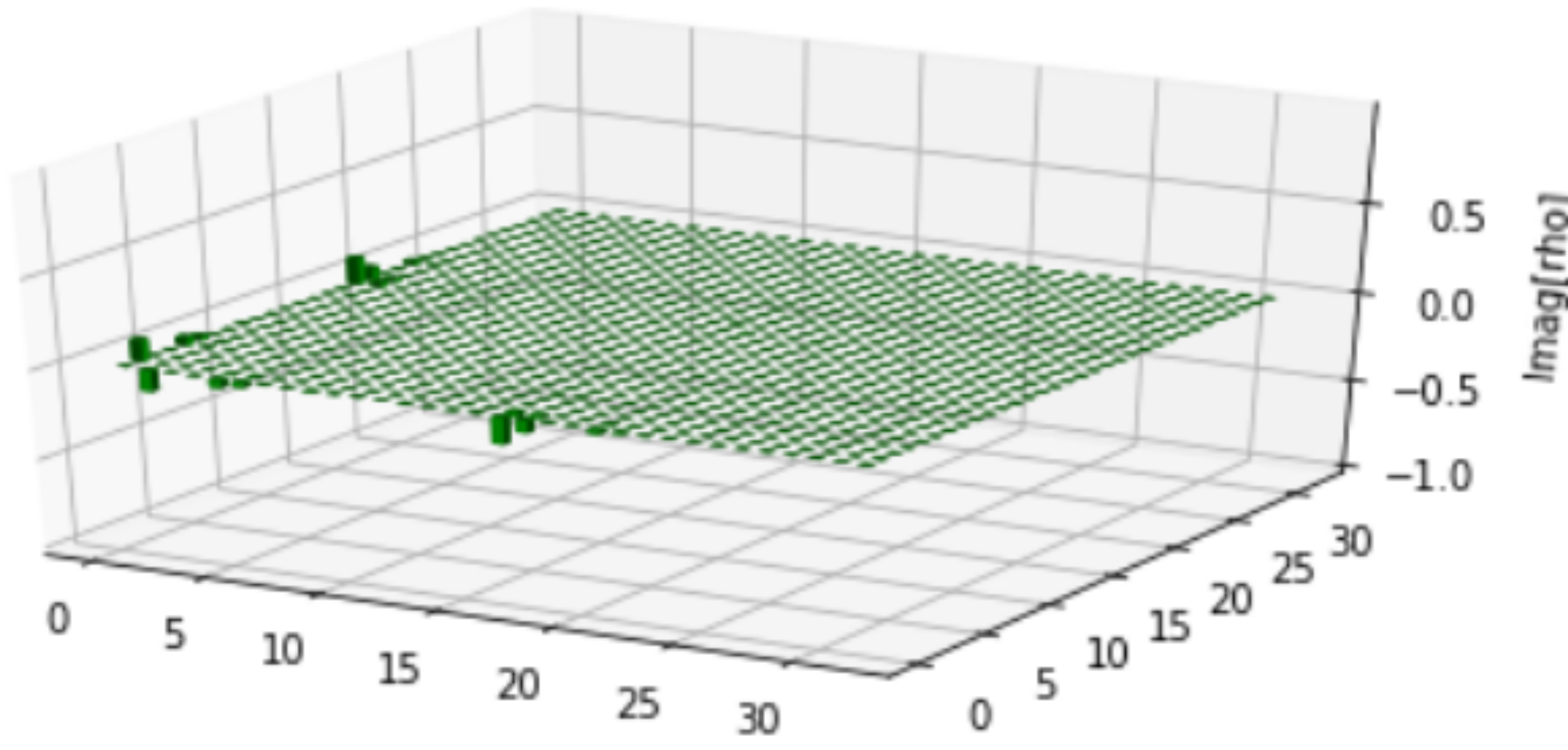

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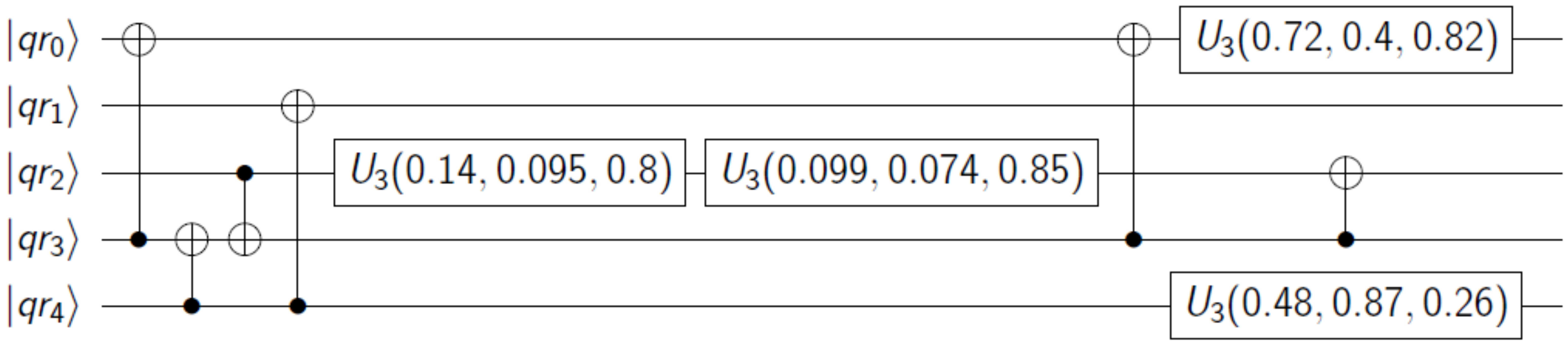


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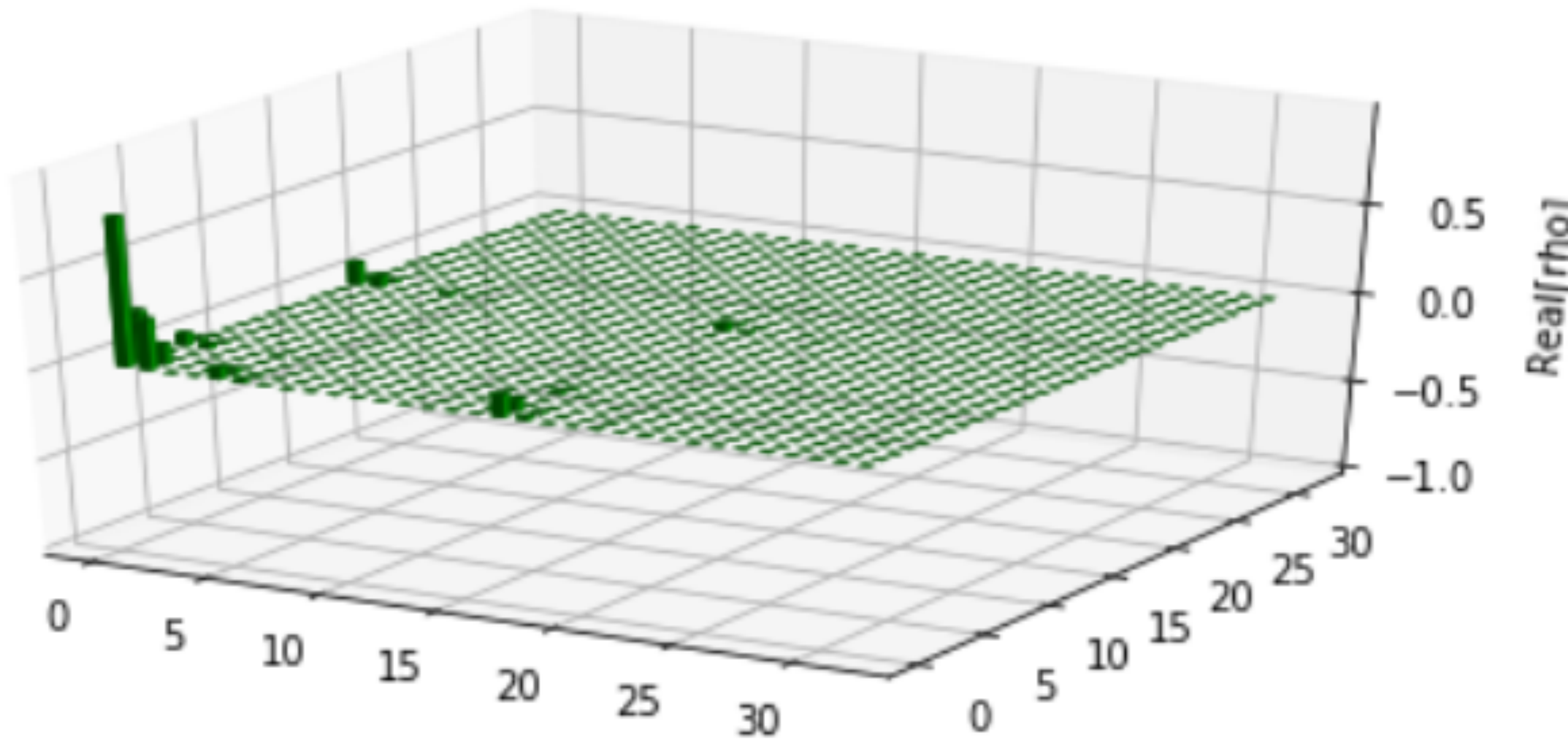

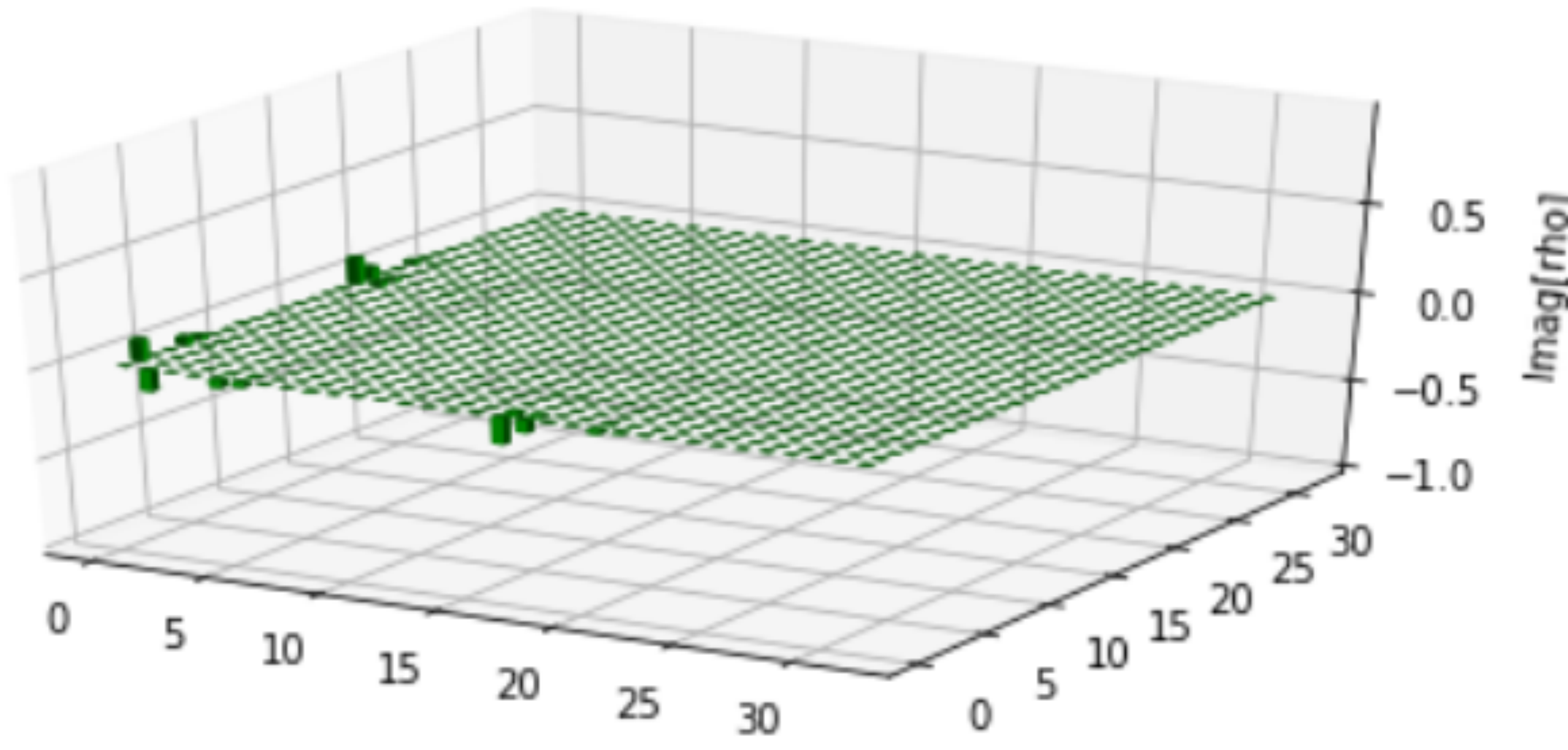

– Goal: Validate the system is in the expected.. state, the computations are completed ..as expected

Quantum state tomography (Much easier than it sounds like..)

- Generative model: $y_i = \langle A_i, X^\star \rangle + w_i = \text{Tr}(A_i X^\star) + w_i$
  - $A_i \in \mathbb{R}^{p \times p}$: 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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(Pauli operators)

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

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

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

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

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

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

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

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

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Quantum state tomography (Much easier than it sounds like..)

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

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

RIP for Pauli operators

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

$$[\mathcal{A}(X)]_i = \mathrm{Tr}(A_i, X)$$

(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)

$$
\begin{aligned}
\min_{X \in \mathbb{R}^{p \times p}} \quad & \frac{1}{2} \sum_{i=1}^{n} \left(y_i - \langle A_i, X \rangle\right)^2 \\
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Nuclear norm min.

– Solution #1: **convexification** + proj. gradient descent

$$\min_{X \in \mathbb{R}^{p \times p}} \quad \frac{1}{2} \sum_{i=1}^{n} (y_i - \langle A_i, X \rangle)^2$$
$$\text{s.t.} \quad \|X\|_* \leq \lambda$$

$\longrightarrow$

$$X_{t+1} = \Pi_{\|\cdot\|_* \leq \lambda} (X_t - \eta \nabla f(X_t))$$

(Pros & Cons?)

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$\longrightarrow$ $X_{t+1} = \Pi_{\|\cdot\|_* \leq \lambda} \left(X_t - \eta \nabla f(X_t) \right)$

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

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Hard-thresholding

– Solution #2: **keep the rank−constraint** + proj. gradient descent (Non−convex)

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(Pros & Cons?)

– Definition of the projection onto low-rank matrices

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

(Requires truncated SVD for its calculation)

But before we proceed..

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

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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``

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(It is just projected gradient descent on low-rank constraints)

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- Now, imagine yourself implementing this.. What are the hyper−parameters?
  - "How do we set the step size?"
  - "How do we select the initial point? (it is non−convex after all)"
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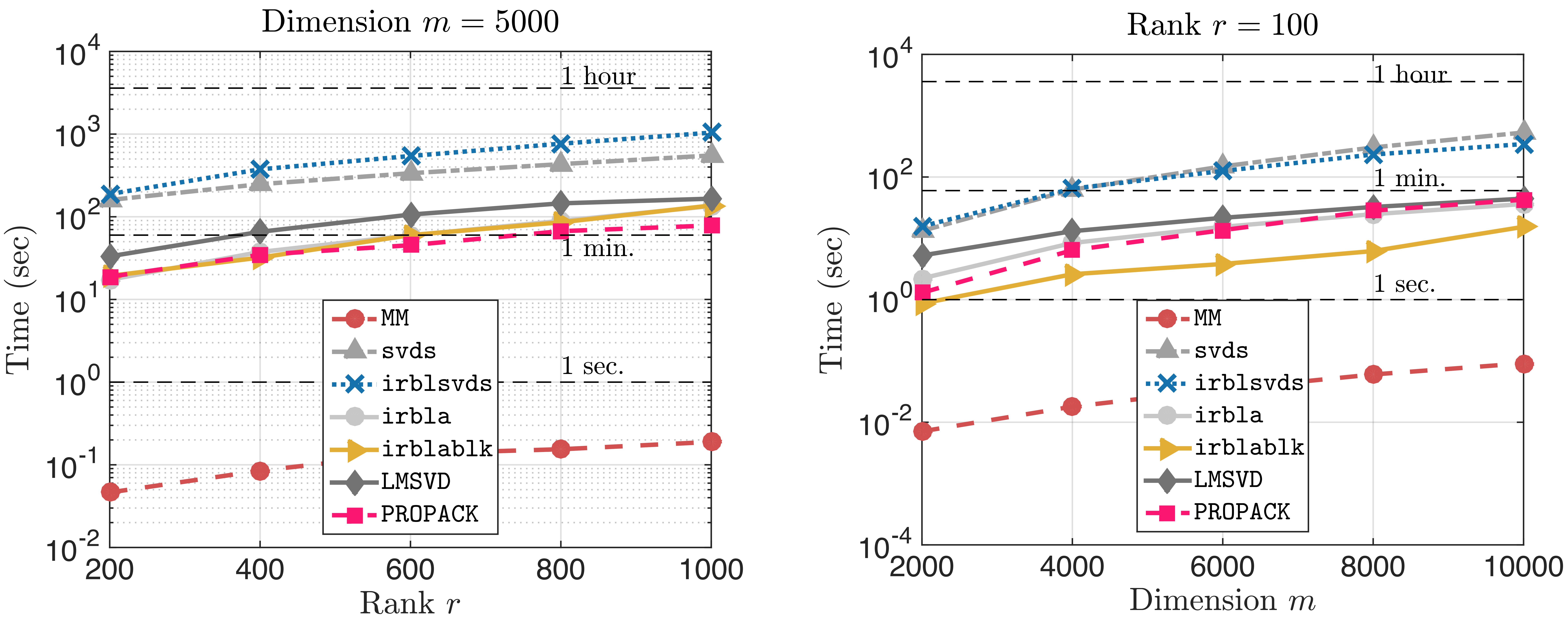
  - ``Are there any other tricks we can pull−off?`` (Answer: see previous Chapter)

Convexification vs. hard−thresholding in practice

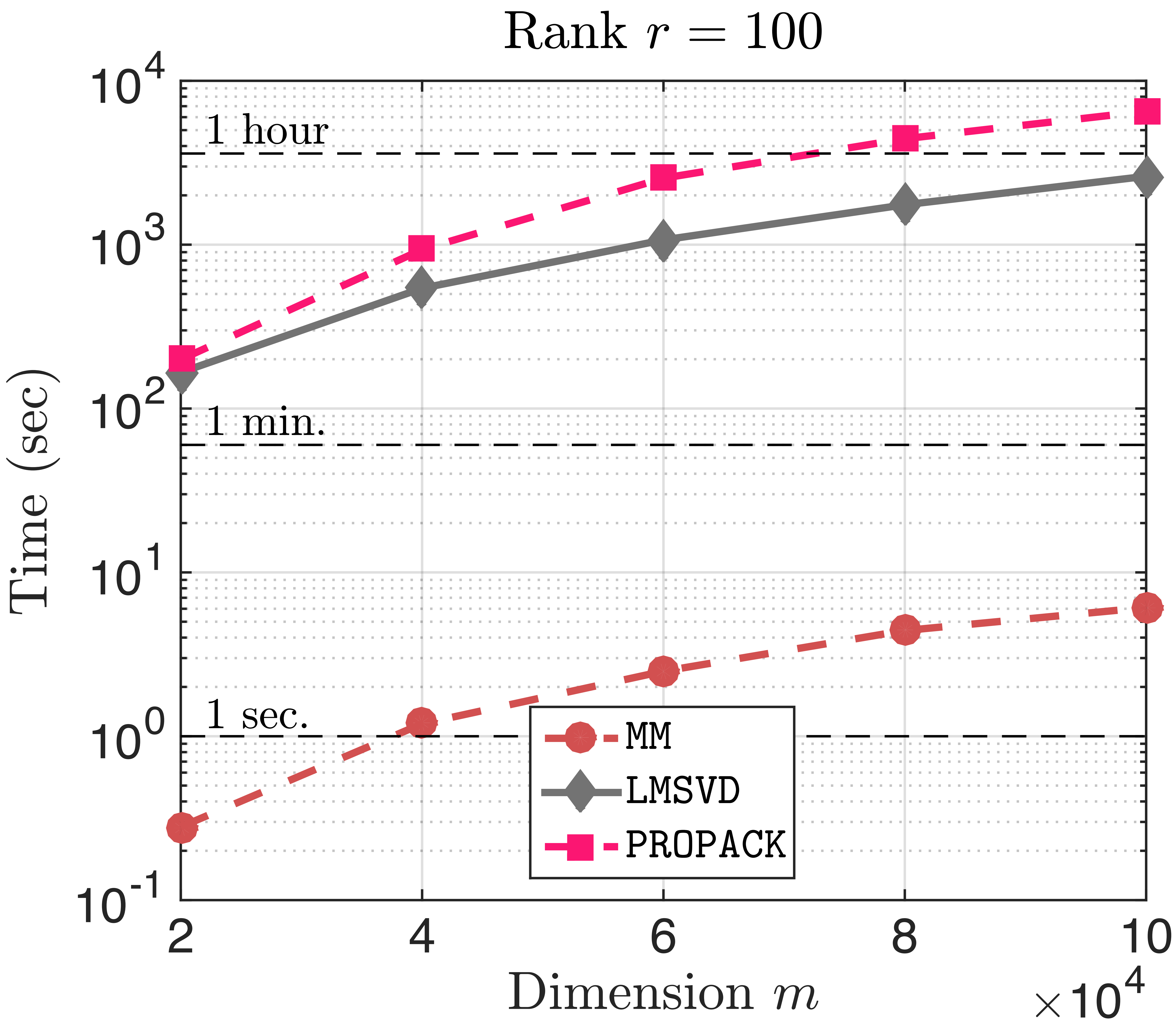
Demo

The price of SVD



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

The price of SVD



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

$$X = UV^\top$$

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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- 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)

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  - Initialization does matter: e.g., for PCA there are initializations that do not lead to convergence

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  - 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 \\
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s.t. ~~$\operatorname{rank}(X) \leq r$~~

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Back to matrix sensing

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Back to matrix sensing

Non-convex!

$$\min_{U \in \mathbb{R}^{n \times r}, V \in \mathbb{R}^{p \times r}} \frac{1}{2} \sum_{i=1}^{n} \left(y_i - \langle A_i, UV^\top \rangle \right)^2$$

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No constraints!

- 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

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

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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?

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

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

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– Factors at $X^\star$ are not unique

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$$f(X) = \frac{1}{2} \cdot \|y - \texttt{vec}(A \cdot X)\|_2^2$$

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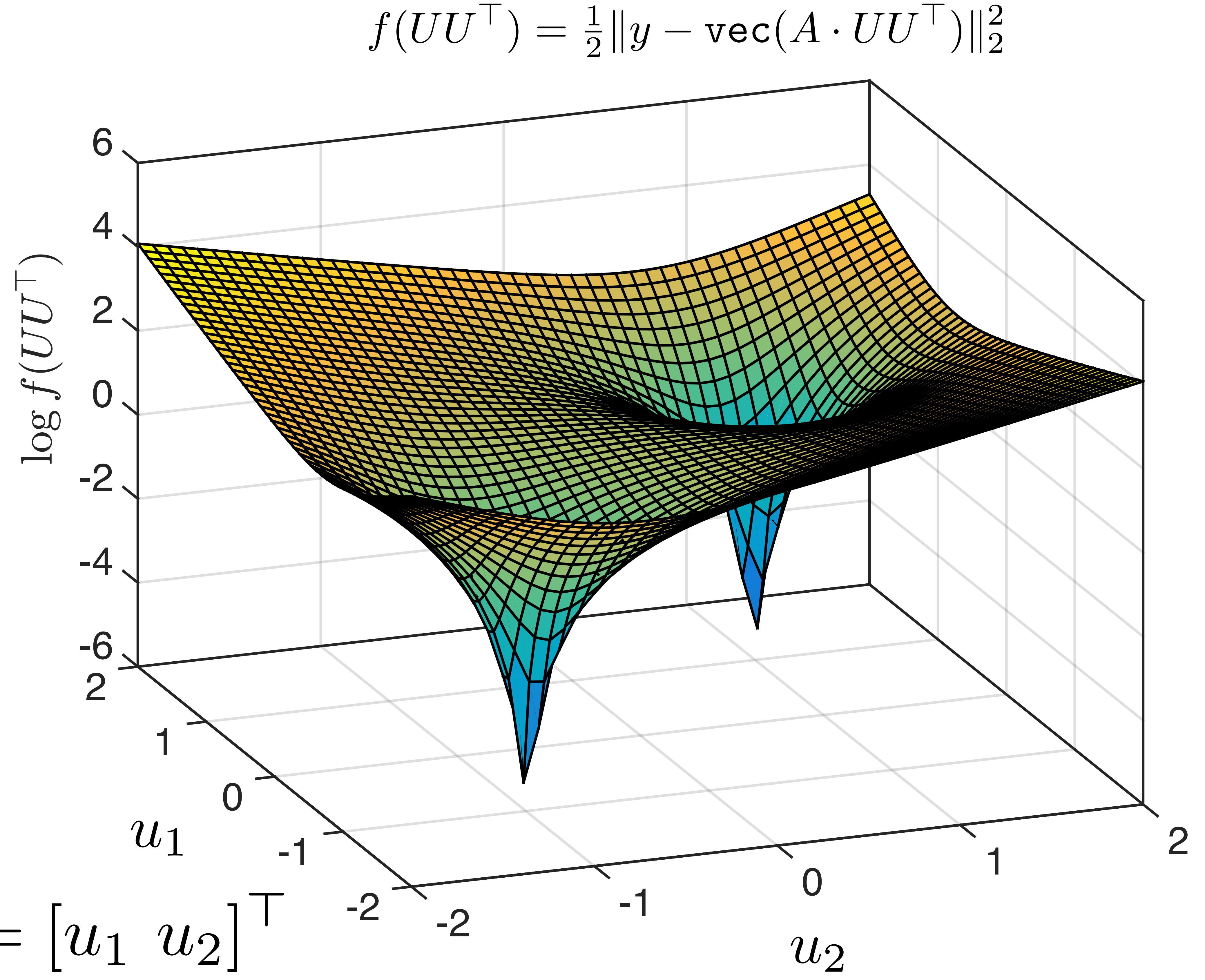

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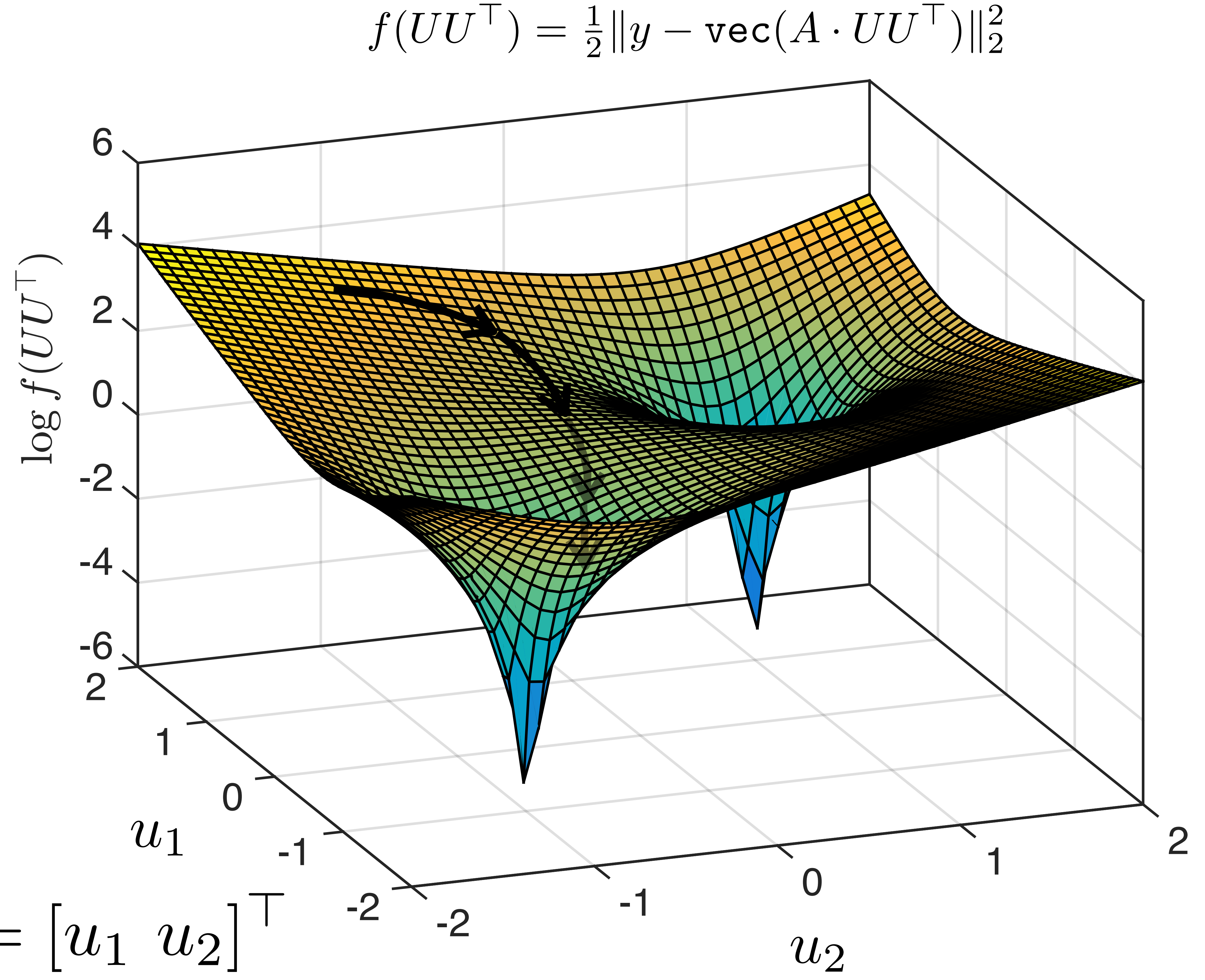

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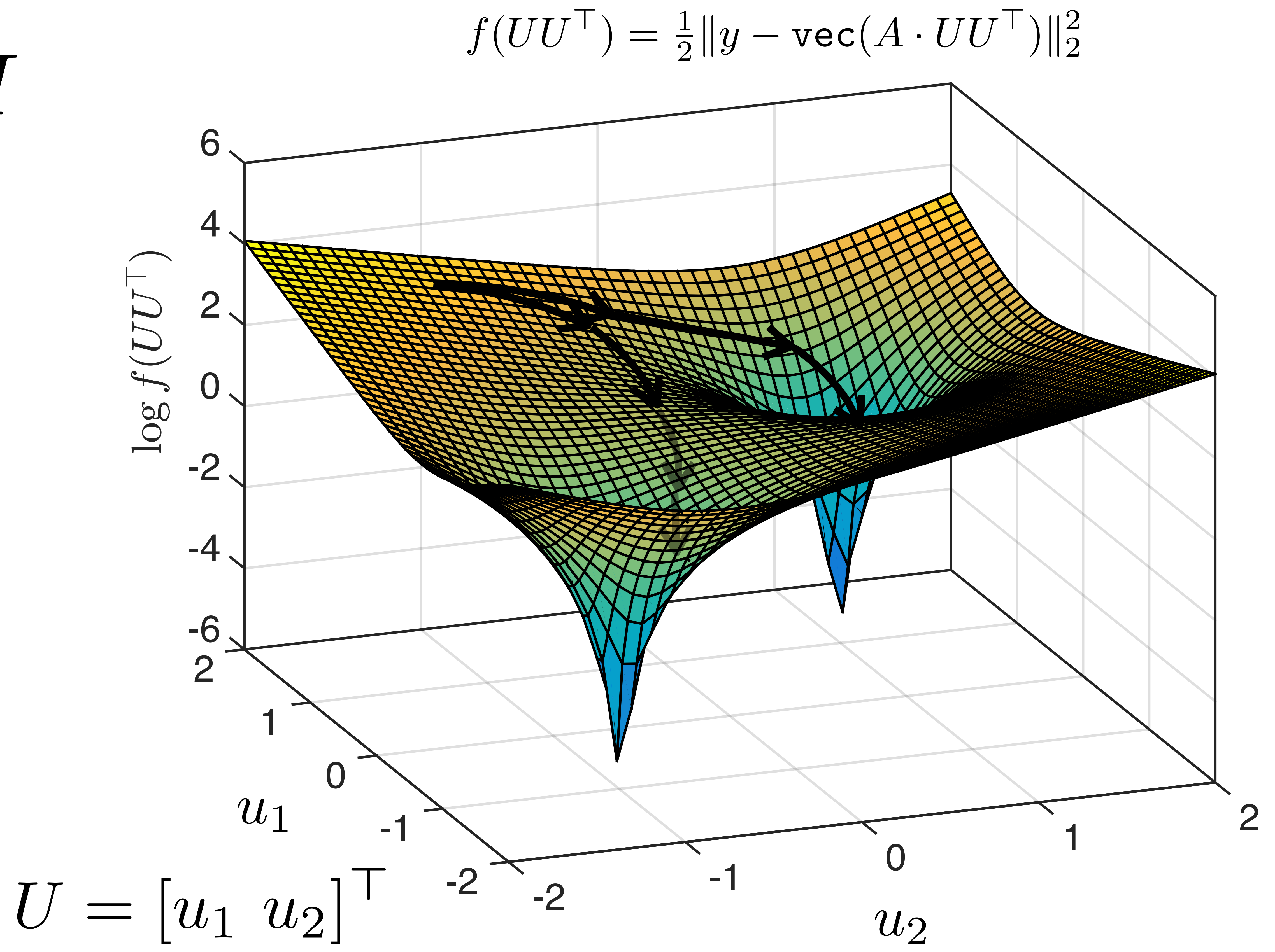

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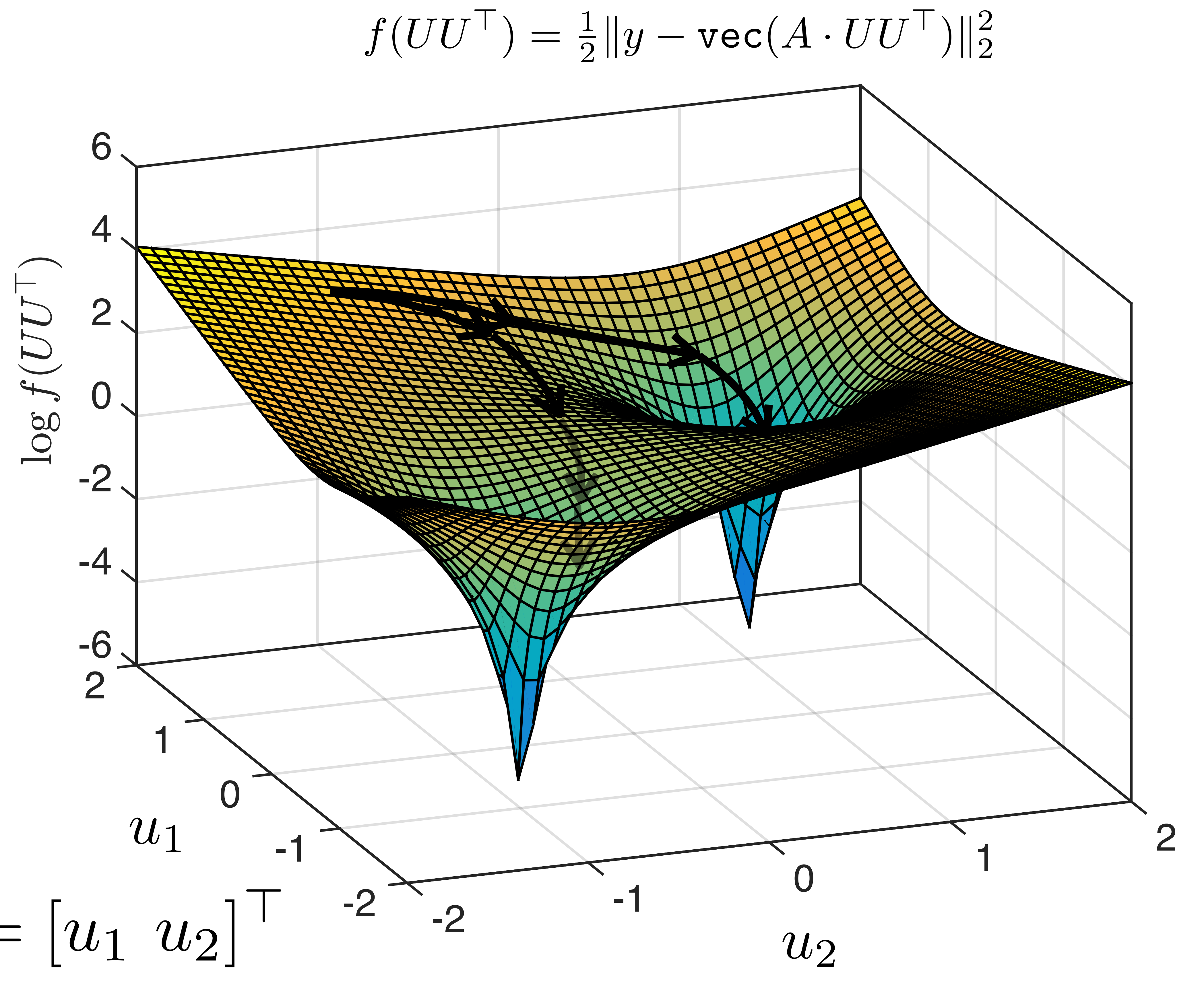
- $X \mapsto UV^\top$ "ruins" convexity
- Even local convergence results are important



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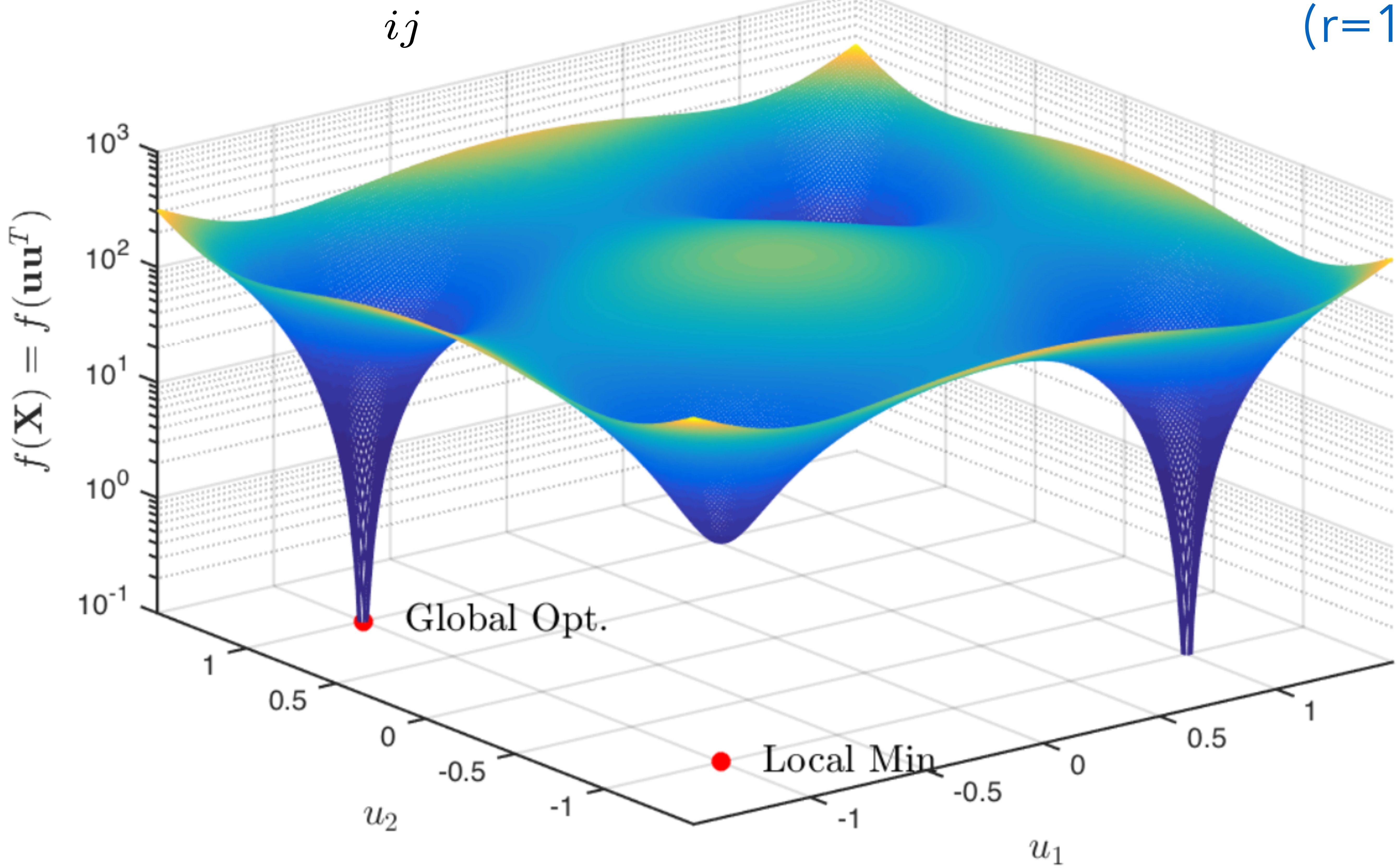

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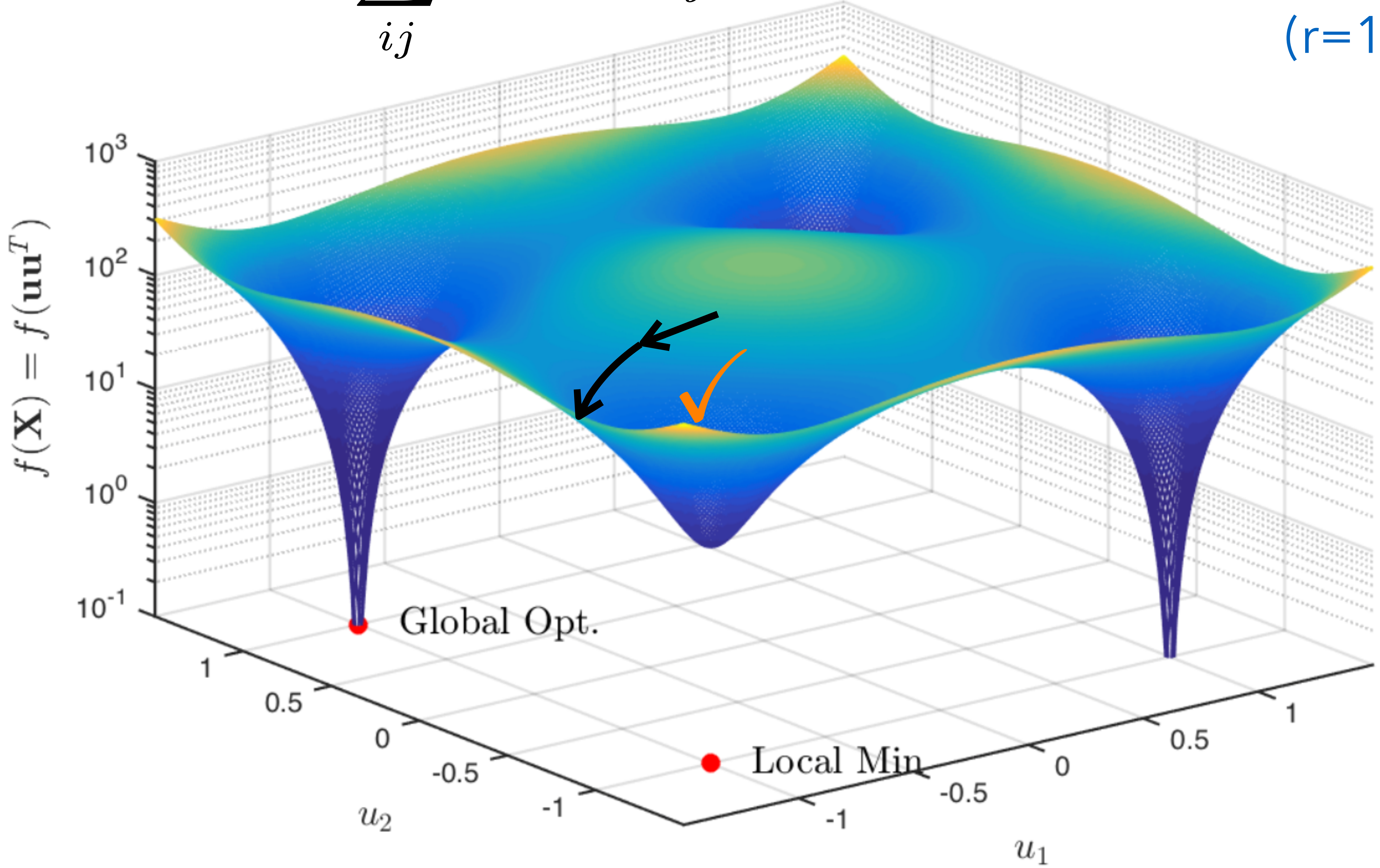

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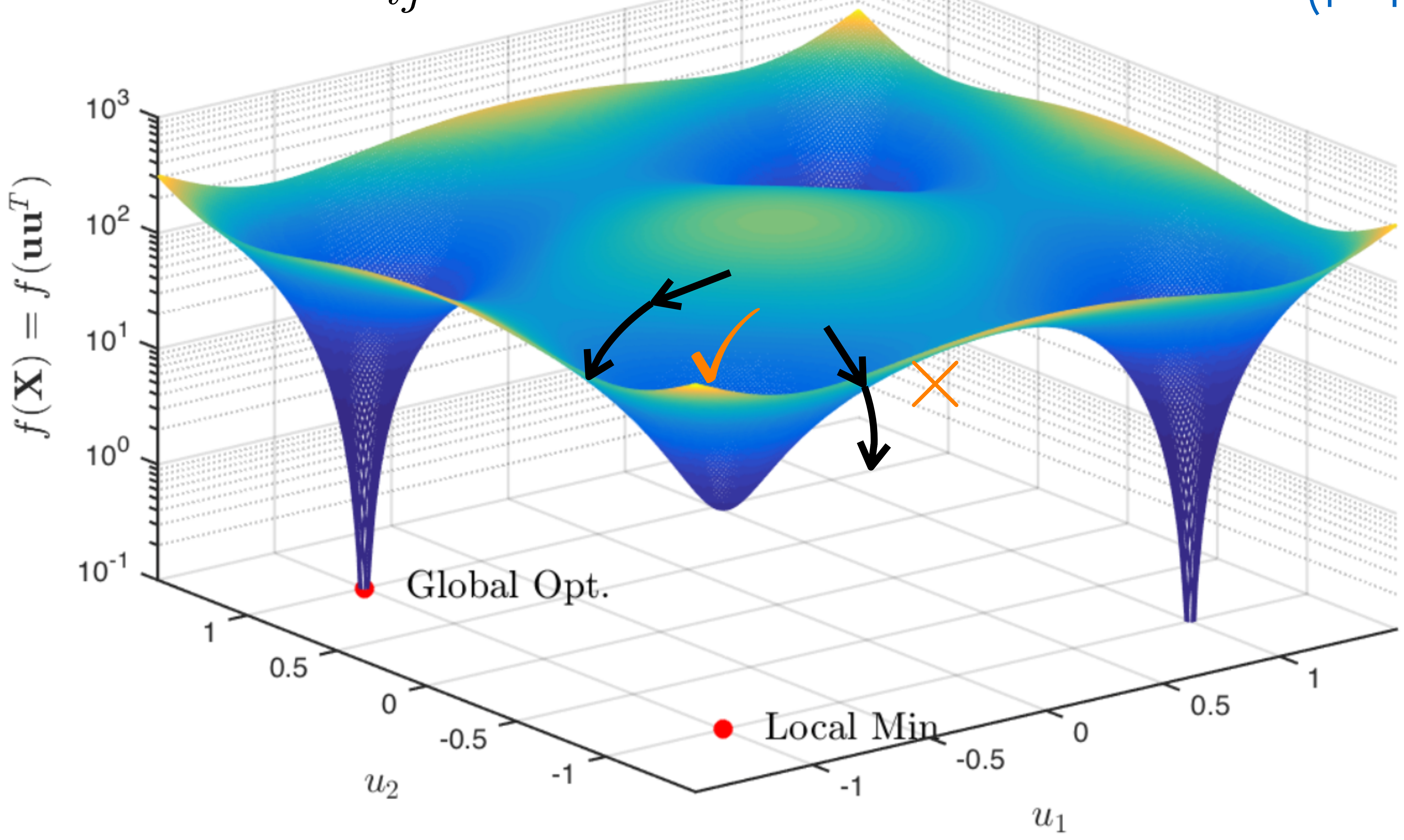

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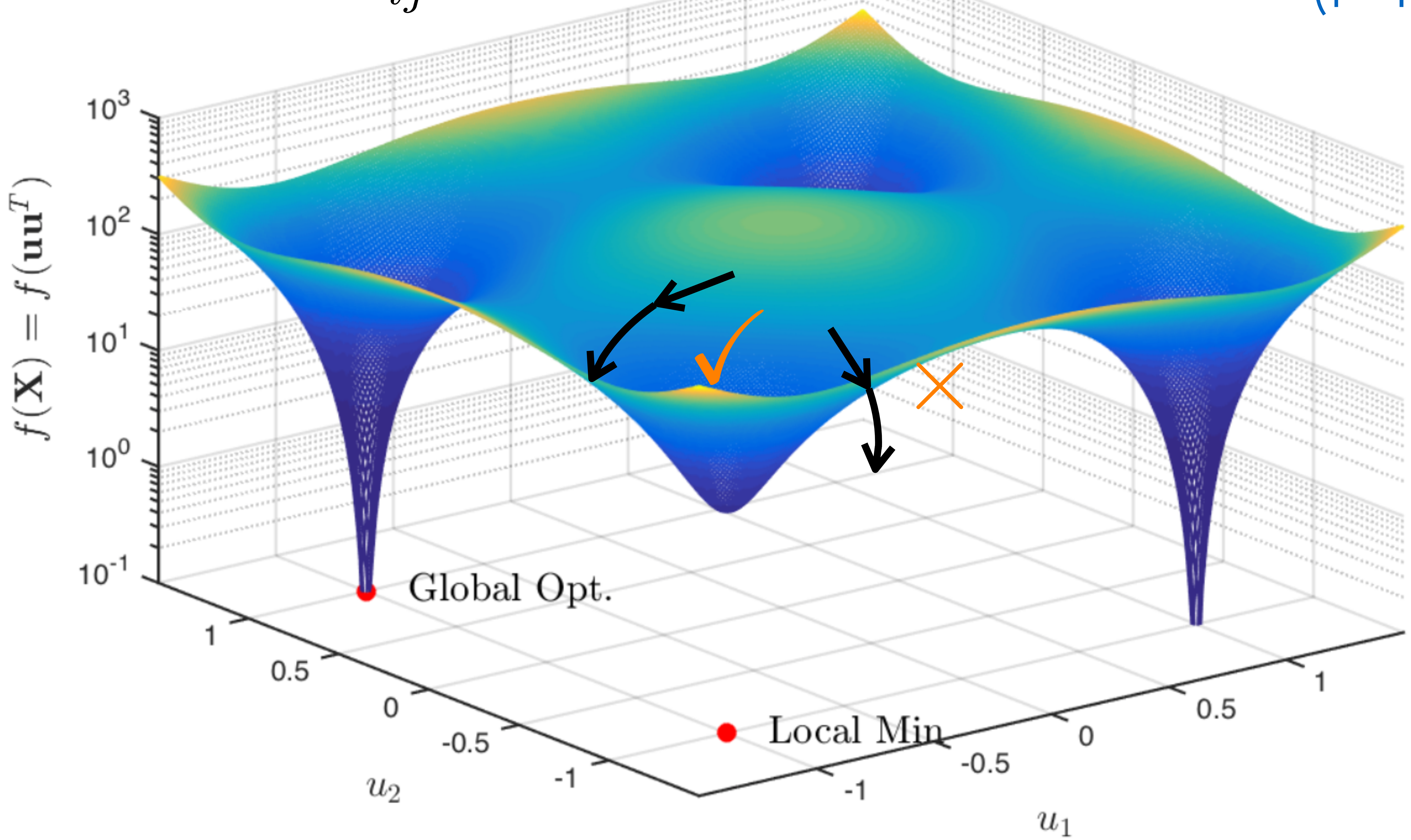

- Even simple objectives can be hard to handle
- Proper initialization is key

Nevertheless, can we hope for some guarantees?

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

- General recipe

$$
\begin{aligned}
\|x_{t+1} - x^\star\|_\sharp^2 &= \|x_t - \eta \nabla f(x_t) - x^\star\|_\sharp^2 \\
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(If we can bound this term to cancel this term)

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

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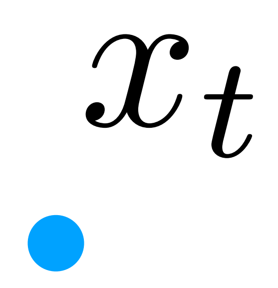

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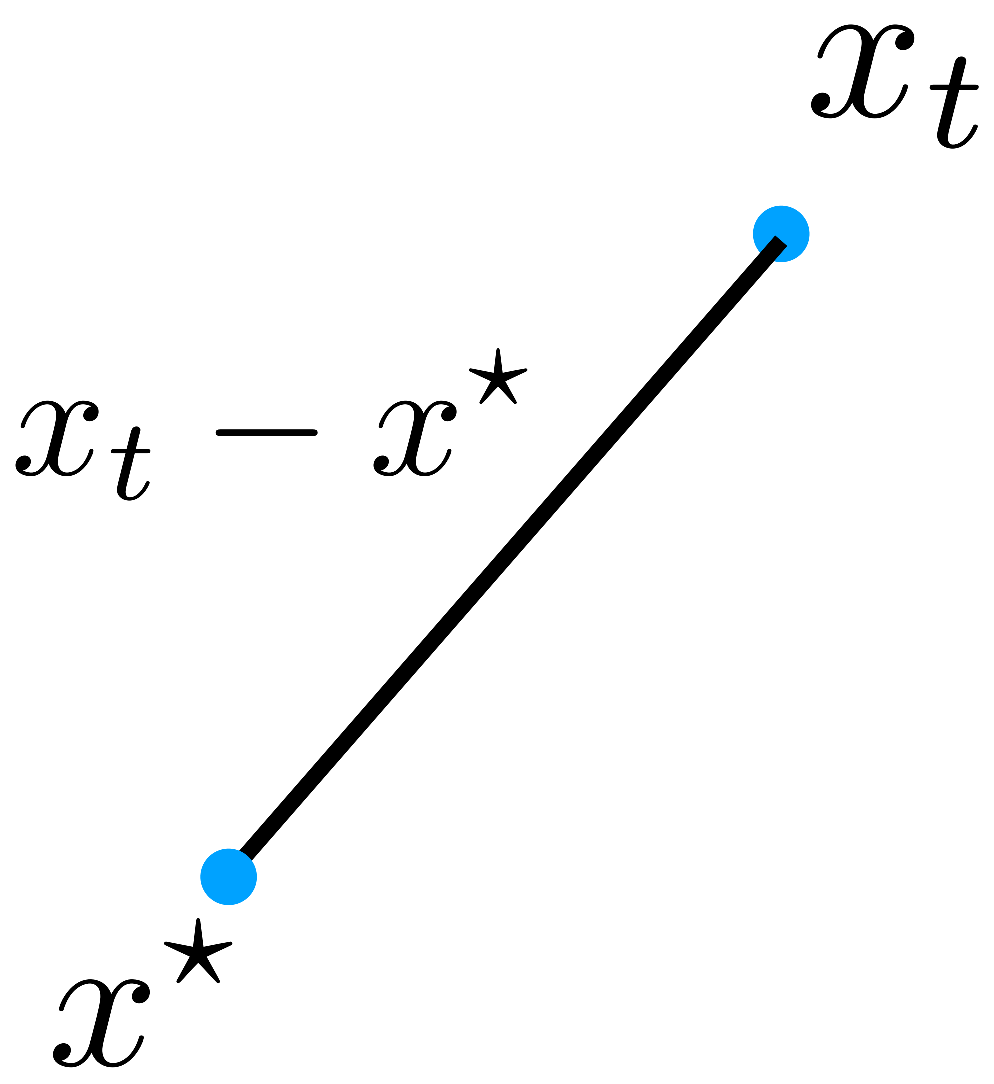

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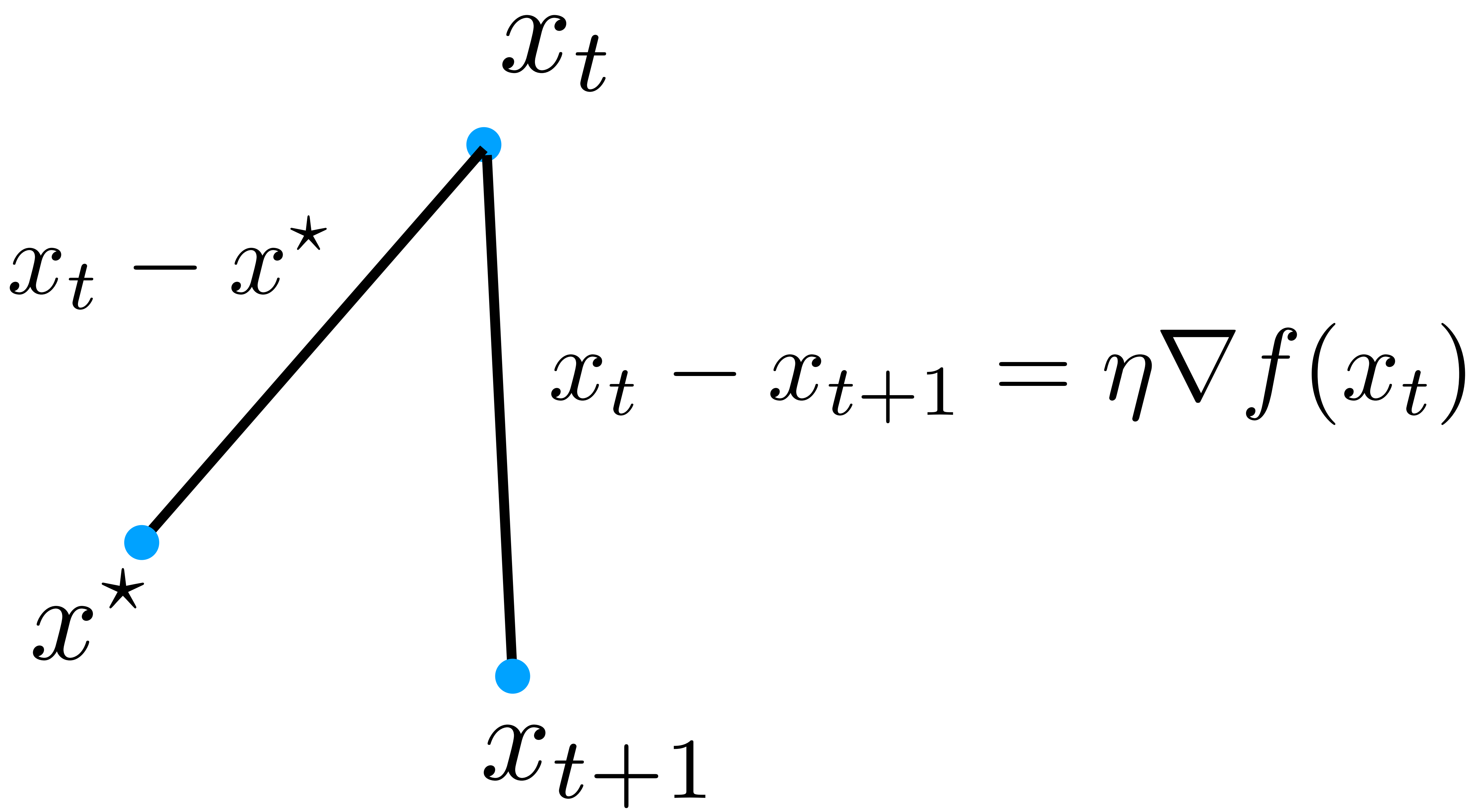

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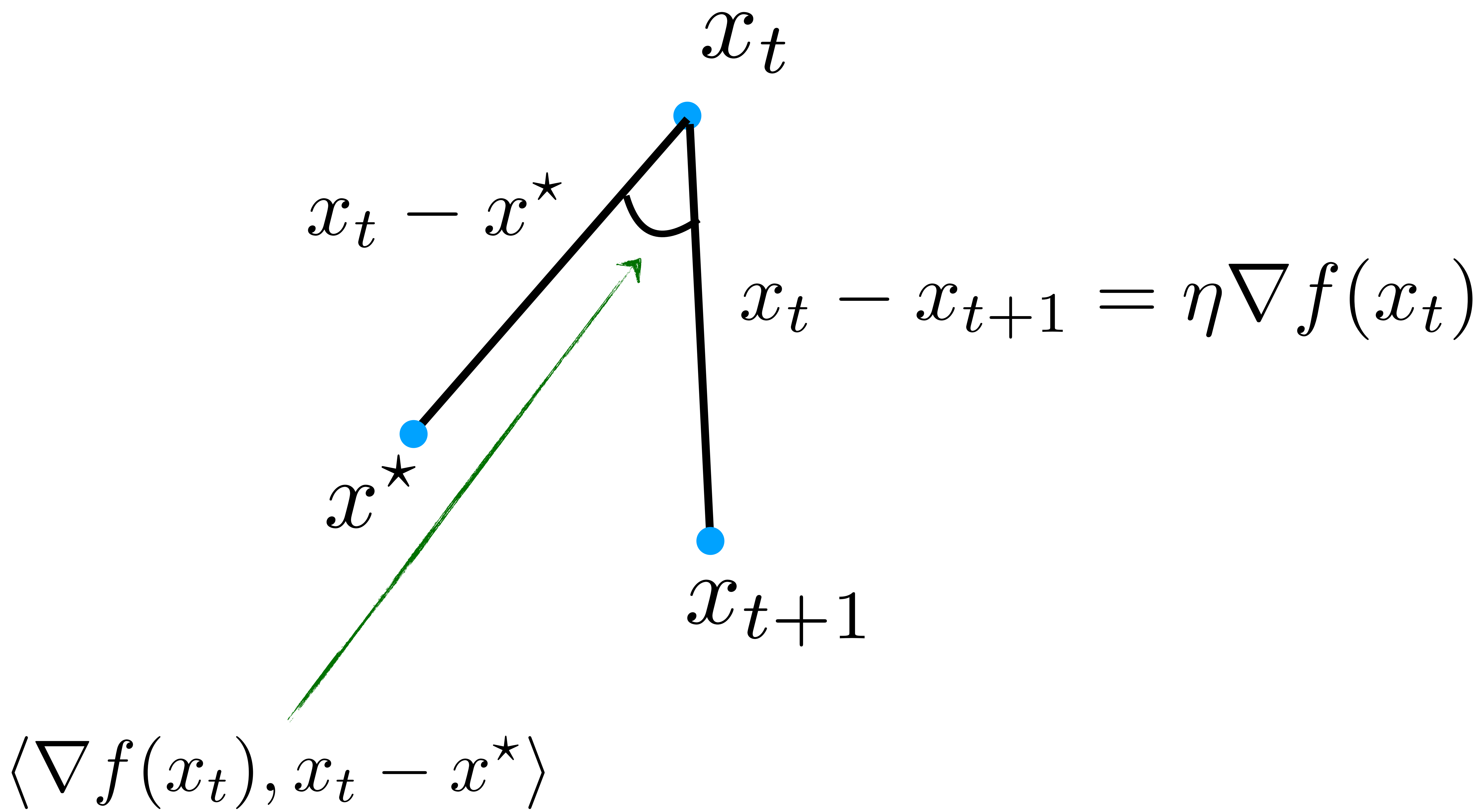

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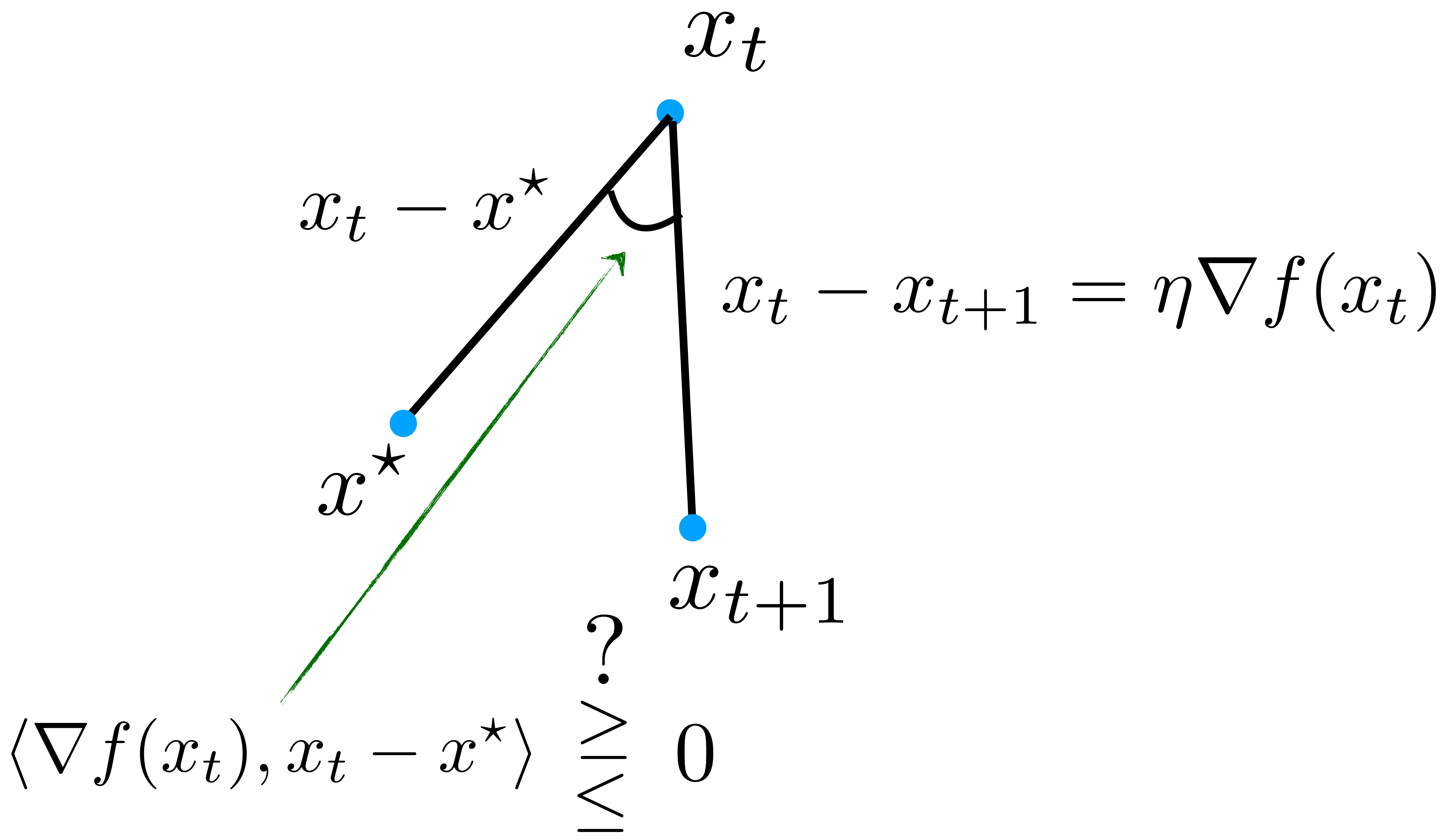

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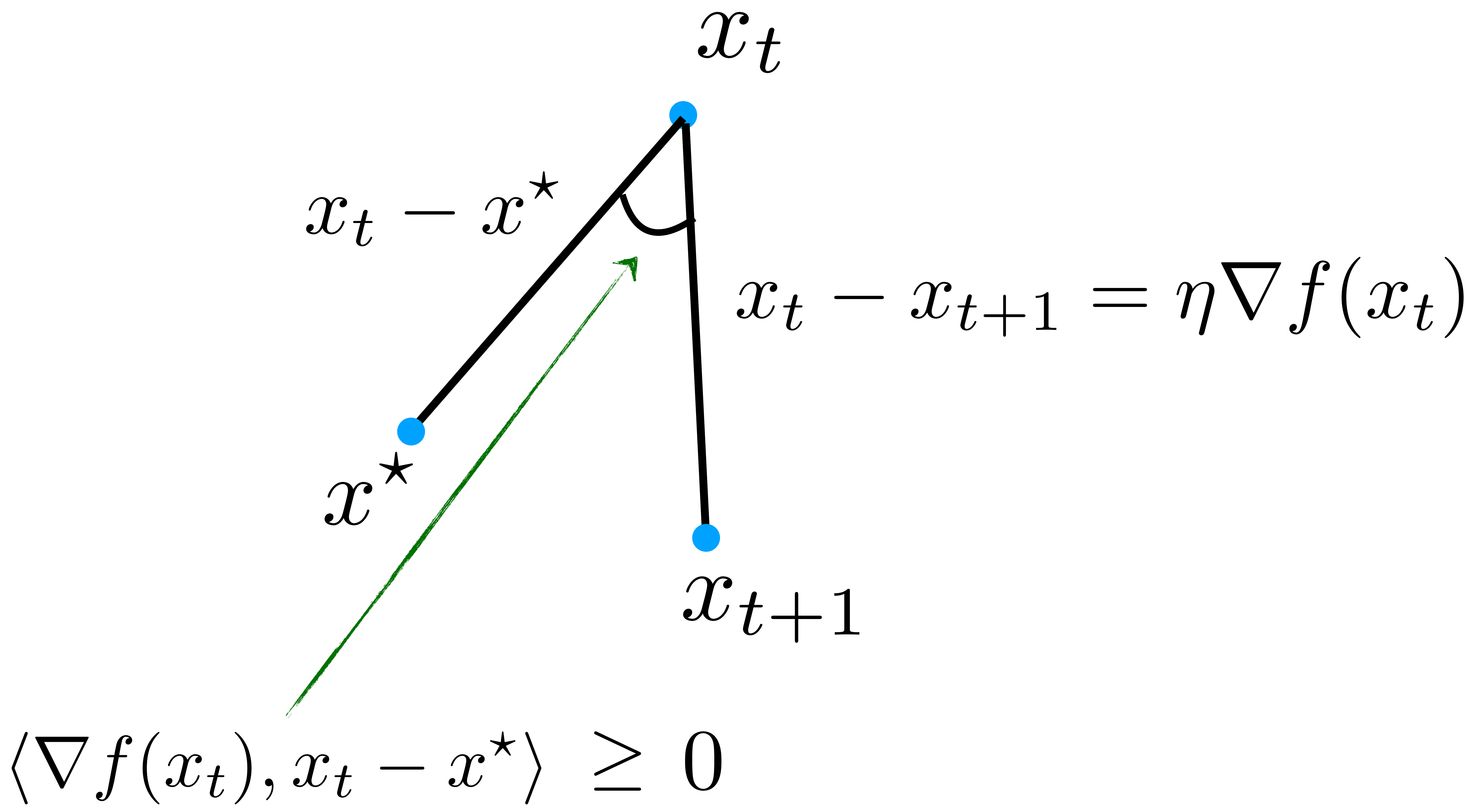

Regulatory condition

– Reminder:

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

$$\|x_t - x^\star\|_\sharp^2 - 2\eta \langle \nabla f(x_t), x_t - x^\star \rangle + \eta^2 \|\nabla f(x_t)\|_\sharp^2$$
$$\leq \|x_t - x^\star\|_\sharp^2 - c\alpha\eta \|x_t - x^\star\|_\sharp^2 - \left(c\eta\beta - \eta^2\right) \|\nabla f(x_t)\|_\sharp^2$$

c is problem dependent

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- We know from convex analysis that

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

$$\langle \nabla f(x), x - x^\star \rangle \geq \frac{\mu L}{\mu + L} \|x - x^\star\|_2^2 + \frac{1}{\mu + L} \|\nabla f(x)\|_2^2$$

  and compare with

$$\langle \nabla f(x_t), x_t - x^\star \rangle \geq \alpha \|x_t - x^\star\|_\sharp^2 + \beta \|\nabla f(x_t)\|_\sharp^2$$

Local convergence guarantees for $UU^\top$

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

– Define **distance function**:

$$\textsc{Dist}(U,\ U^\star R) := \min_R \|U - U^\star R\|_F$$

(This is the $\|\cdot\|_\sharp$ distance for this problem)

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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 $(U^\star, V^\star)$, then **non-convex** alternating gradient descent **i)** converges to $(U^\star, V^\star)$, 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*

i.e., if we are sufficiently close to the optimal point.

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Convergence to global minimum for non-convex optimization!

Main result: Proper initialization and global convergence

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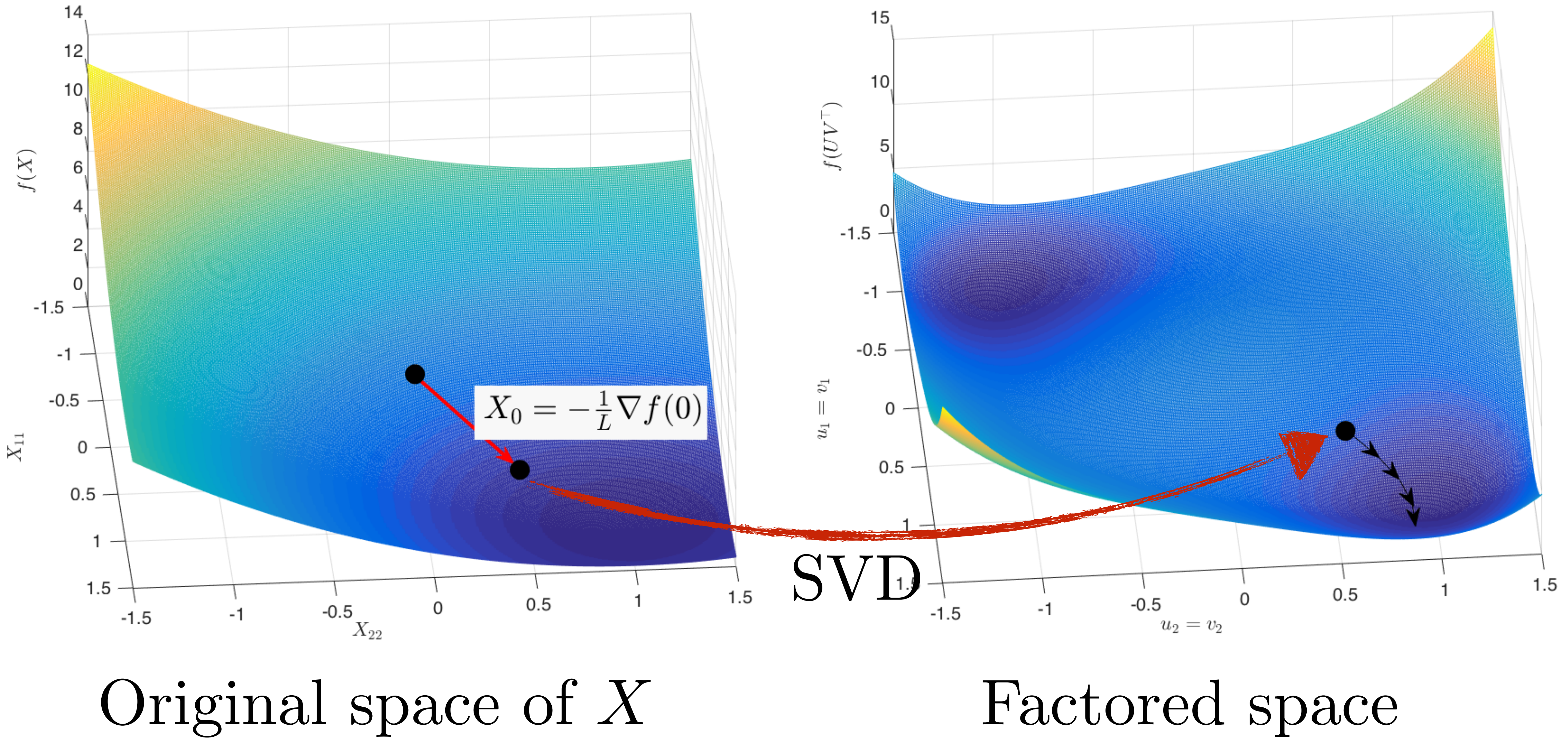
- **Proposed initialization:**
  - Compute $X_0 \propto -\nabla f(0)$
  - Perform one SVD calculation:

$$X_0 = U_0 V_0^\top$$



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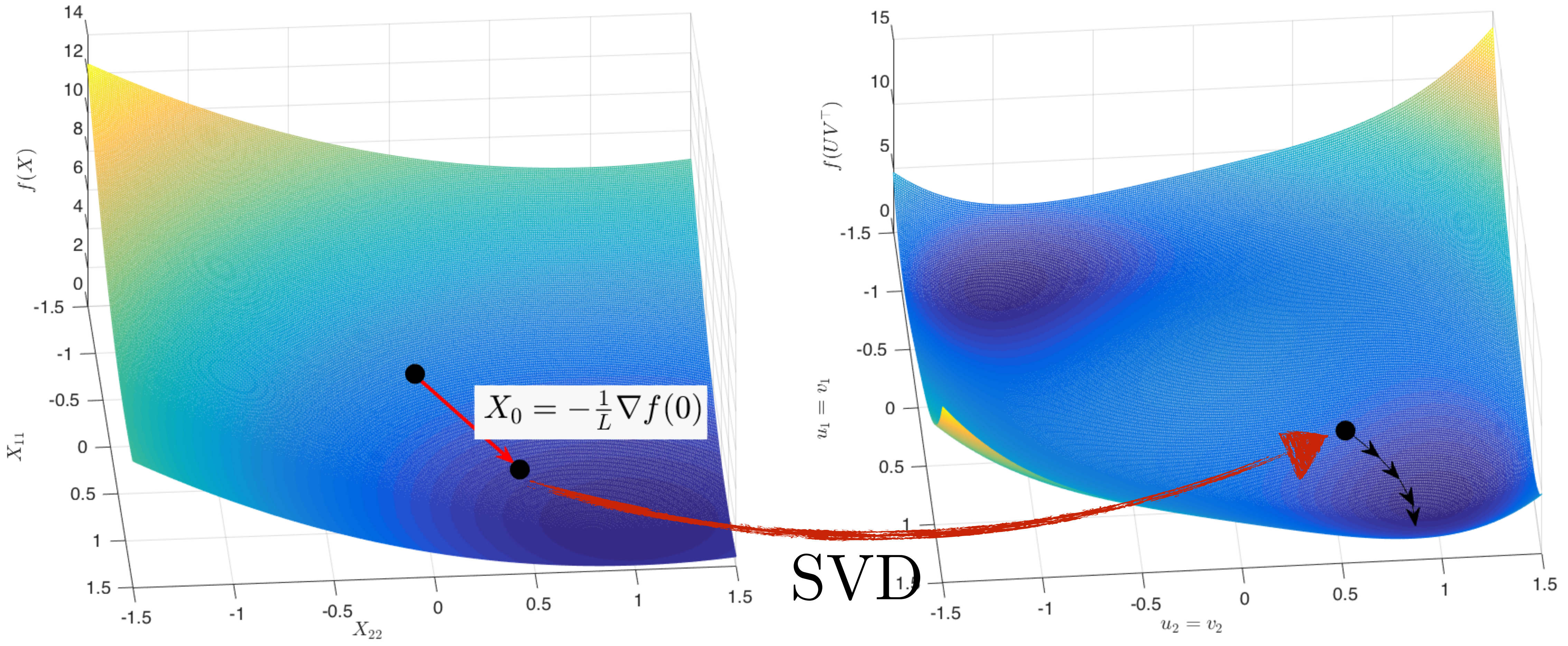

Original space of X

Factored space

THEOREM: GLOBAL CONVERGENCE

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

Condition number: ratio of smoothness over strong convexity parameters

Main result: Proper initialization and global convergence

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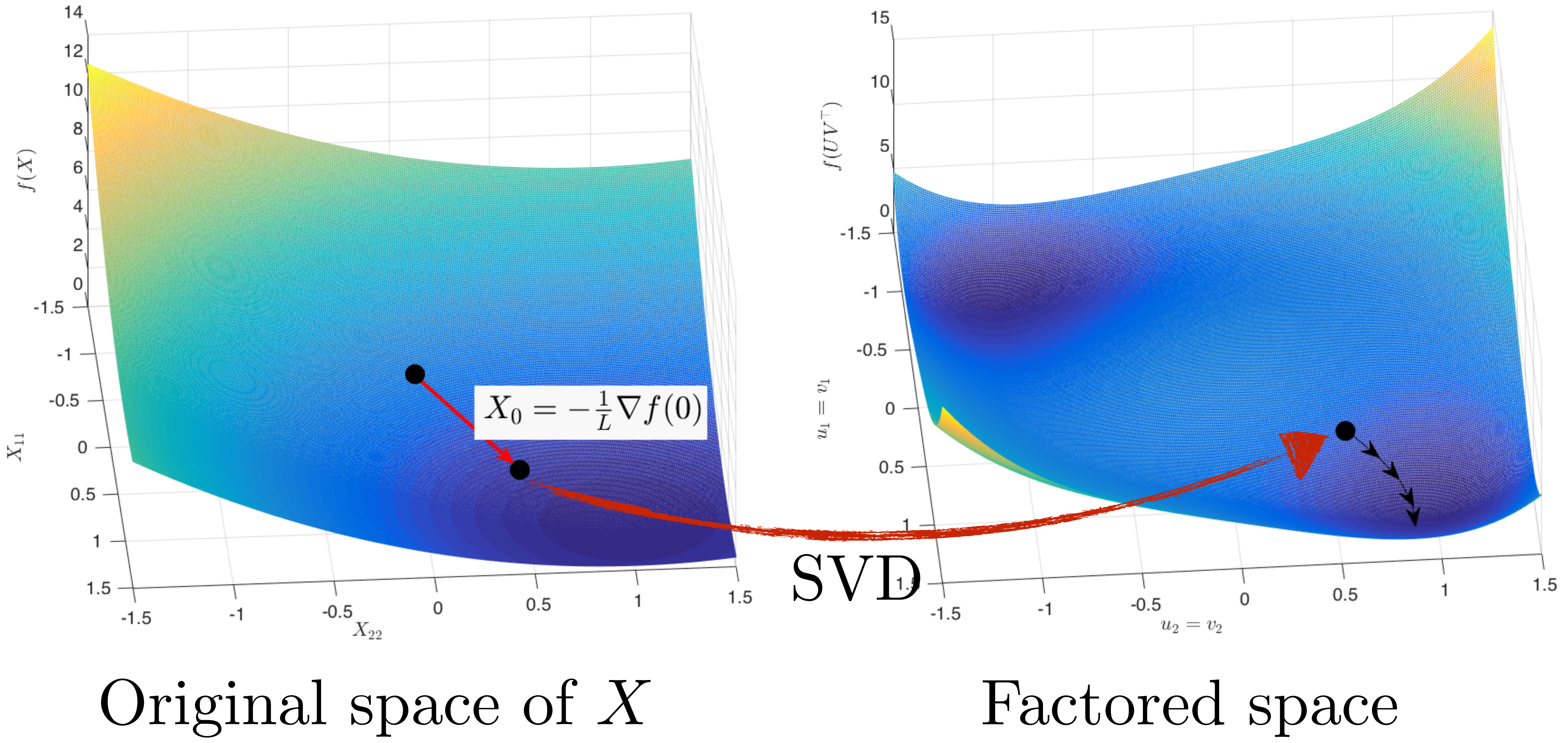

PRACTICAL IMPACT

One SVD *(non-convex)* **vs.** **SVD per iteration!** *(convex)*

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

.. by using $(U_{t+1}, V_{t+1}) = (U_t, V_t) - \eta(\nabla f(U_t V_t^\top) V_t, \nabla f(U_t V_t)^\top U_t)$

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– There are initializations that come with some convergence guarantees

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

(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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– What if we don't know the exact rank? (Open question)

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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 scenaria