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

Lecture 2

Overview

- Different objective classes
- Different strategies within each problem
- Different approaches based on computational capabilities
- Different approaches based on constraints

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

And, always having in mind applications in machine learning, AI and signal processing

About what we have talked so far

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

About what we have talked so far

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

$$\cancel{\text{s.t.} \quad x \in \mathcal{C}}$$

Unconstrained

About what we have talked so far

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

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Unconstrained

About what we have talked so far

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- There is a lot of work on such settings (mostly in the convex domain)

(Early stage of modern ML, but out of scope of this course)

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Unconstrained

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(Early stage of modern ML, but out of scope of this course)

- We focused though on complex ways to deal with such problems: **asynchrony**

(We proved convergence under standard conditions and staleness conditions)

The focus of this lecture

Huge!

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The focus of this lecture

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  - Inspired by modern ML (neural networks), we will describe alternatives to SGD:
    - Accelerated SGD
    - AdaGrad
    - RMSProp
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  - Inspired by modern ML (neural networks), we will describe alternatives to SGD:
    - Accelerated SGD
    - RMSProp
    - AdaGrad
    - Adam
  - Bonus discussion: **The marginal value of adaptive methods**

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- Why SGD is preferable over full−batch GD?
  - Full−batch GD performs **redundant computations** for large datasets
  - SGD's fluctuations enables it to **jump to potentially better local minima**

- However, SGD's proof for non−convex settings is more **complicated + weaker**

SGD convergence result in non−convex scenaria

Whiteboard

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- Key observations:
  - For convergence, this theory assumes a small step size $O\left(\frac{1}{\sqrt{T}}\right)$
    - In a sense, we need to know a priori the number of iterations to achieve ε−approximation
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    - In a sense, we need to know a priori the number of iterations to achieve ε-approximation
    - Step size can be bad at the beginning – other step sizes used in practice
  - Nevertheless, in practice SGD performs favorably compared to full-batch GD.
  - Assuming more structure (e.g., PL condition), one can achieve better rates with constant step sizes (independent on the number of iterations)

Acceleration in SGD in non-convex scenaria

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Acceleration: "get better than ε^{-2}"

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(Results for specific cases – Still an open question in its most generality)

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(To get to a point such that $\|\nabla f(\cdot)\|_2 \leq \varepsilon$)

(We assume no variance reduction variants)

Acceleration in SGD in non-convex scenaria

Nevertheless, this does not prevent us from using acceleration in non-convex scenarios

https://www.tensorflow.org/api_docs/python/tf/train/MomentumOptimizer

Recall: Momentum acceleration

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– Heavy ball method

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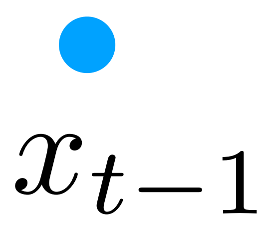

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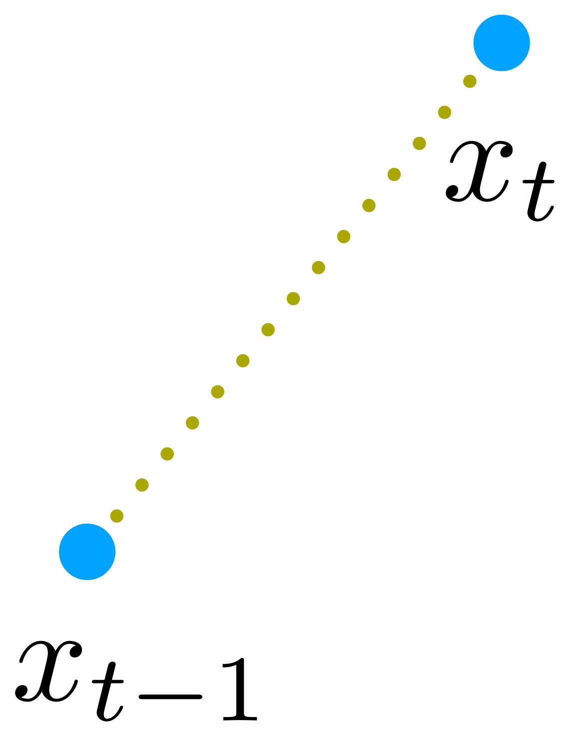
Standard gradient step   Momentum step



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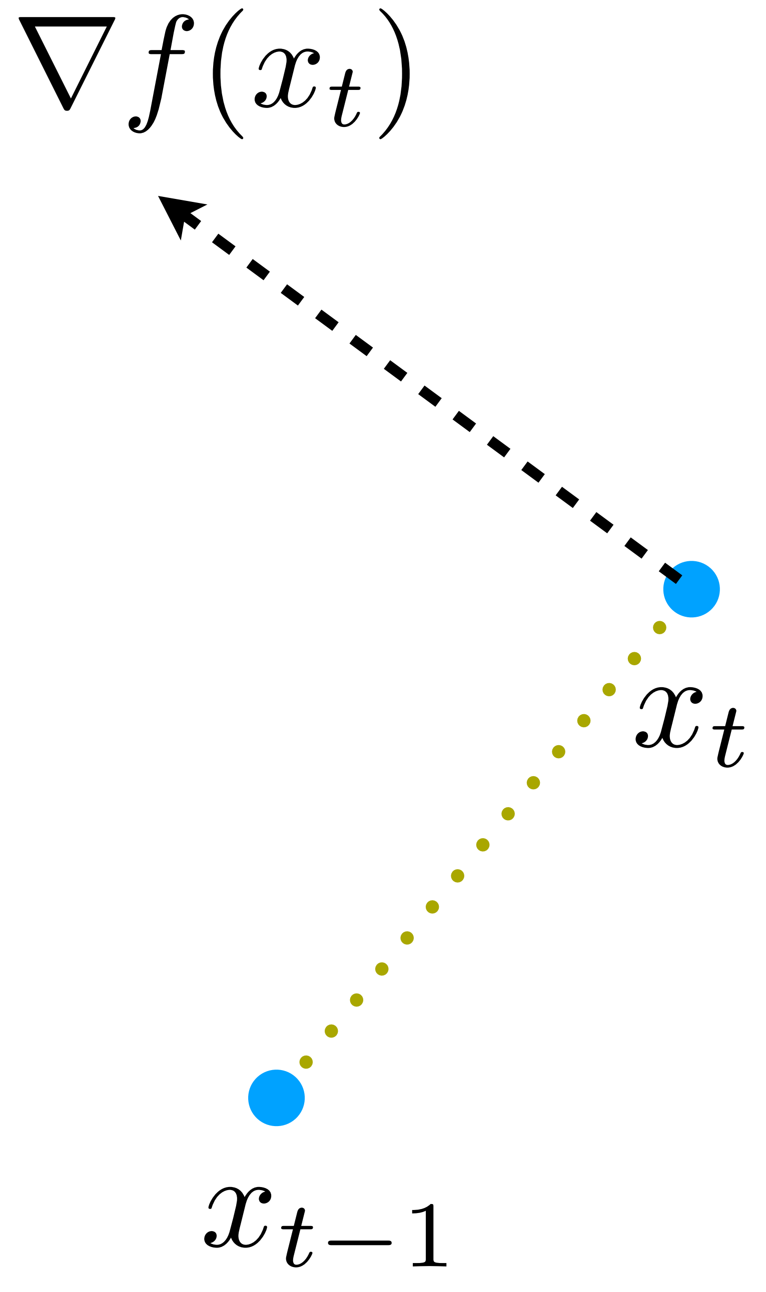

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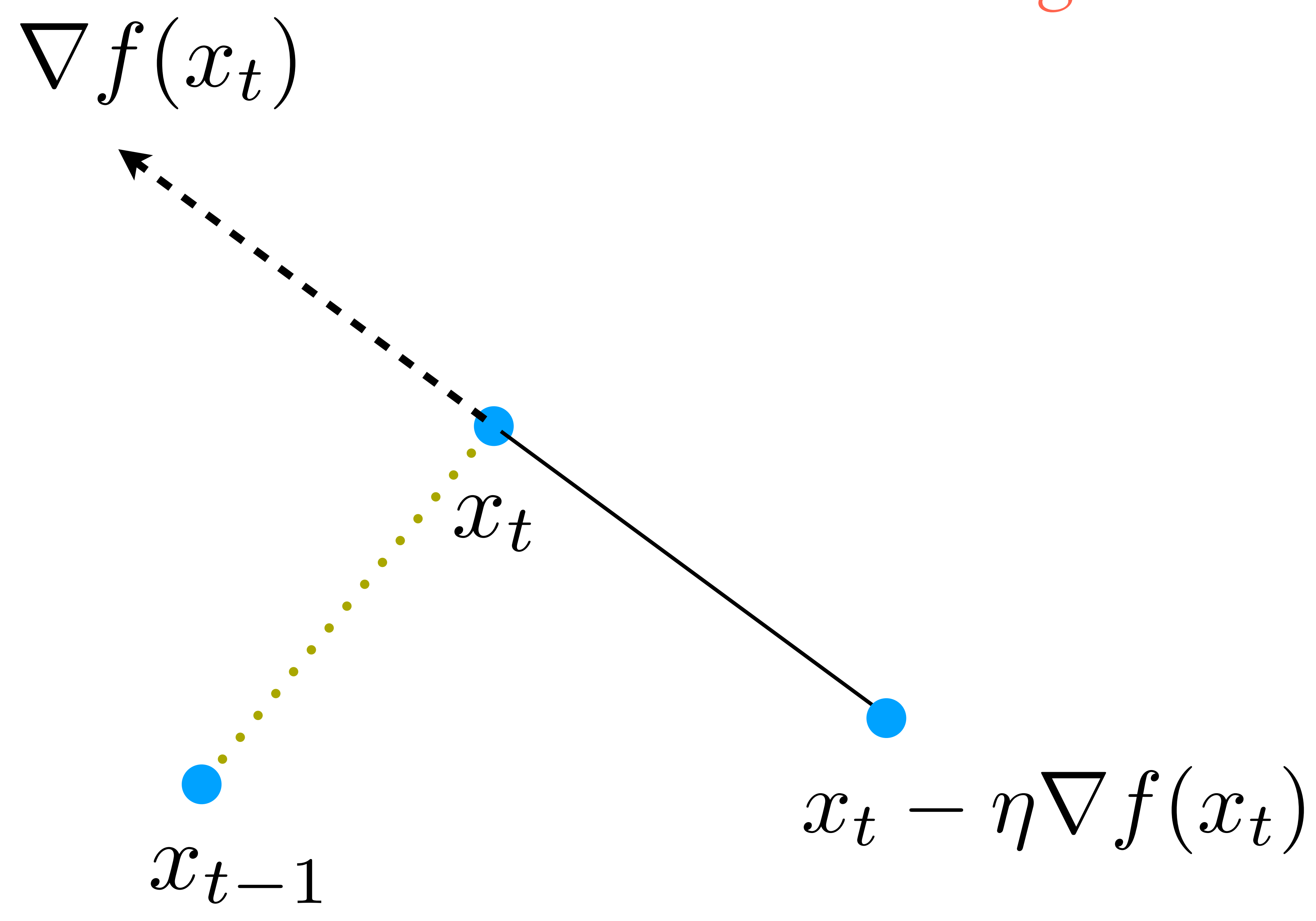

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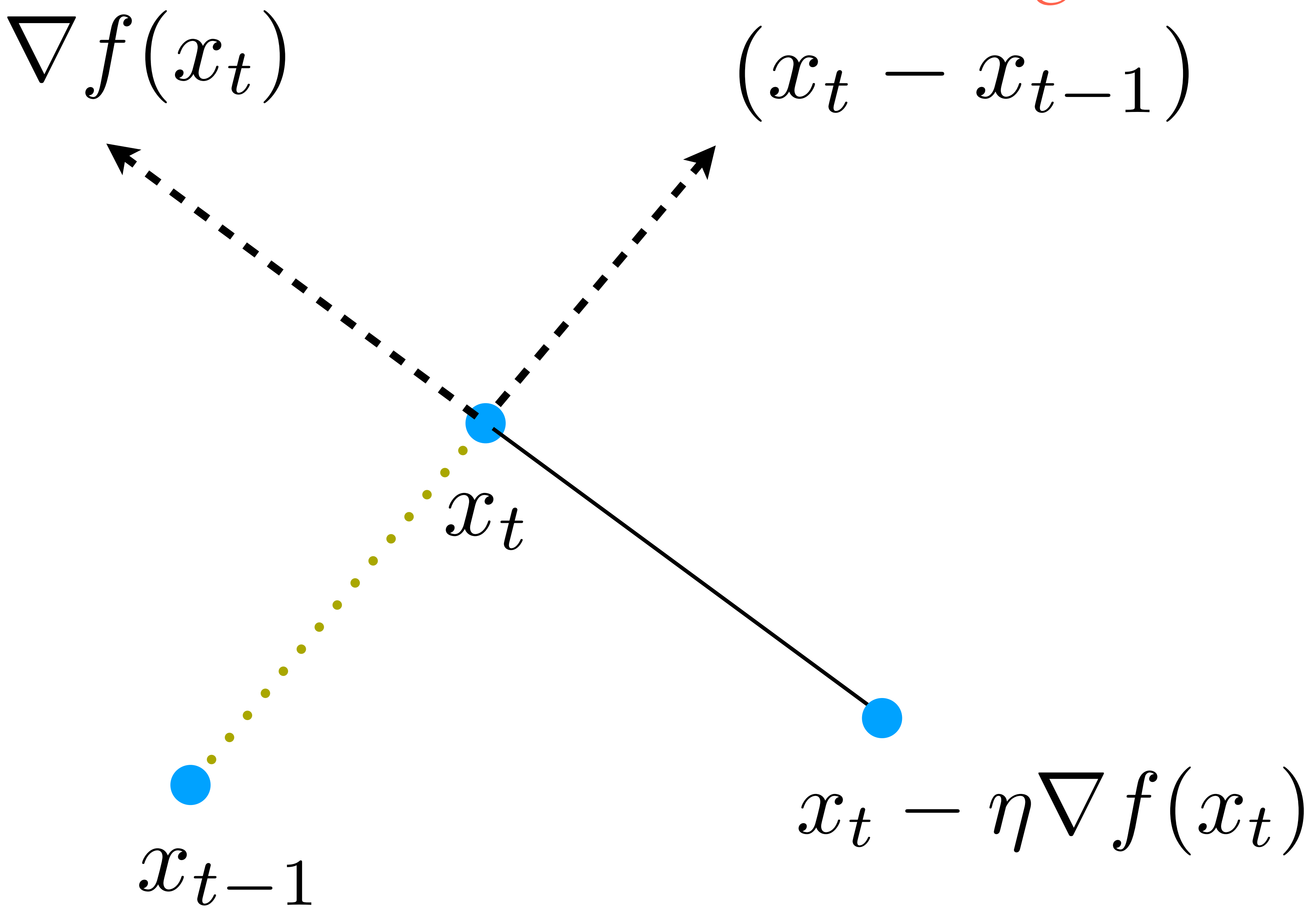

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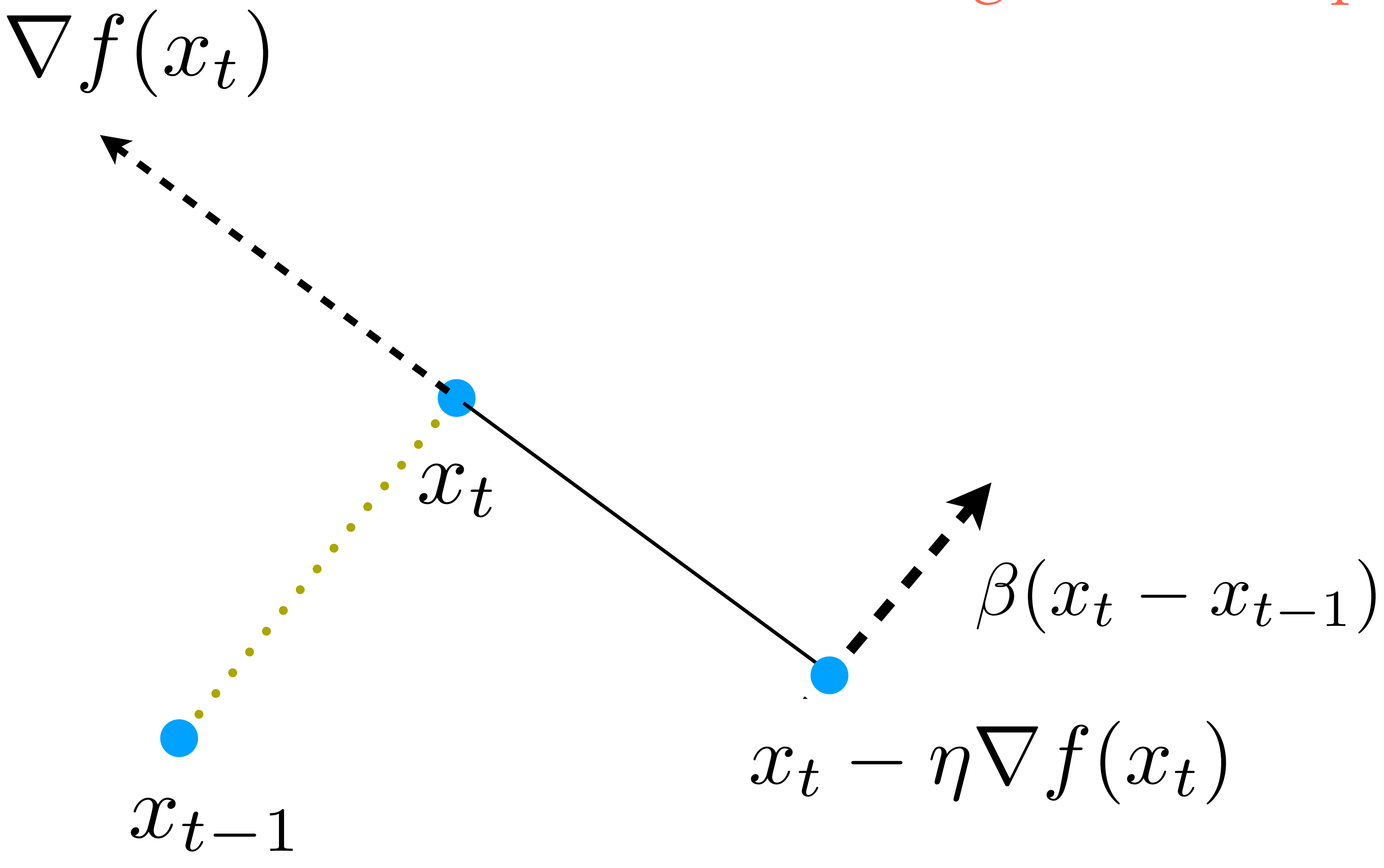

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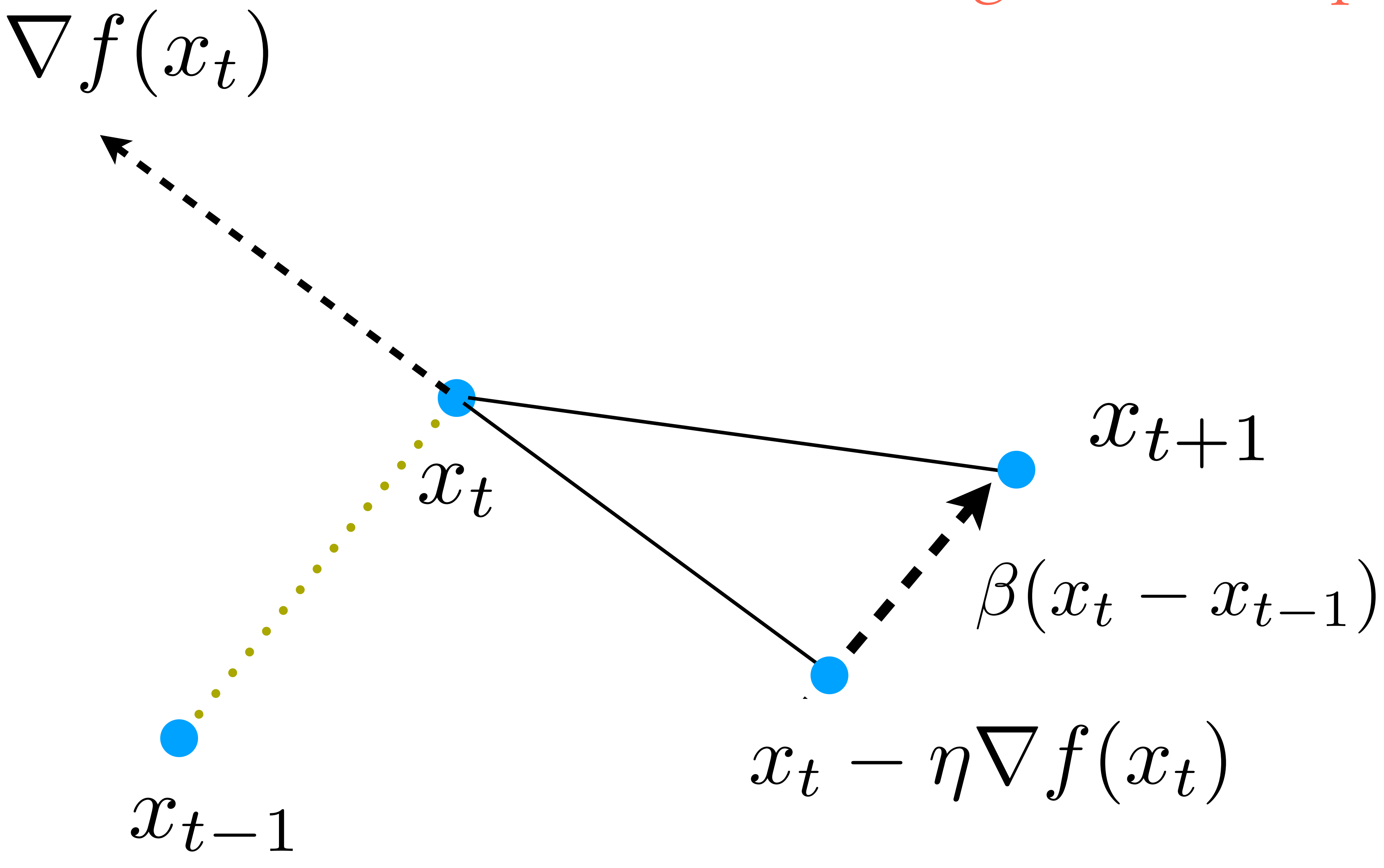

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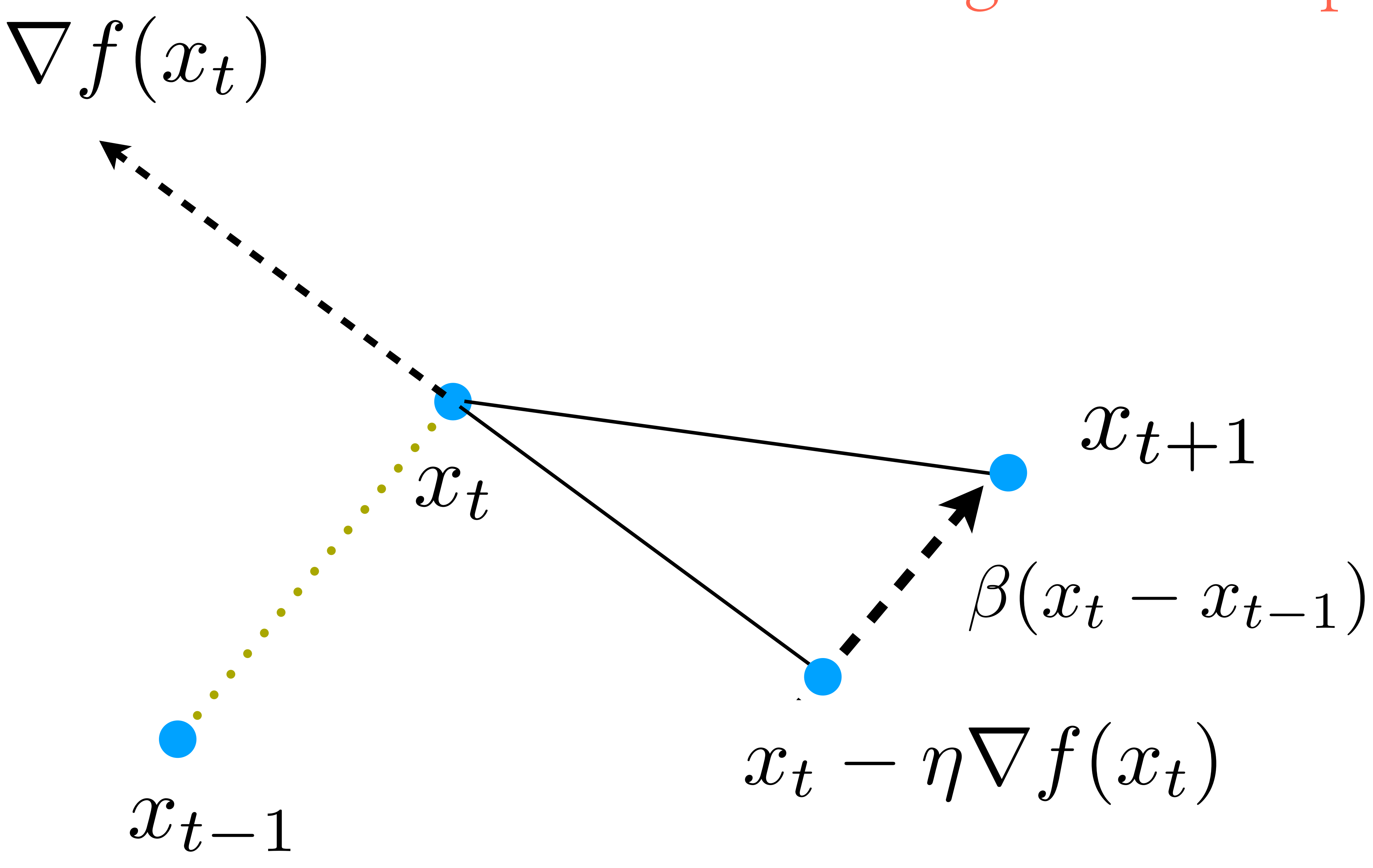

Any analogy in the physical world?

– 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 $\eta = \frac{4}{\sqrt{L} + \sqrt{\mu}}$ *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

Non−convex!

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$$\Downarrow$$

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

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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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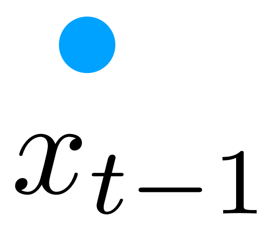

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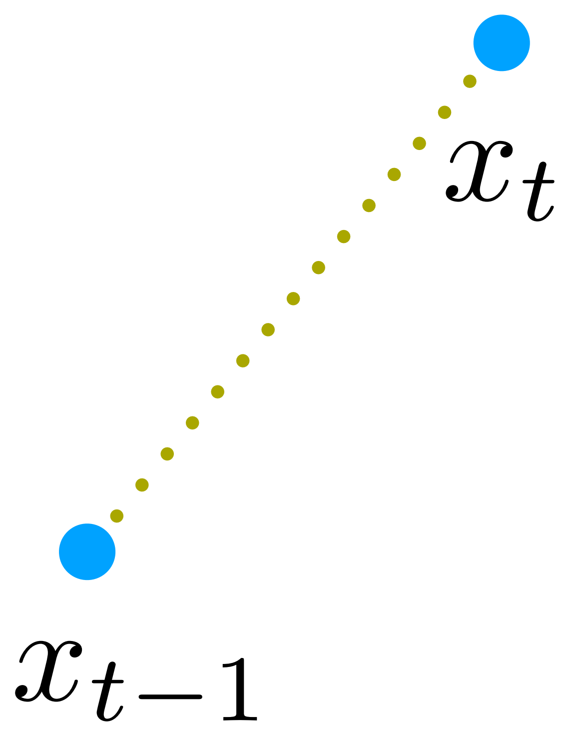

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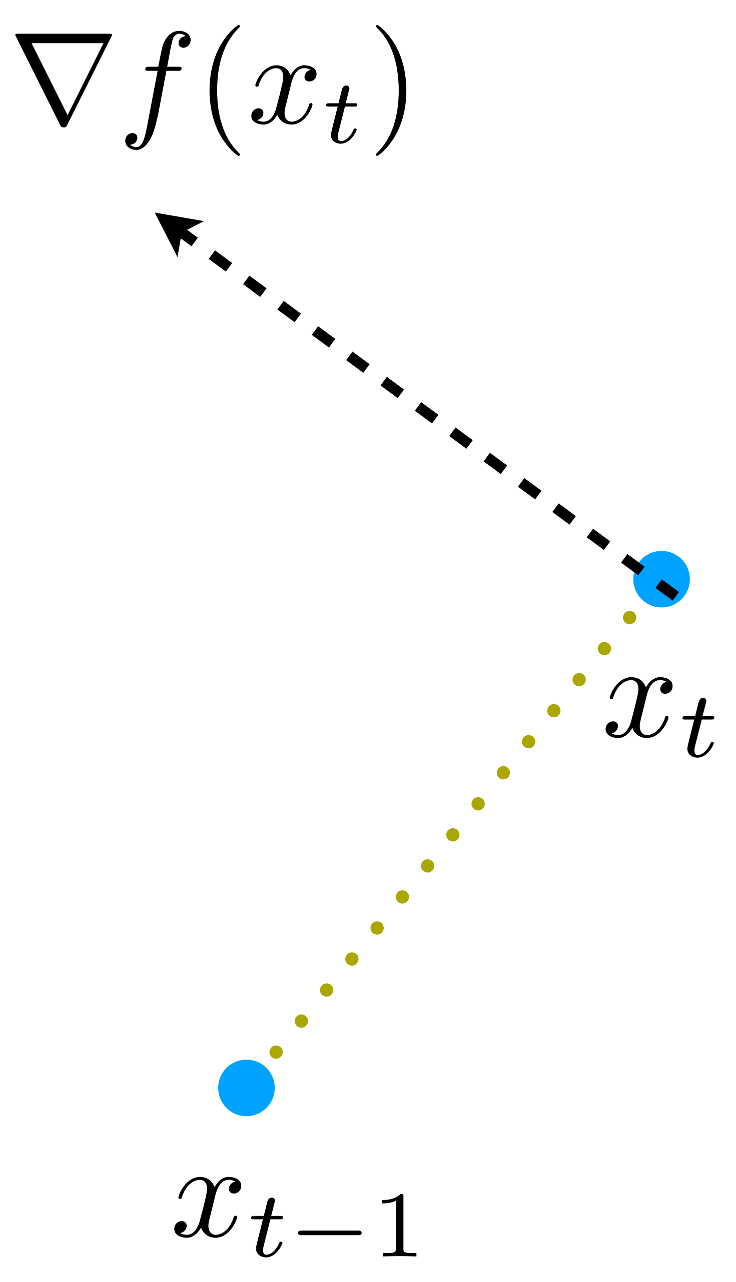

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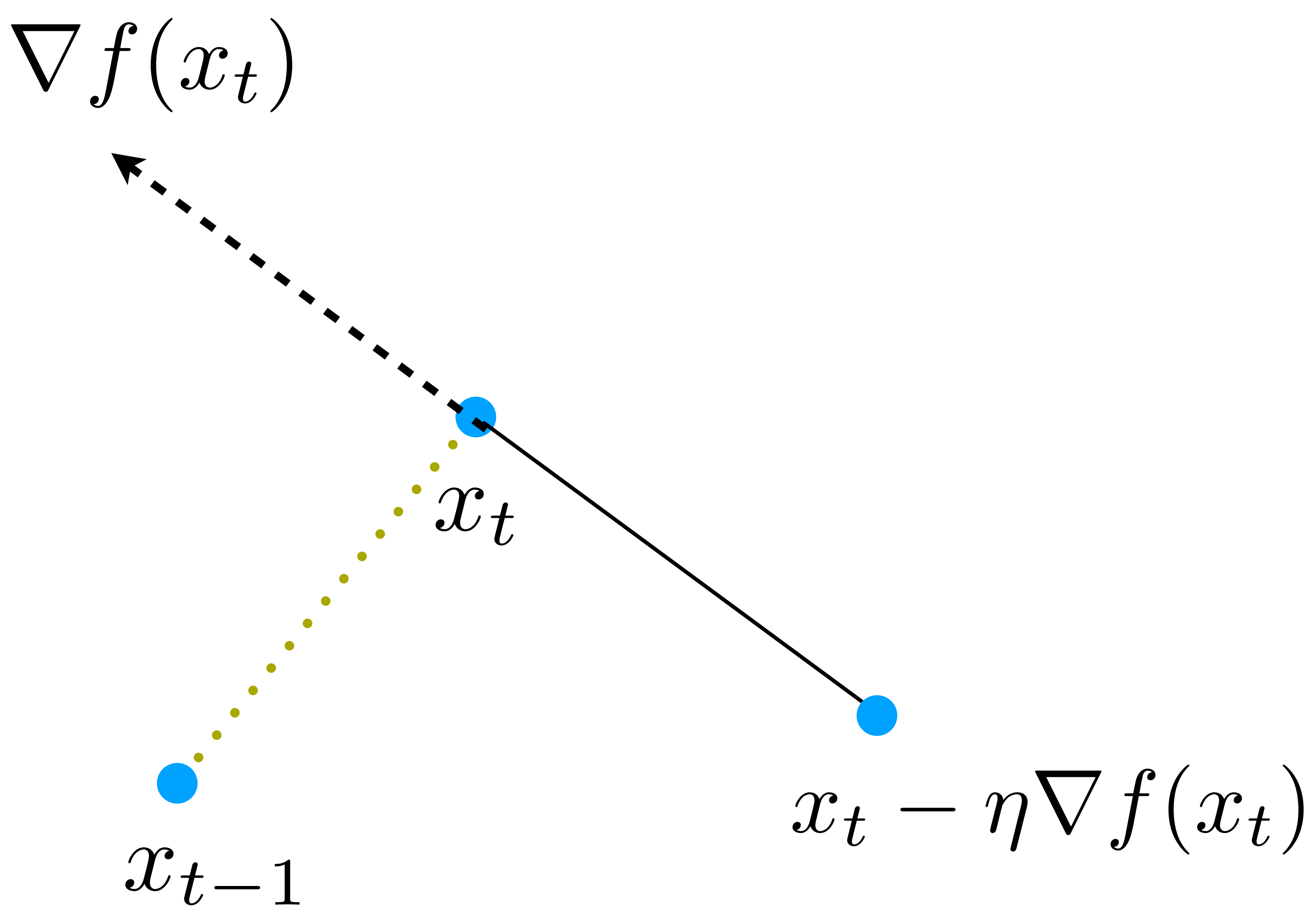

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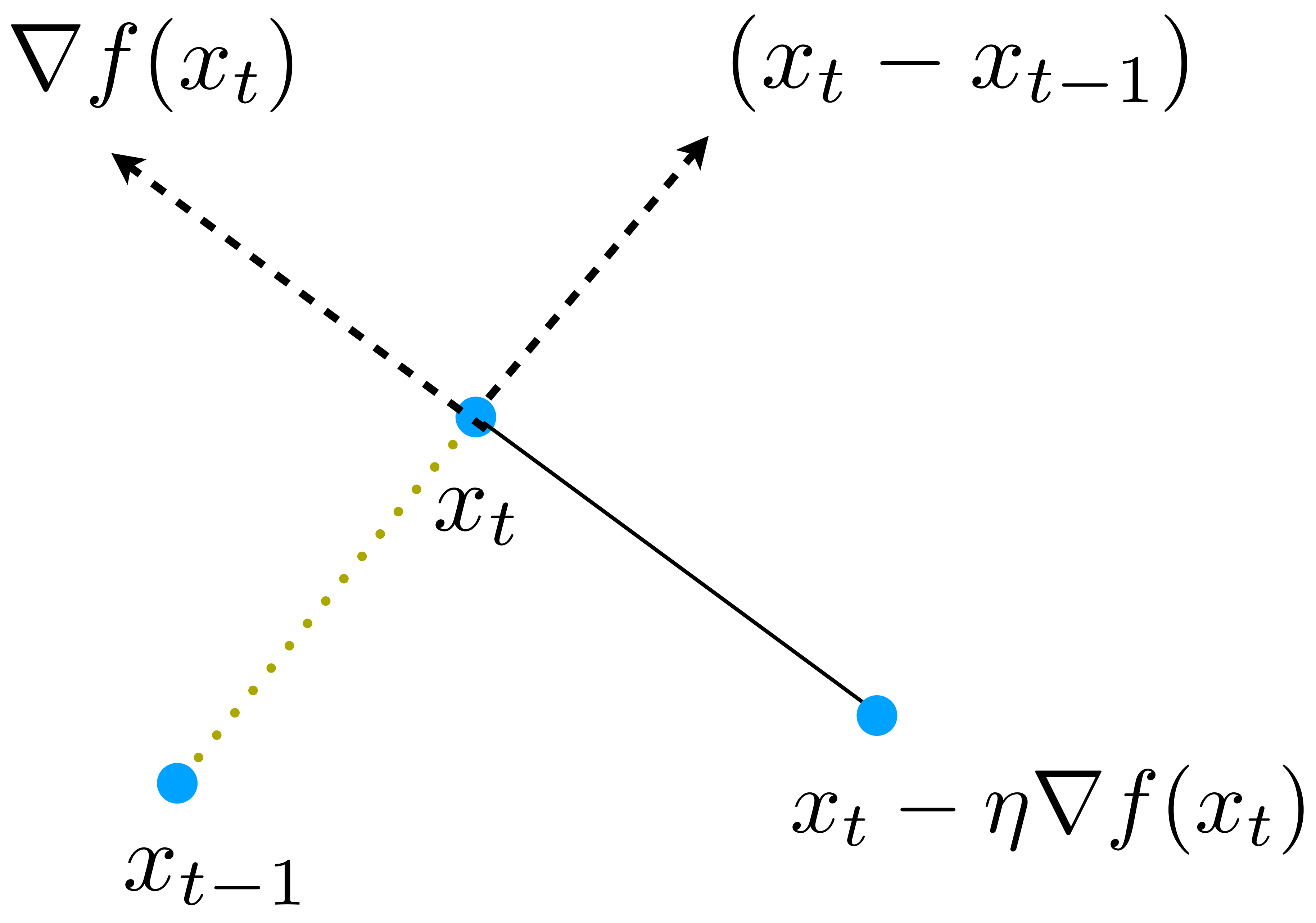

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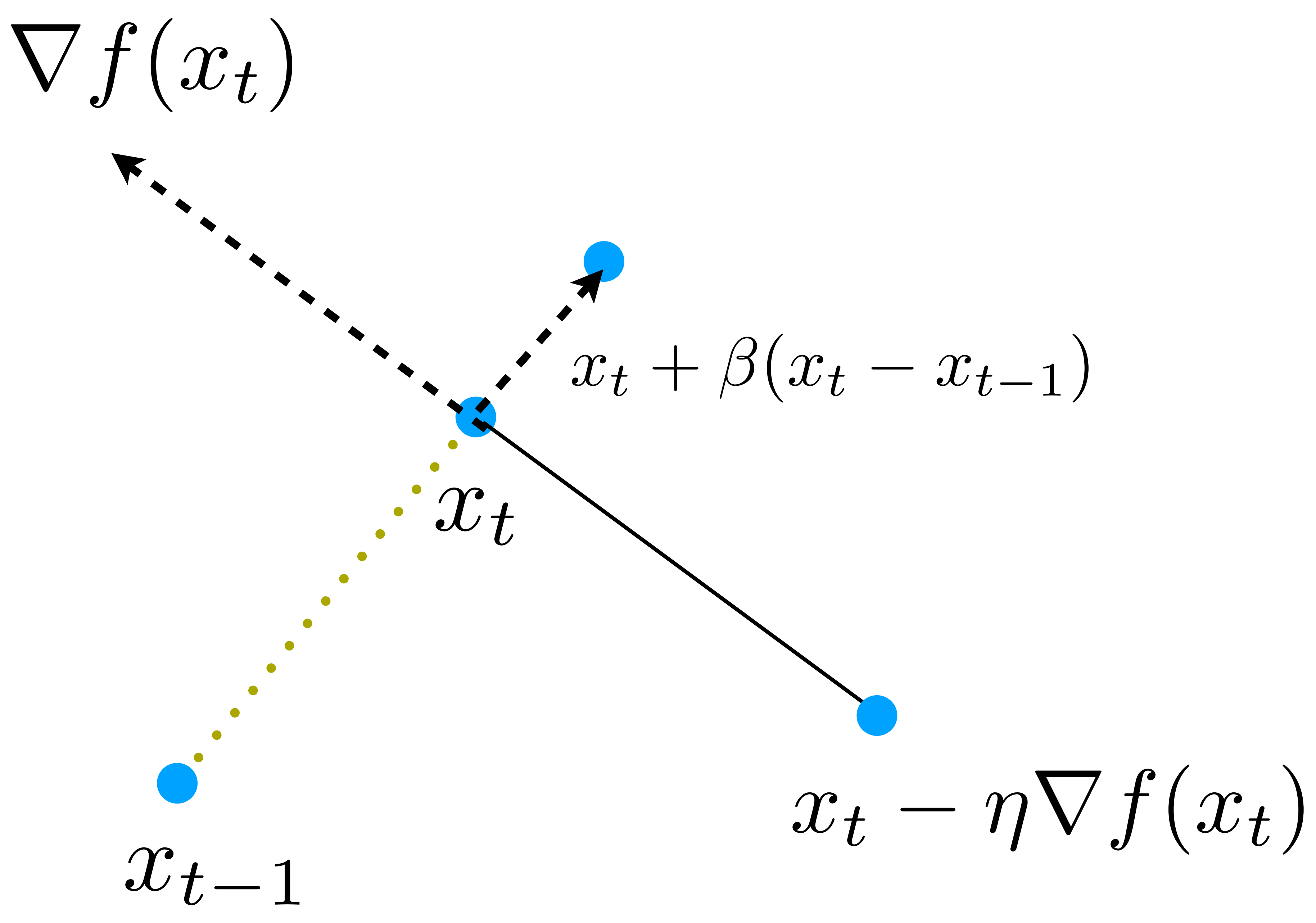

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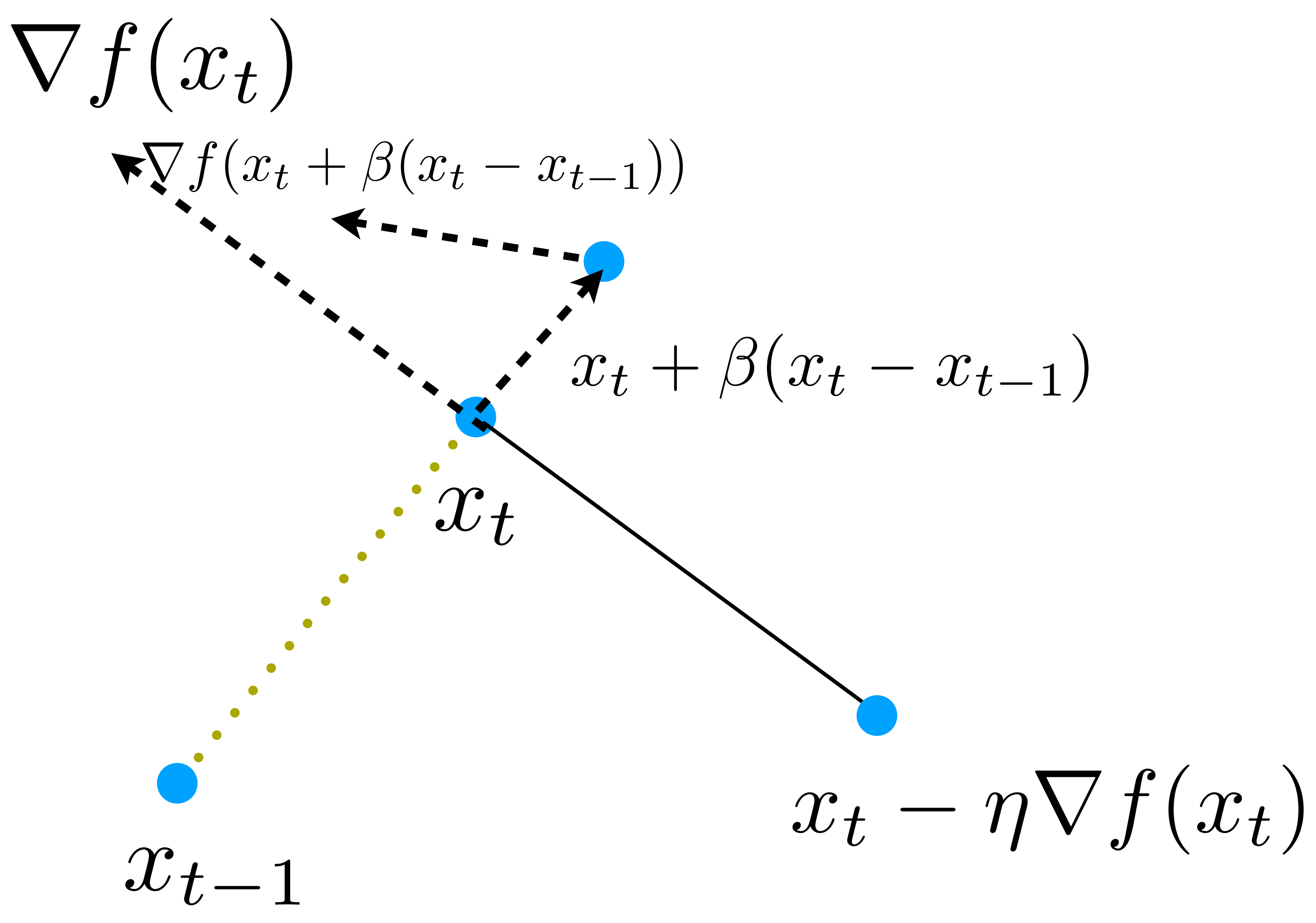

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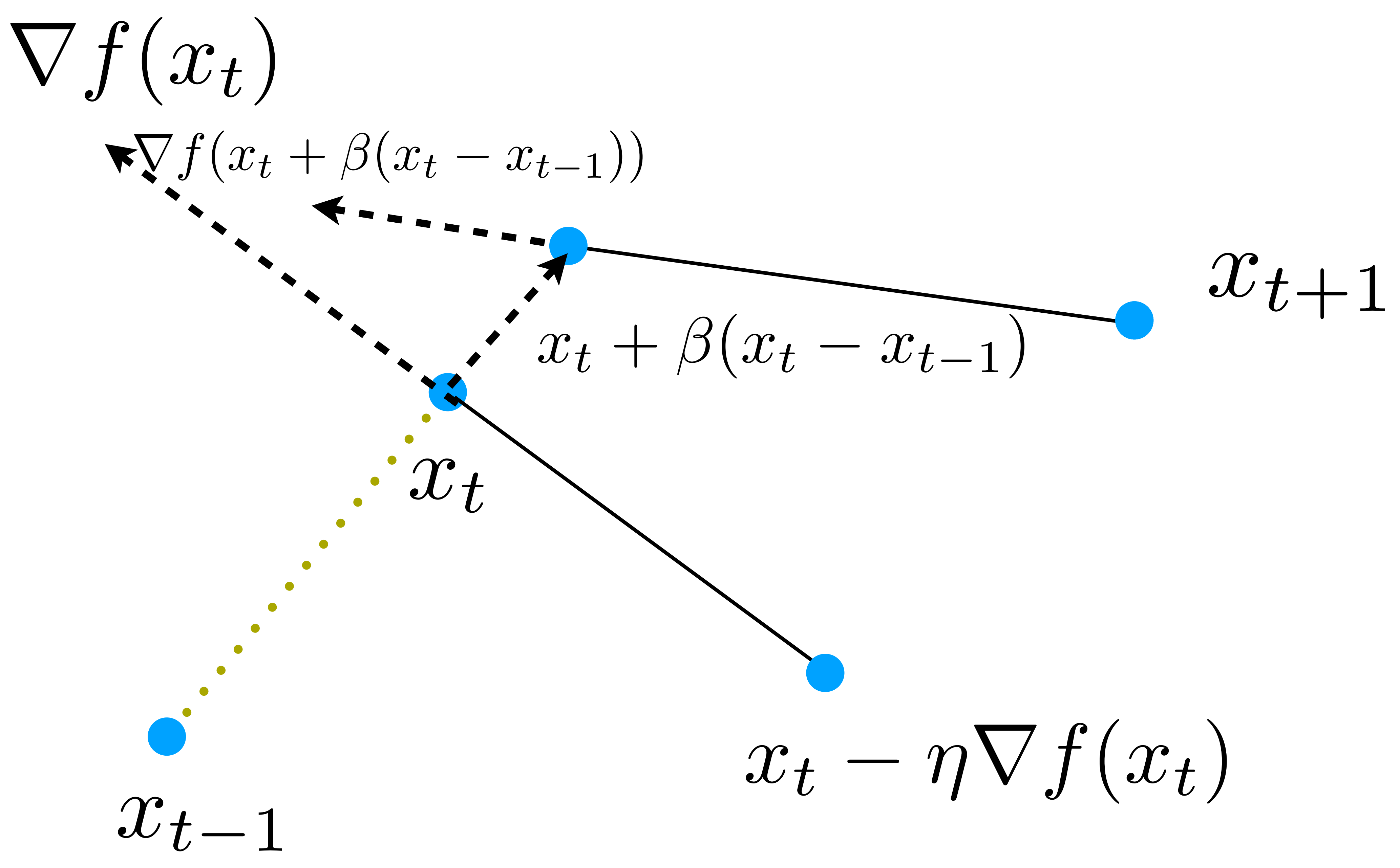

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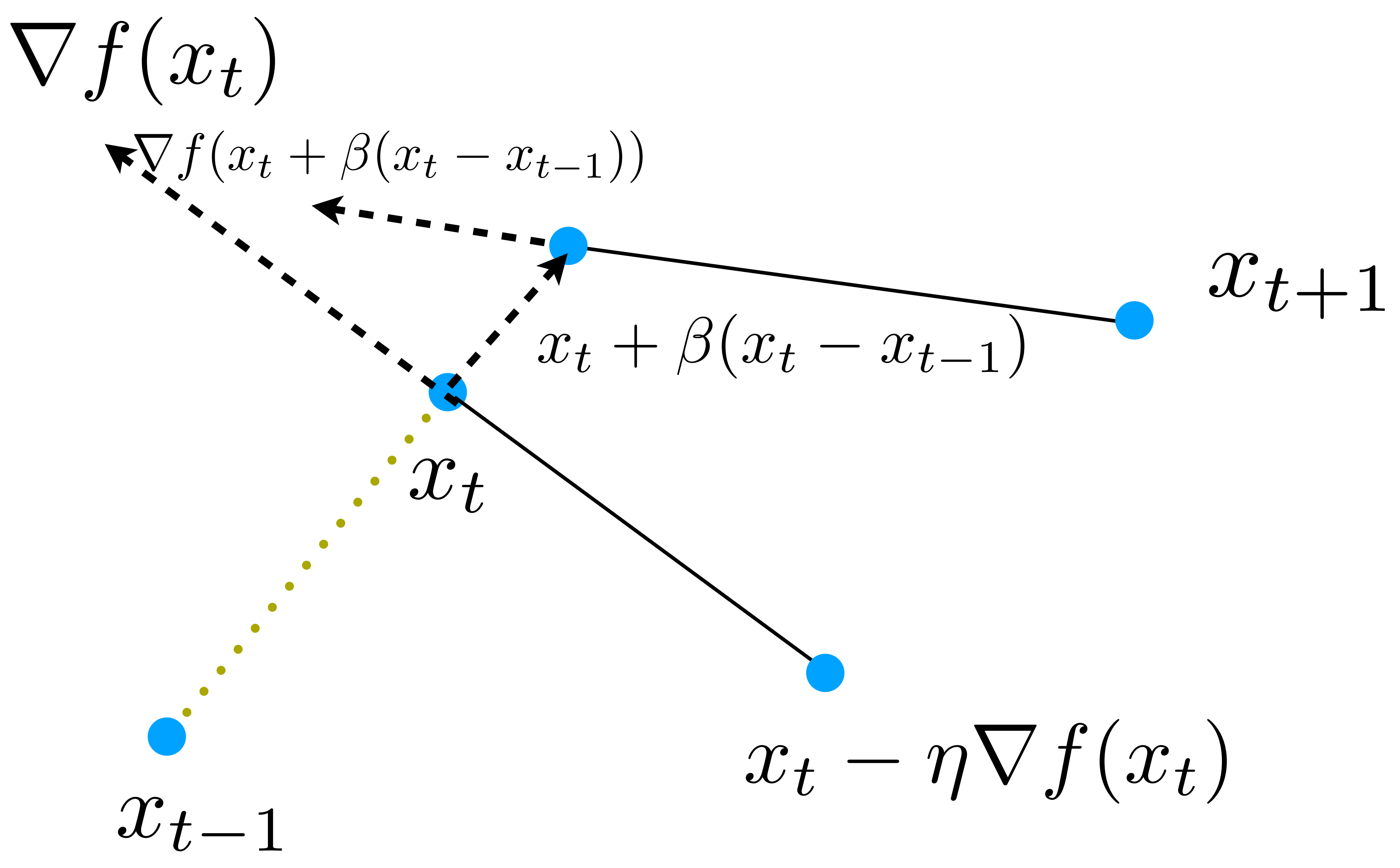

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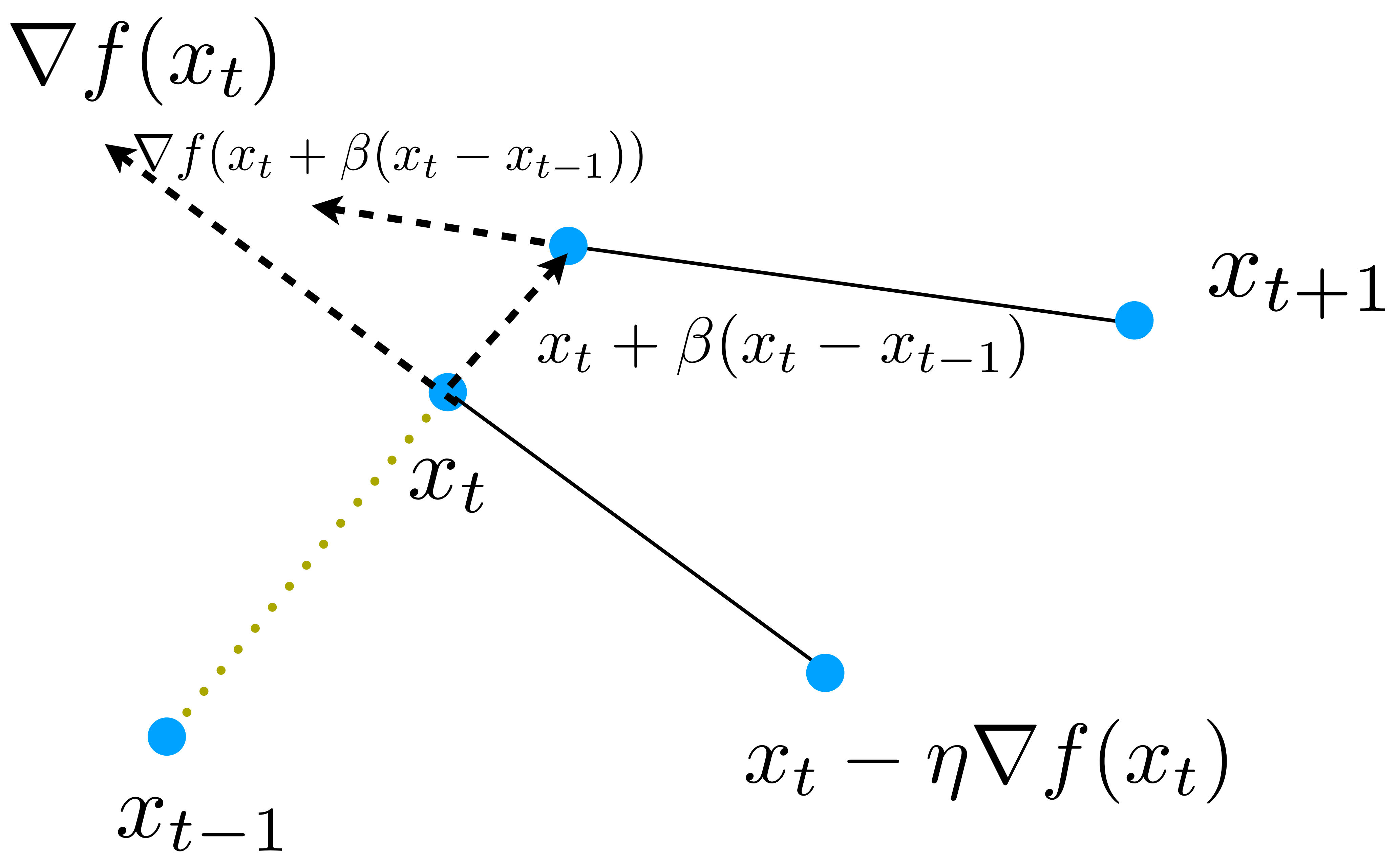

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- Heavy ball can fail converging in cases where Nesterov's scheme still succeeds

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One of the mysteries of optimization..

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(A Google algorithm that found application to "Large-scale distributed deep networks" paper)

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What is this quantity?

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Recall: Preconditioning algorithms (BFGS, SR1) in lecture 3

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Avoids division with zero

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– "Are there guarantees for AdaGrad?"

– Yes, in the convex case, using regret bounds – see Literature section

AdaGrad pseudocode

while stopping criterion not met **do**

Sample a minibatch of m examples from the training set $\{\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(m)}\}$ with corresponding targets $\boldsymbol{y}^{(i)}$.

Compute gradient: $\boldsymbol{g} \leftarrow \frac{1}{m} \nabla_{\boldsymbol{\theta}} \sum_i L(f(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}), \boldsymbol{y}^{(i)})$

Accumulate squared gradient: $\boldsymbol{r} \leftarrow \boldsymbol{r} + \boldsymbol{g} \odot \boldsymbol{g}$

Compute update: $\Delta\boldsymbol{\theta} \leftarrow -\frac{\epsilon}{\delta + \sqrt{\boldsymbol{r}}} \odot \boldsymbol{g}$. (Division and square root applied element-wise)

Apply update: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \Delta\boldsymbol{\theta}$

end while

AdaGrad in practice

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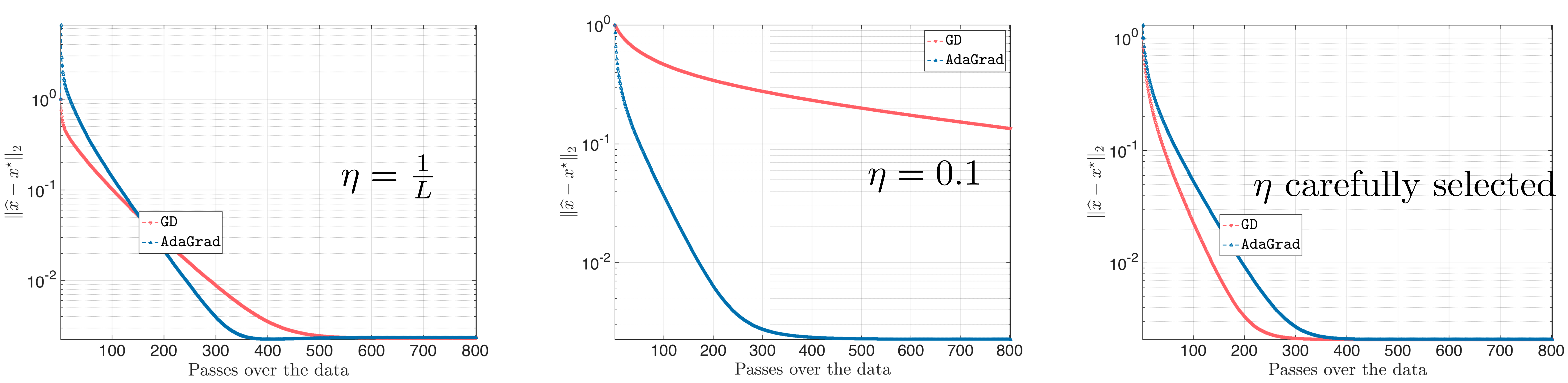
Well-conditioned
linear regression



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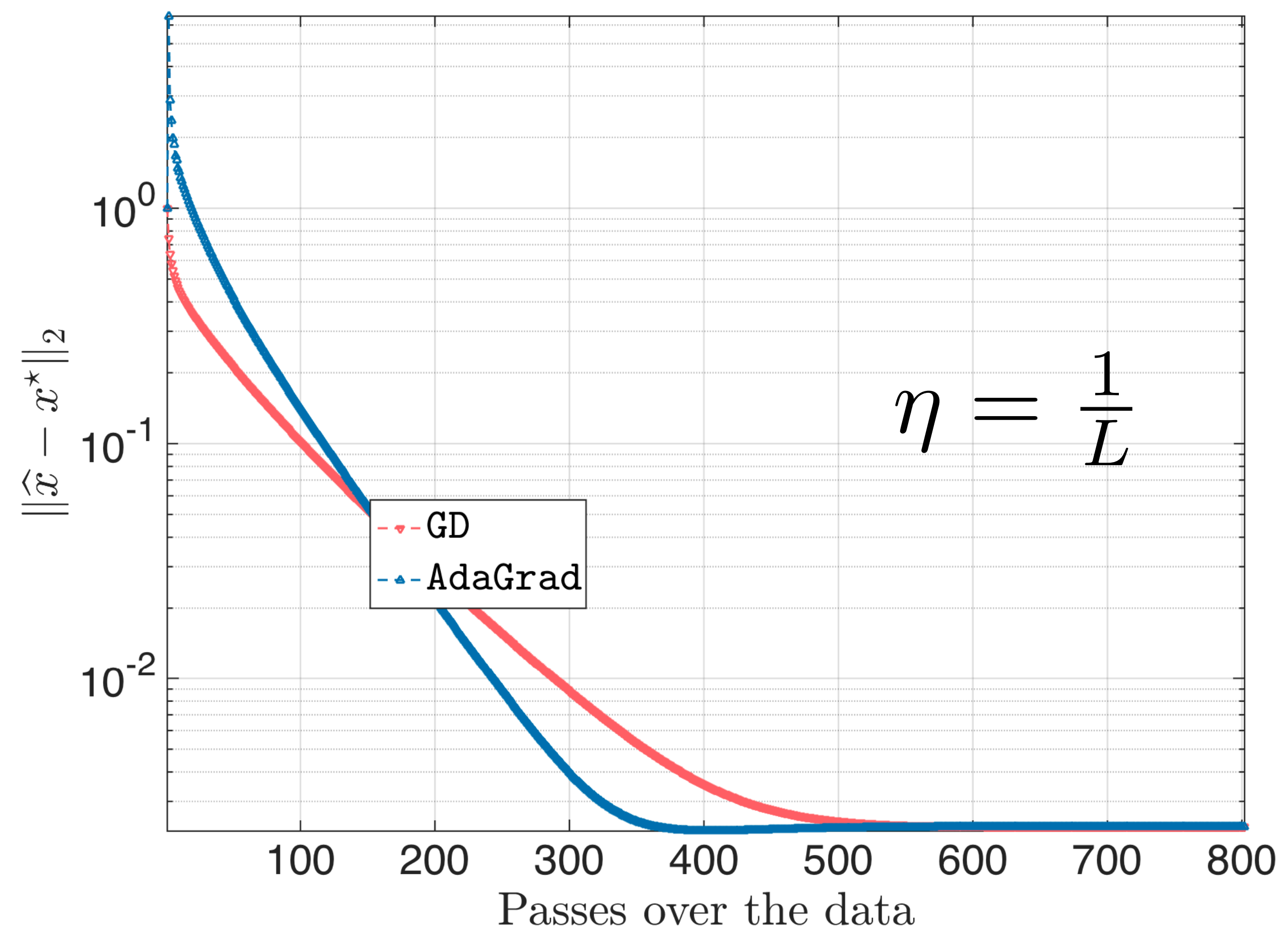

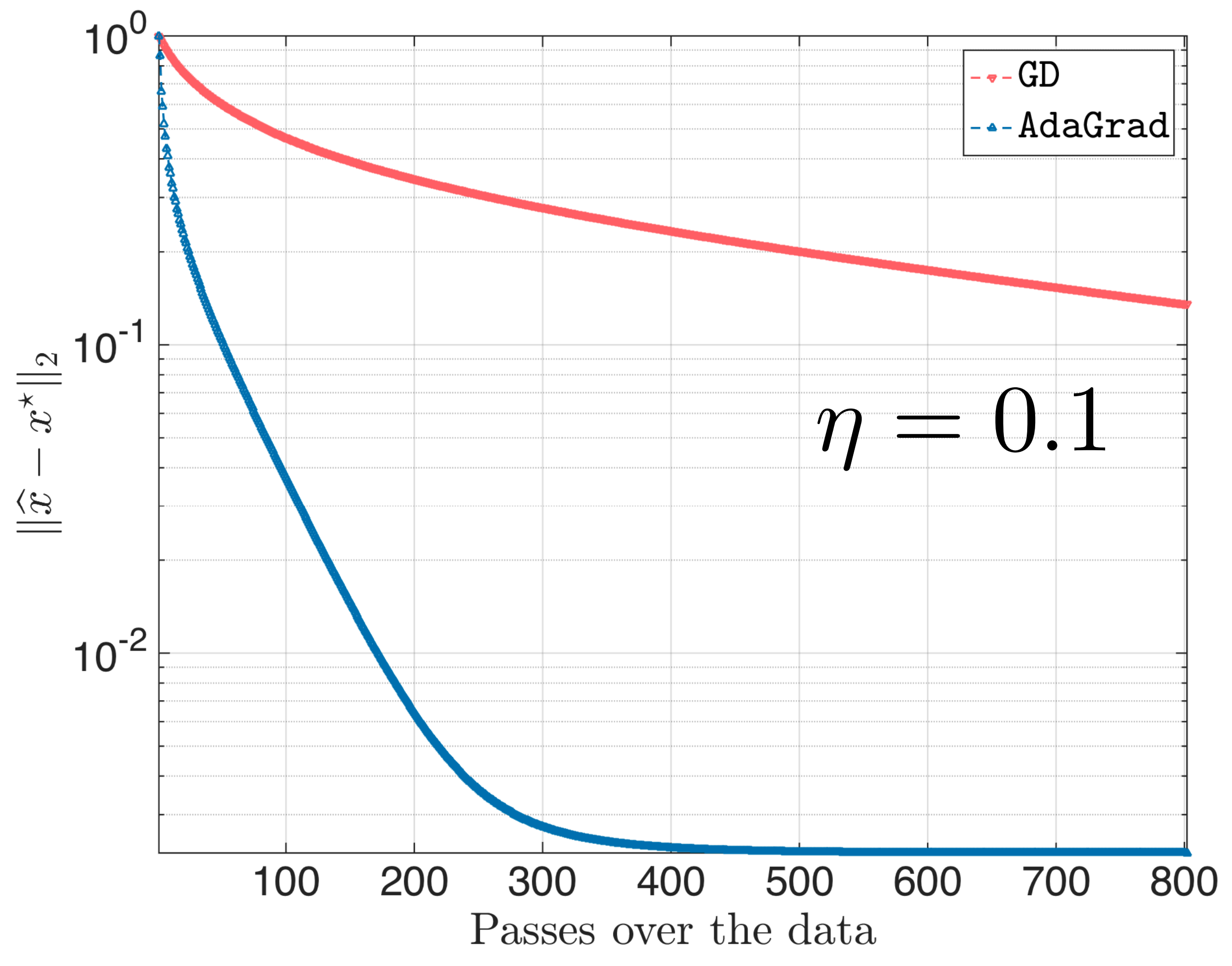

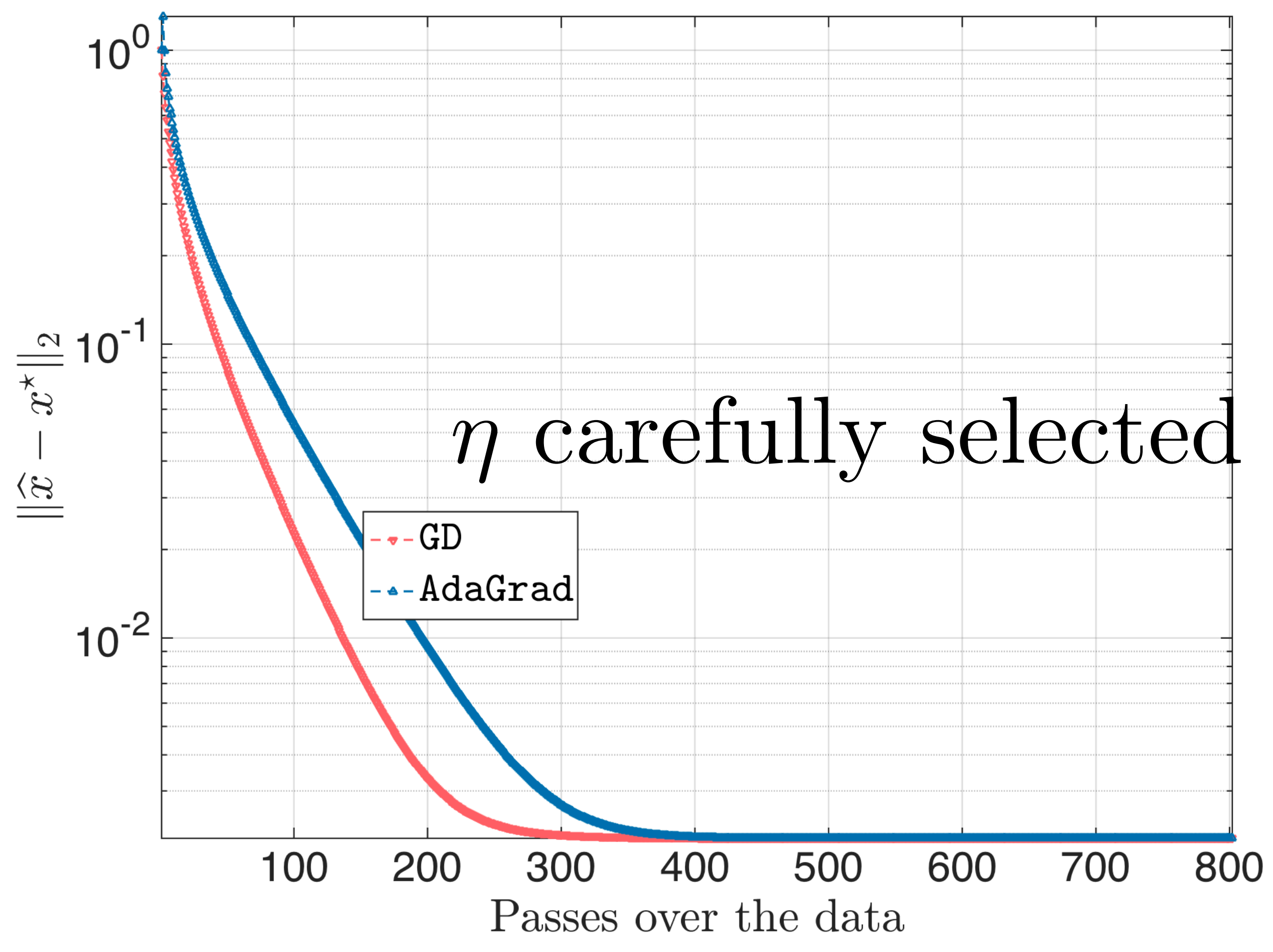

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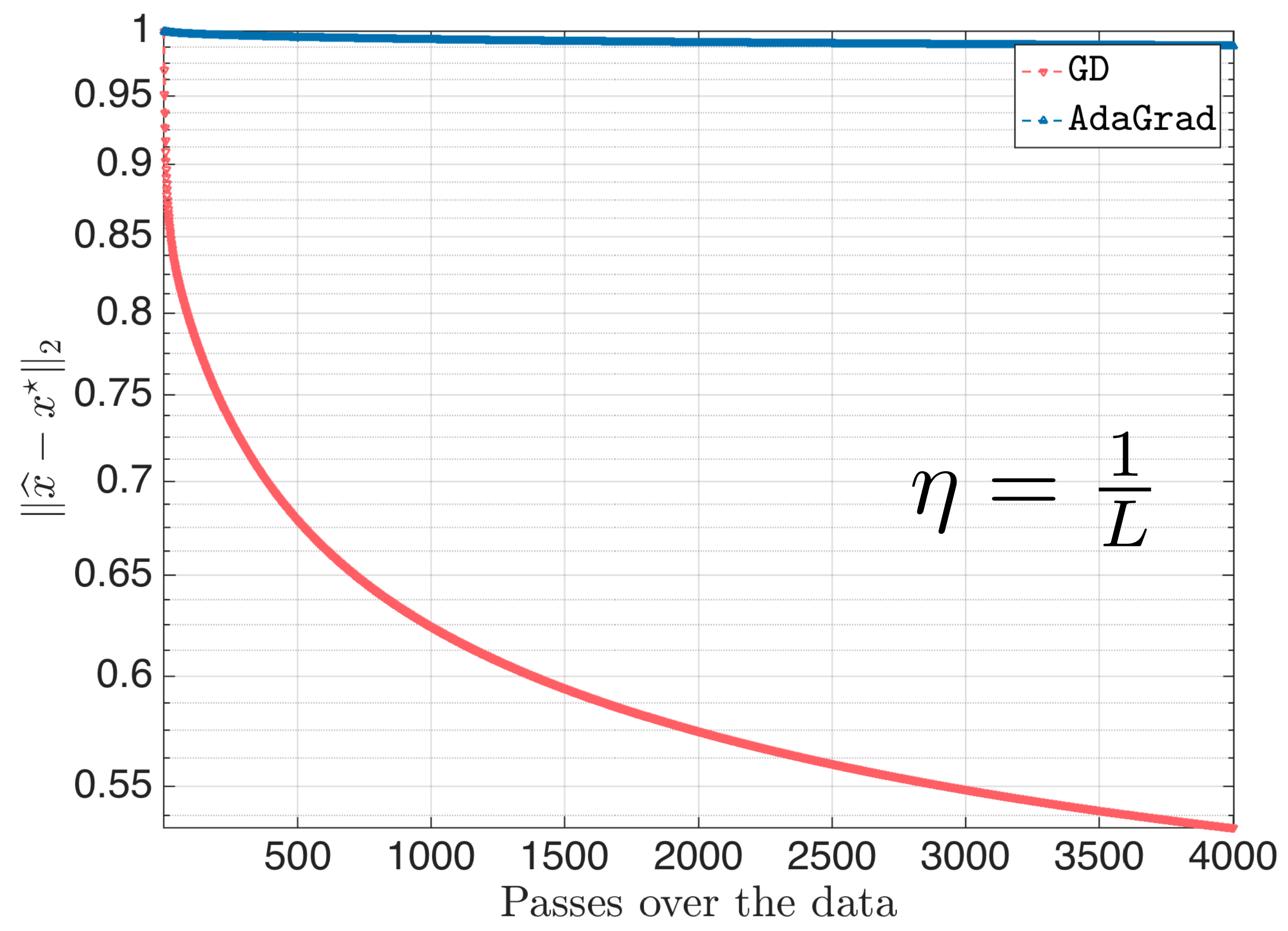
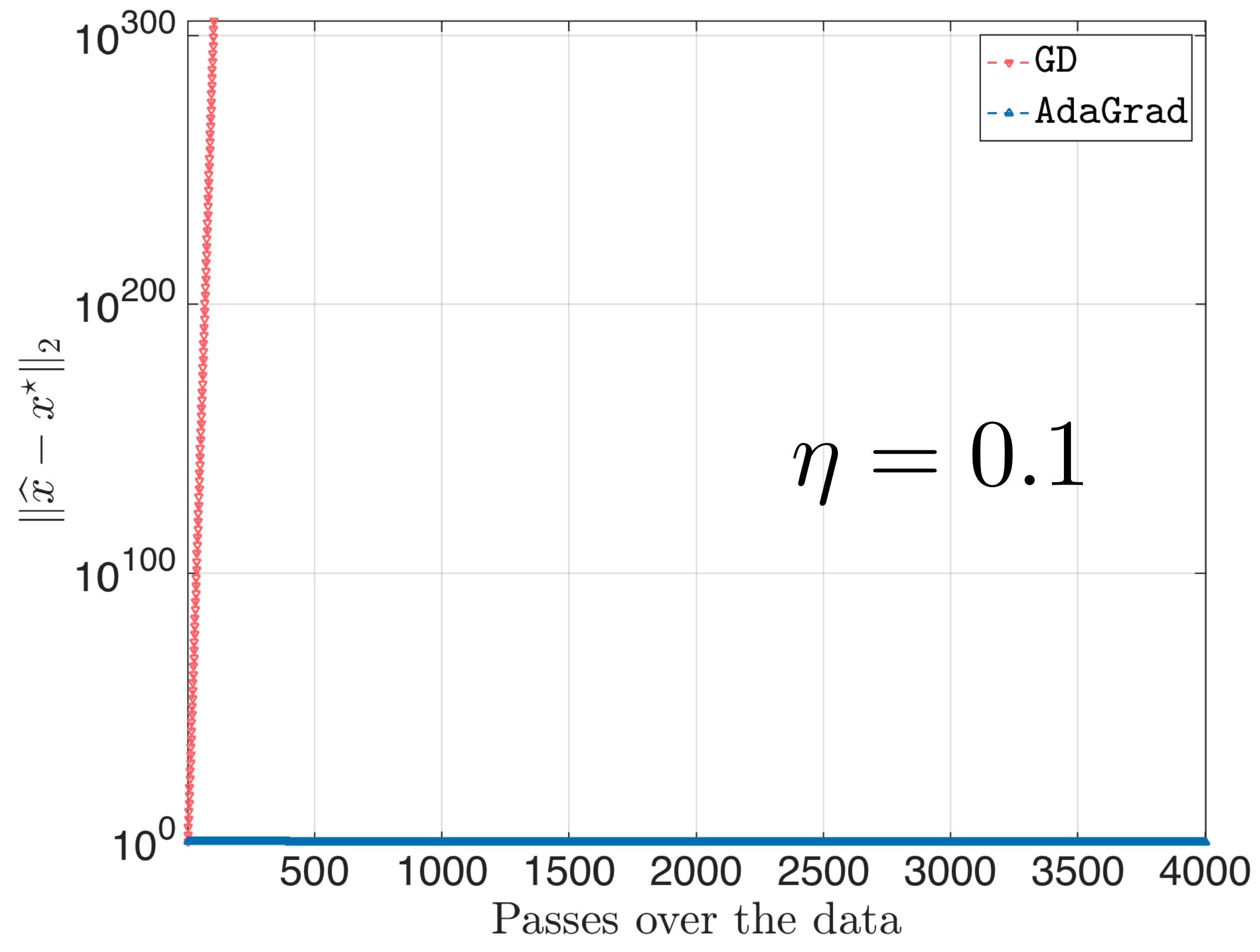
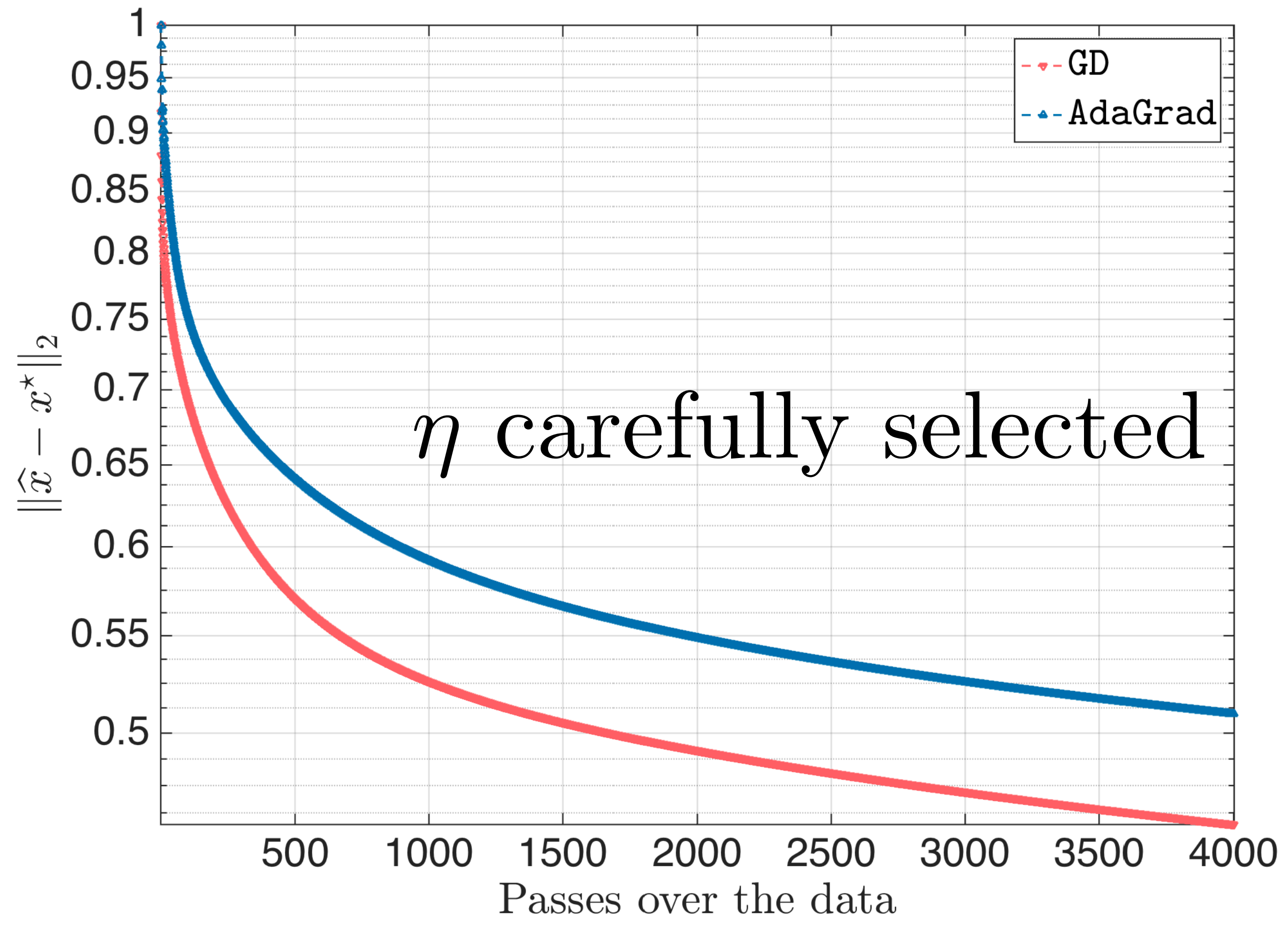


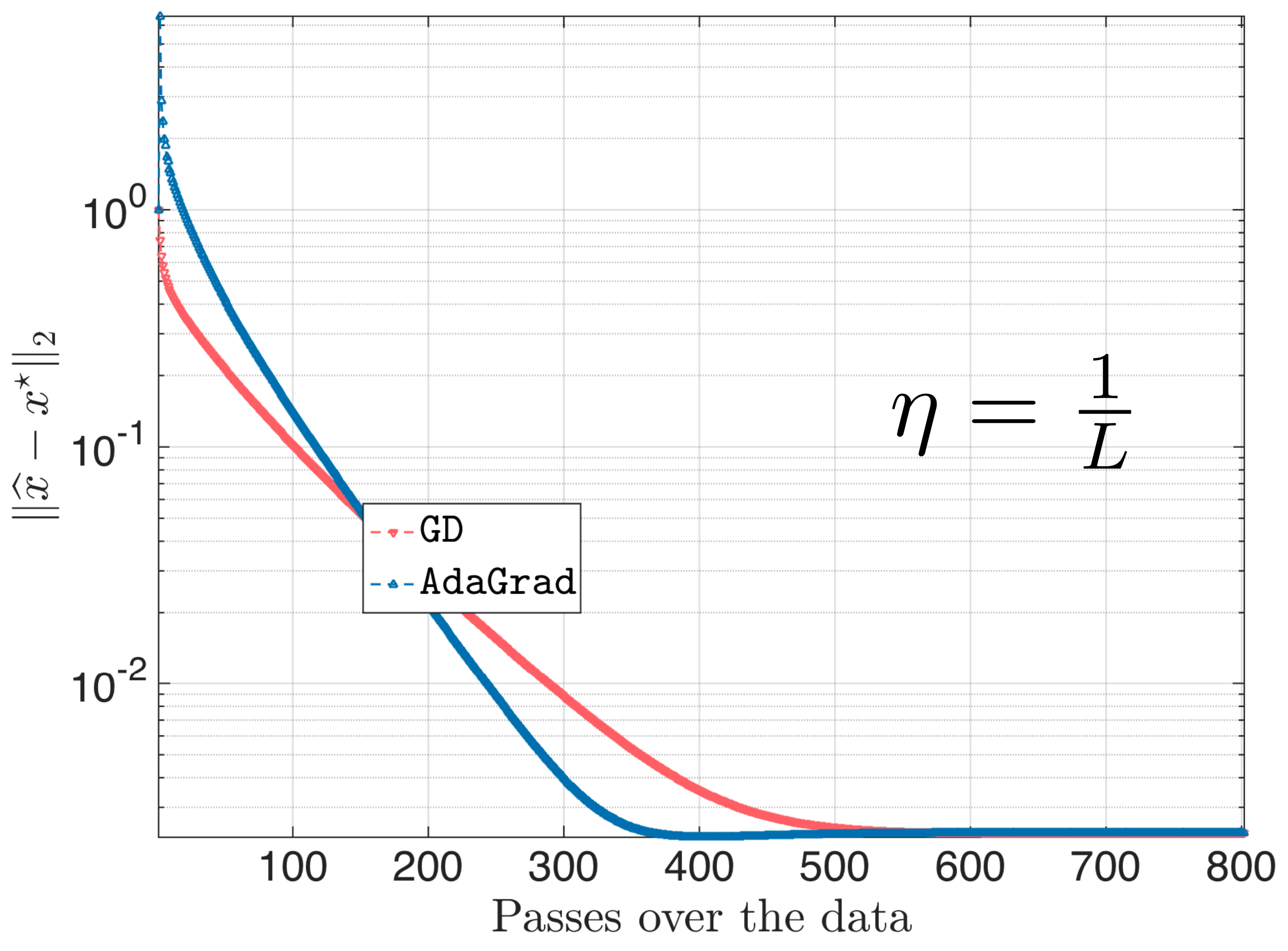


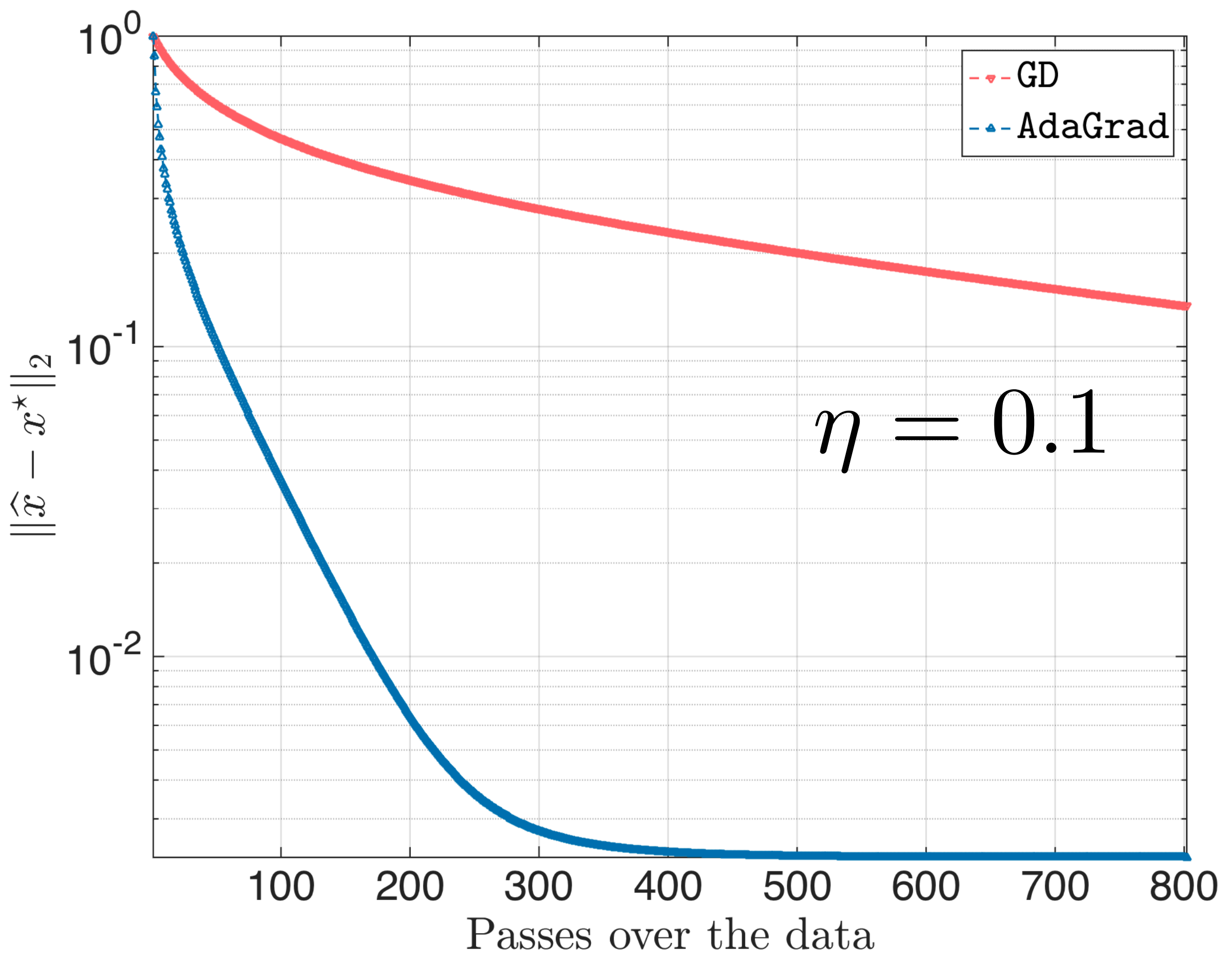


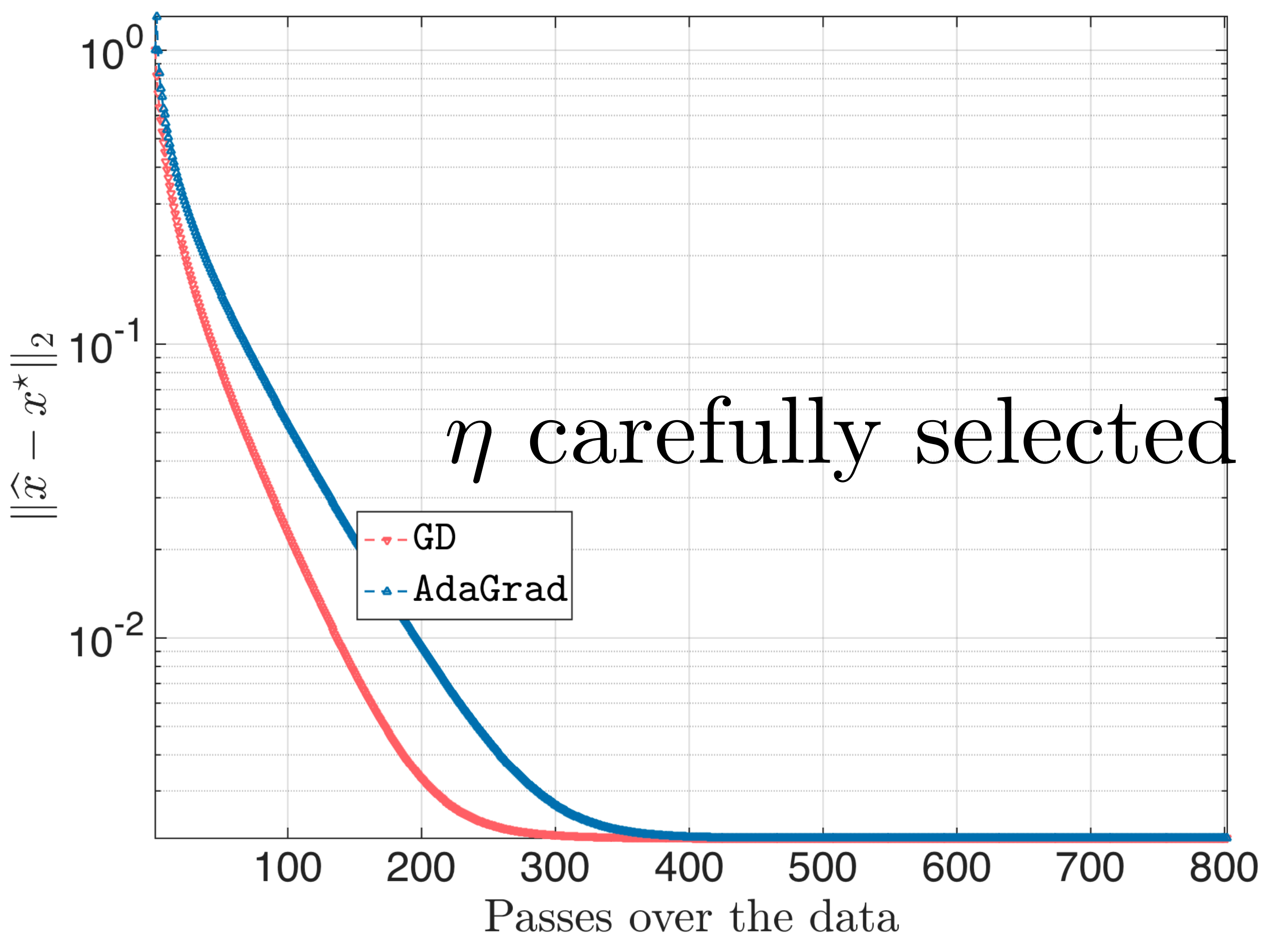
AdaGrad in practice

(Similar performance in logistic regression)

Well−conditioned linear regression







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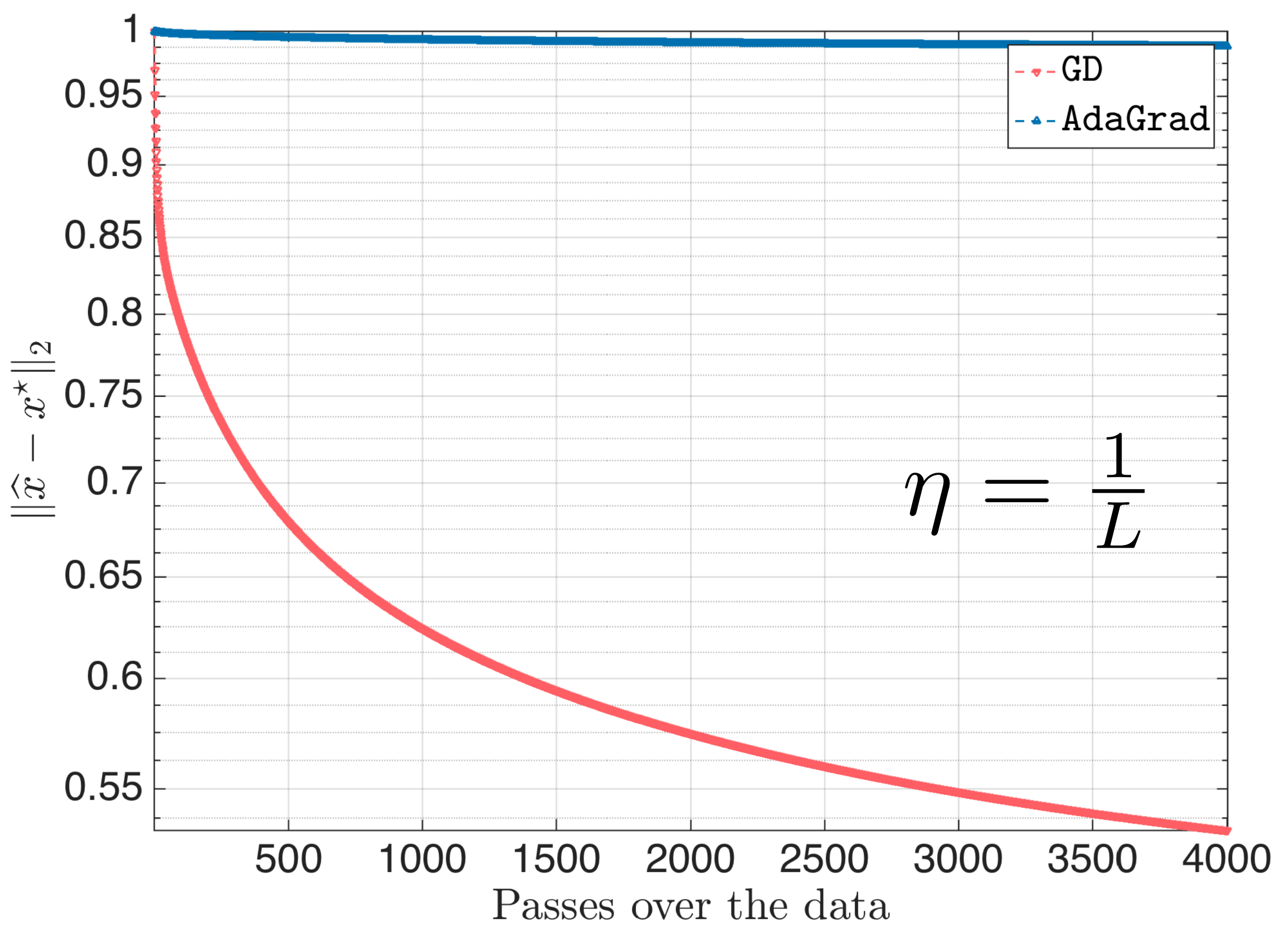
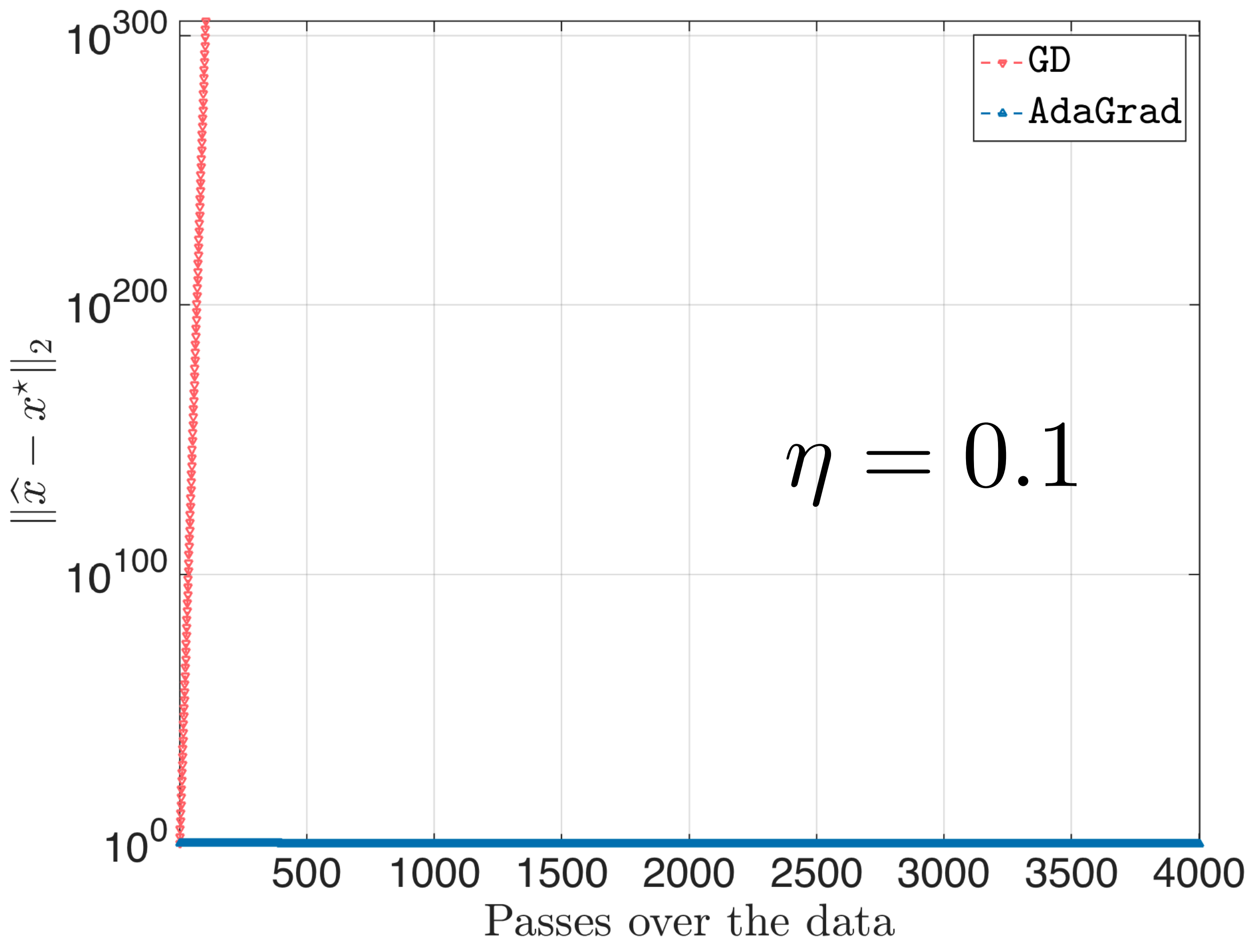
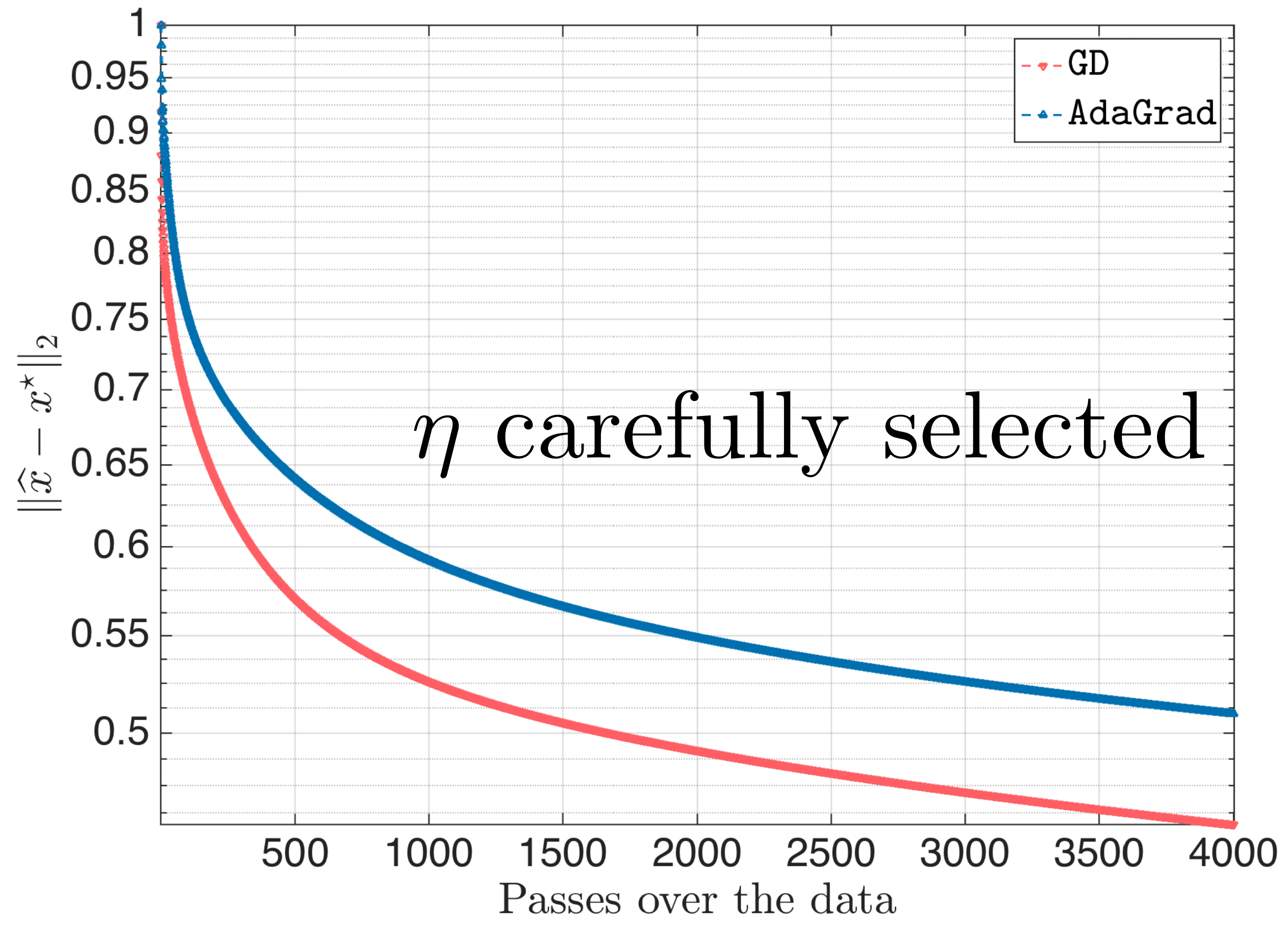
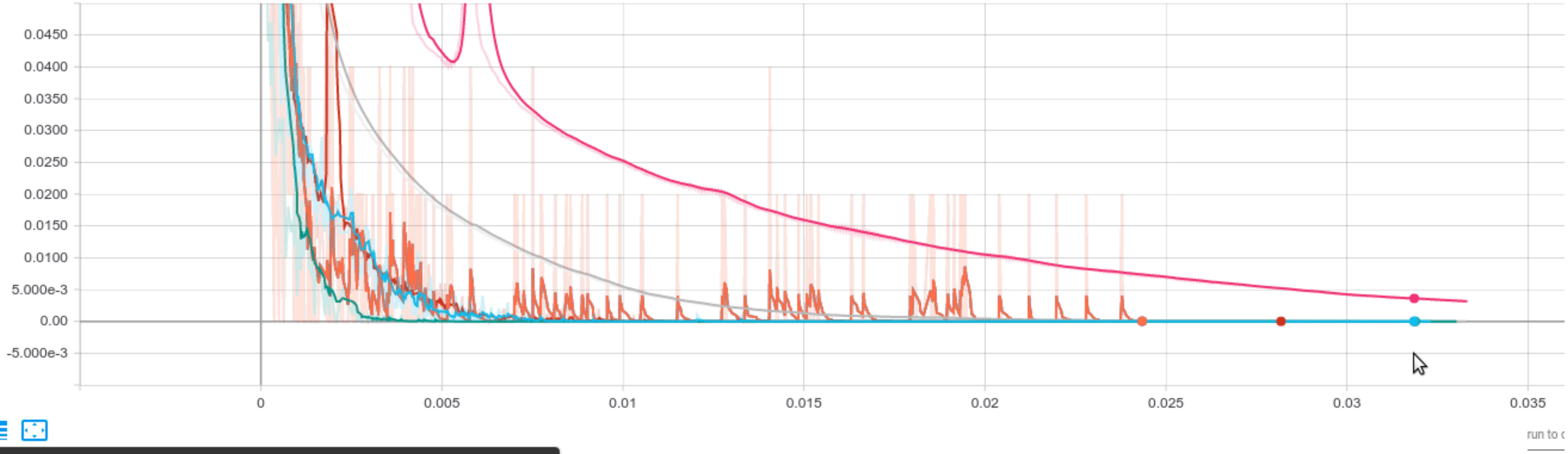






AdaGrad in practice



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AdaGrad2	-1.1921e-7	-1.1921e-7	5.381k	Sun Dec 10, 15:17:05	1m 54s
AdaGrad3	3.6024e-3	3.5634e-3	764.0	Sun Dec 10, 15:19:02	1m 54s
Nesterov2	-1.1921e-7	-1.1921e-7	5.303k	Sun Dec 10, 15:28:30	1m 54s
Nesterov3	-2.3665e-7	-2.3842e-7	764.0	Sun Dec 10, 15:30:29	1m 54s
SGD1	2.1986e-5	0.000	5.486k	Sun Dec 10, 15:01:31	1m 27s
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SGD2	-1.1921e-7	-1.1921e-7	5.486k	Sun Dec 10, 15:03:13	1m 41s

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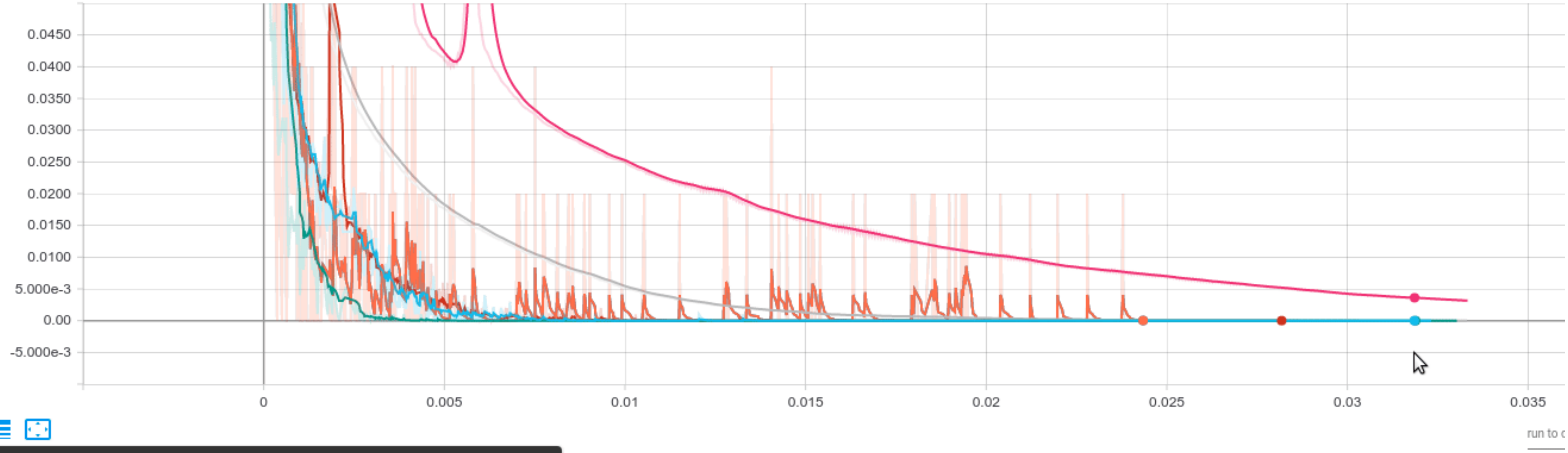

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Introducing exponentially weighted averages

(Adapted from Ng's lectures)

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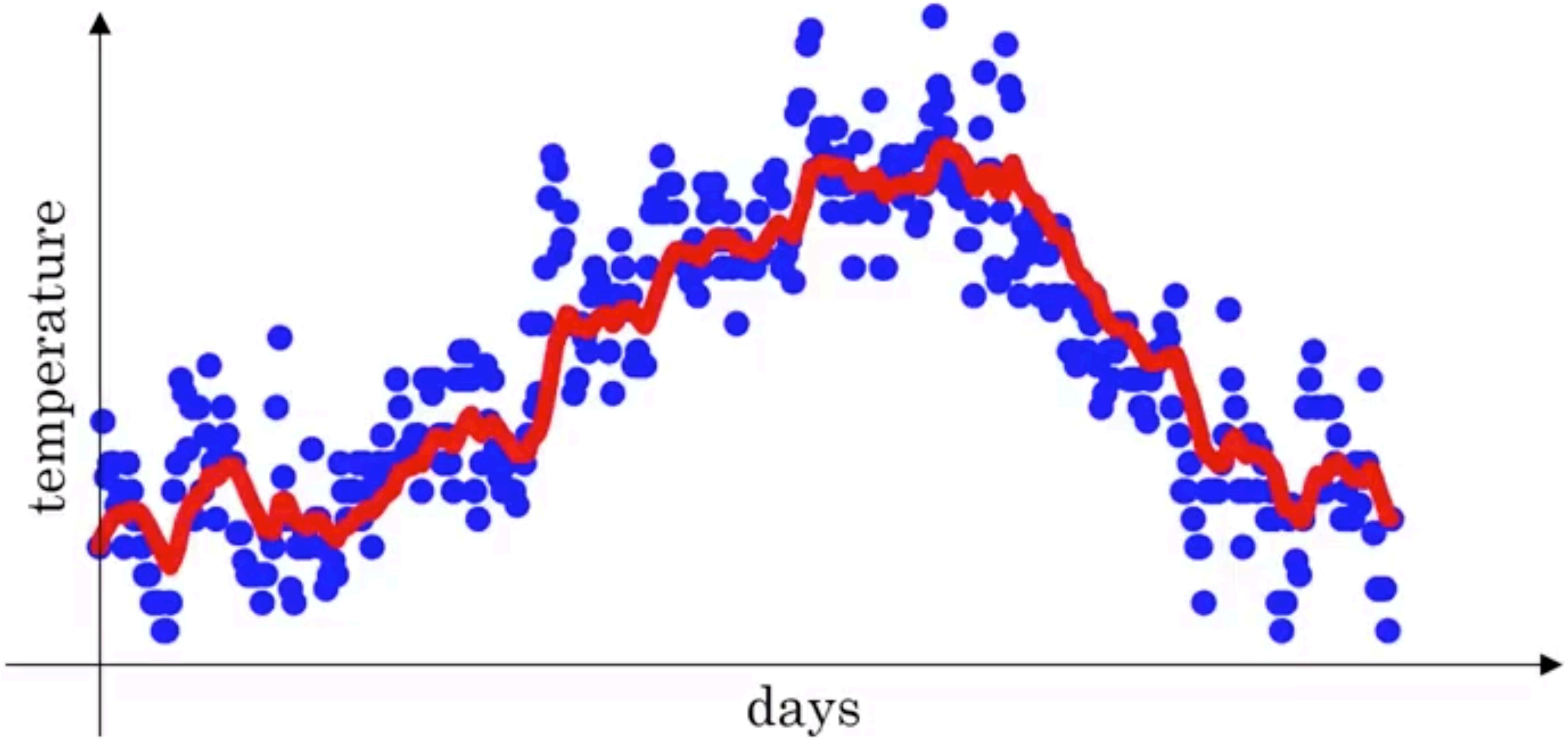

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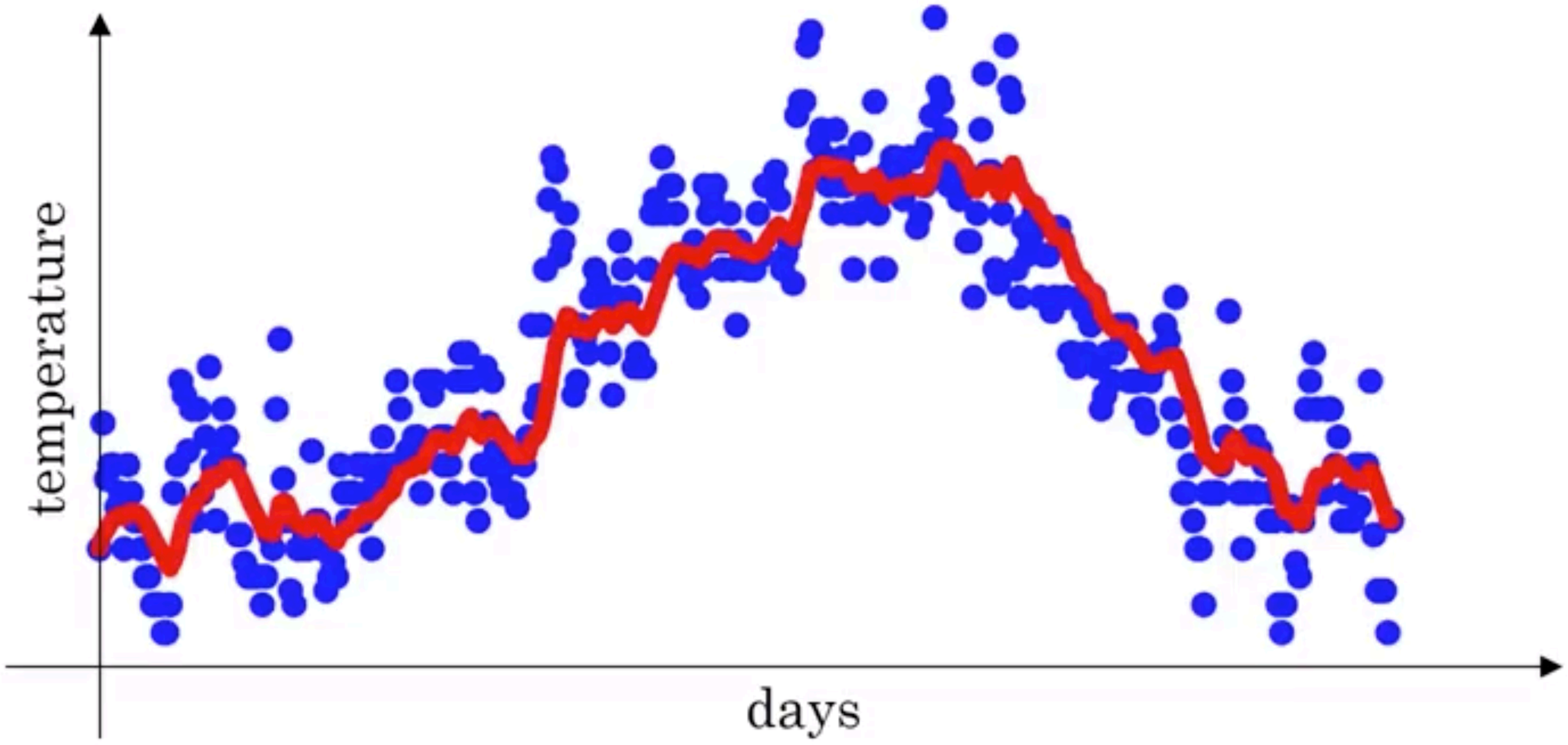

- Computing trends: local averages and how they evolve

$$V_0 = 0$$
$$V_1 = 0.9V_0 + 0.1\theta_1$$
$$V_2 = 0.9V_1 + 0.1\theta_2$$
$$\vdots$$
$$V_t = 0.9V_{t-1} + 0.1\theta_t$$

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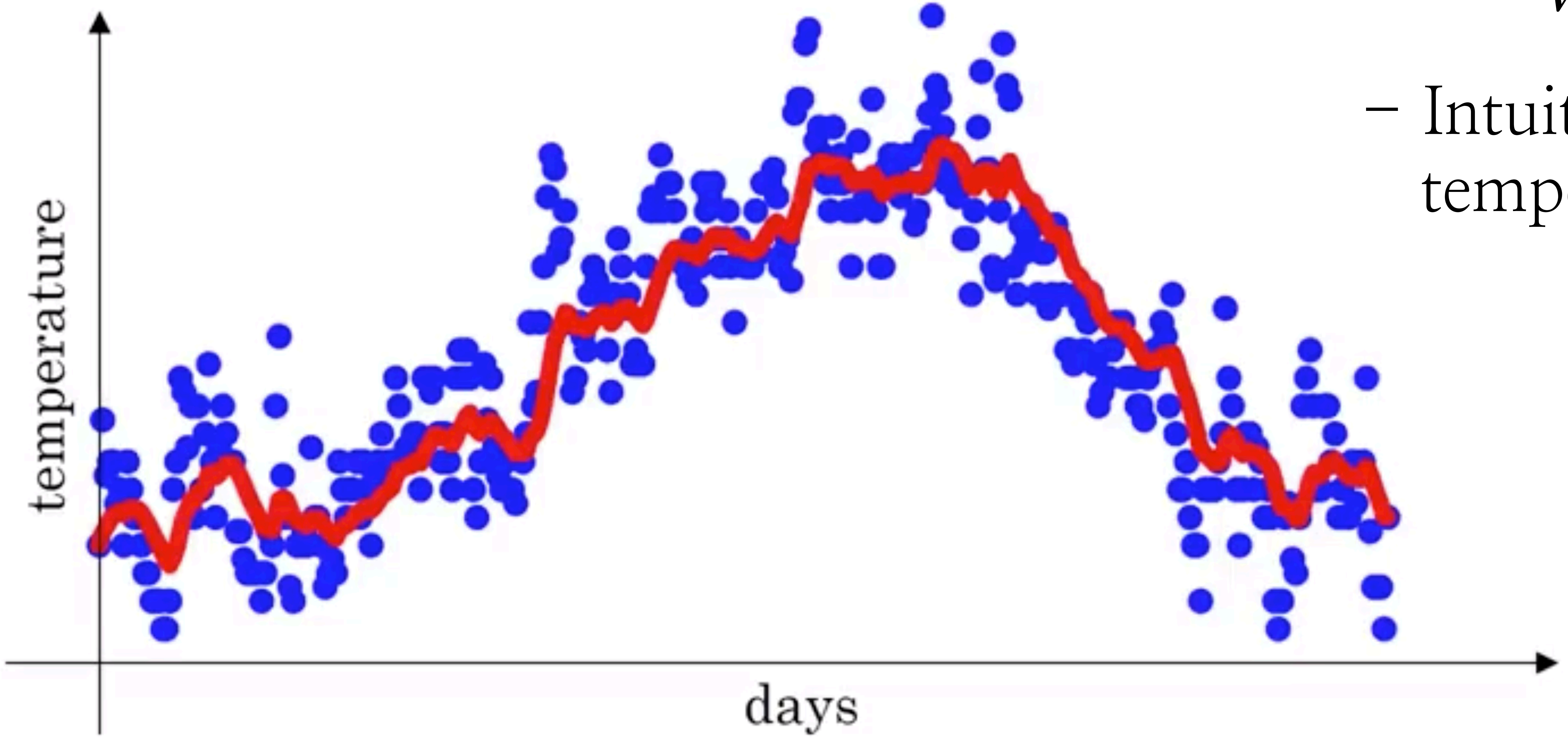

- General formula:

$$V_t = \beta V_{t-1} + (1 - \beta)\theta_t$$

- Intuition: V_t approximates temperature over

$$\approx \frac{1}{1-\beta} \text{ days}$$

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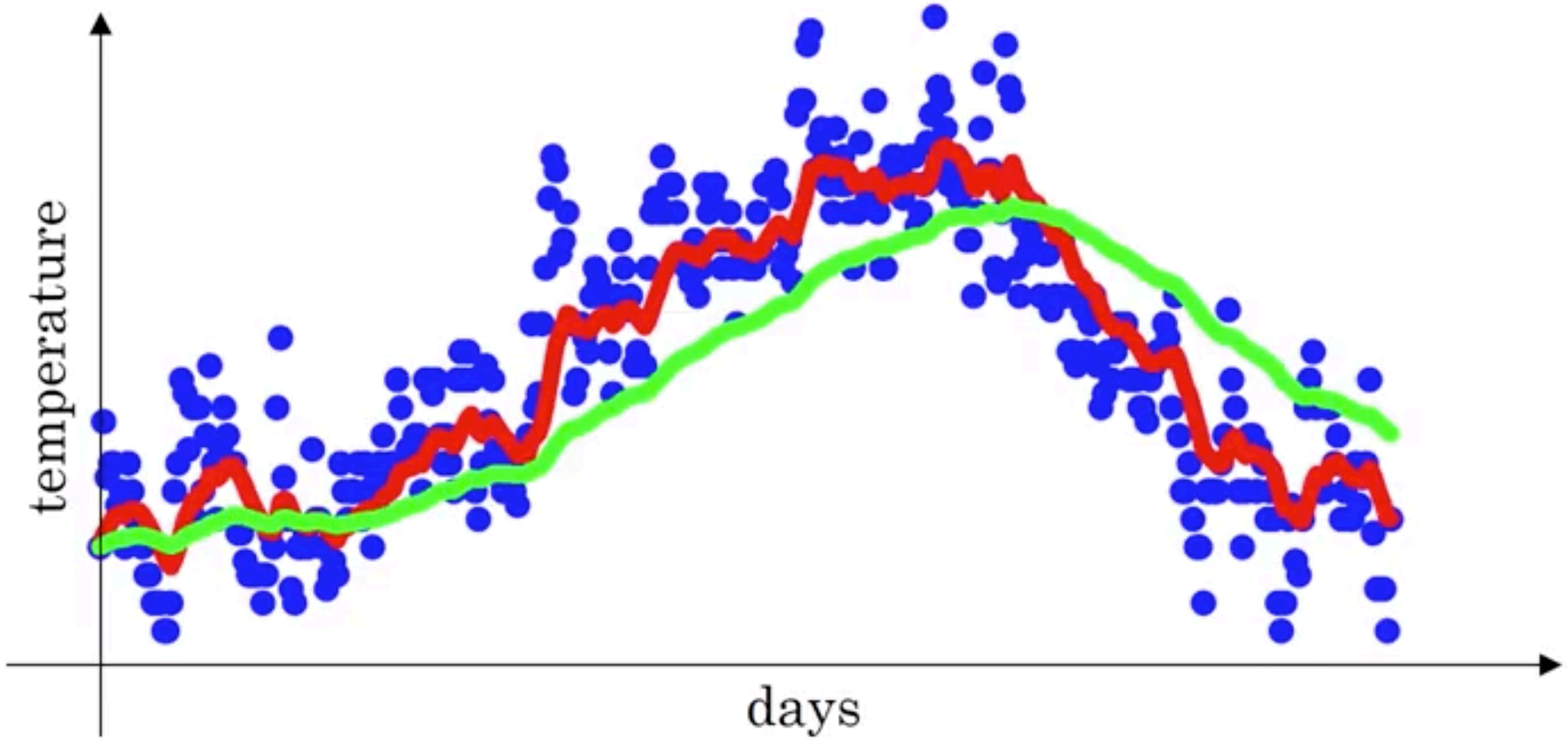

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$\beta = 0.98 \rightarrow \quad \approx 50$ days

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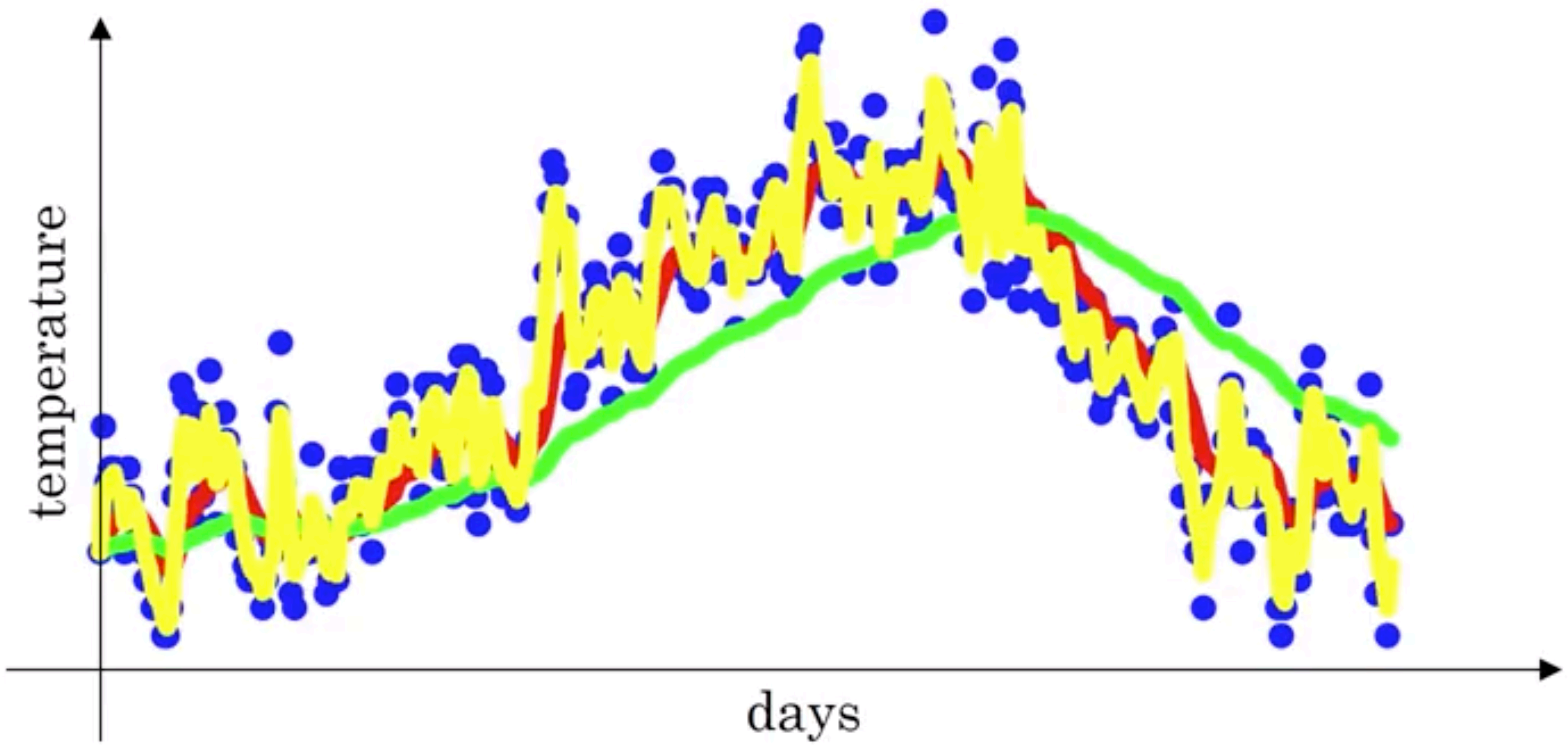

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+ **Adam** rule: $$E[g^2]_t = \beta_2 \cdot E[g^2]_{t-1} + (1 - \beta_2) \cdot g_t^2$$

and

$$m_t = \beta_1 \cdot m_{t-1} + (1 - \beta_1) \cdot \nabla f_{i_t}(x_t)$$

"Moving averages are essentially about averaging many previous values in order to become independent of local fluctuations and focus on the overall trend"

Going beyond RMSprop: **Adam** algorithm

- Idea: Use weighted moving average in gradient also:
  - + **RMSprop** rule: $E[g^2]_t = \frac{9}{10} \cdot E[g^2]_{t-1} + \frac{1}{10} \cdot g_t^2$
  - + **Adam** rule: $E[g^2]_t = \beta_2 \cdot E[g^2]_{t-1} + (1 - \beta_2) \cdot g_t^2$

"Moving averages are essentially about averaging many previous values in order to become independent of local fluctuations and focus on the overall trend"

and

$$m_t = \beta_1 \cdot m_{t-1} + (1 - \beta_1) \cdot \nabla f_{i_t}(x_t)$$

Further: $$\widehat{m}_t = \frac{m_t}{1 - \beta_1^t}, \quad \widehat{v}_t = \frac{E[g^2]_t}{1 - \beta_2^t}$$

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"Moving averages are essentially about averaging many previous values in order to become independent of local fluctuations and focus on the overall trend"

Further: $$\widehat{m}_t = \frac{m_t}{1-\beta_1^t}, \quad \widehat{v}_t = \frac{E[g^2]_t}{1-\beta_2^t}$$

– Algorithm: $$x_{t+1} = x_t - \frac{\eta}{\sqrt{\widehat{v}_t} + \epsilon} \cdot \widehat{m}_t$$

$\beta_1 = 0.9, \ \beta_2 = 0.999$

Bias correction in weighted averages

(Adapted from Ng's lectures)

- How to explain these ``weird`` denominators?

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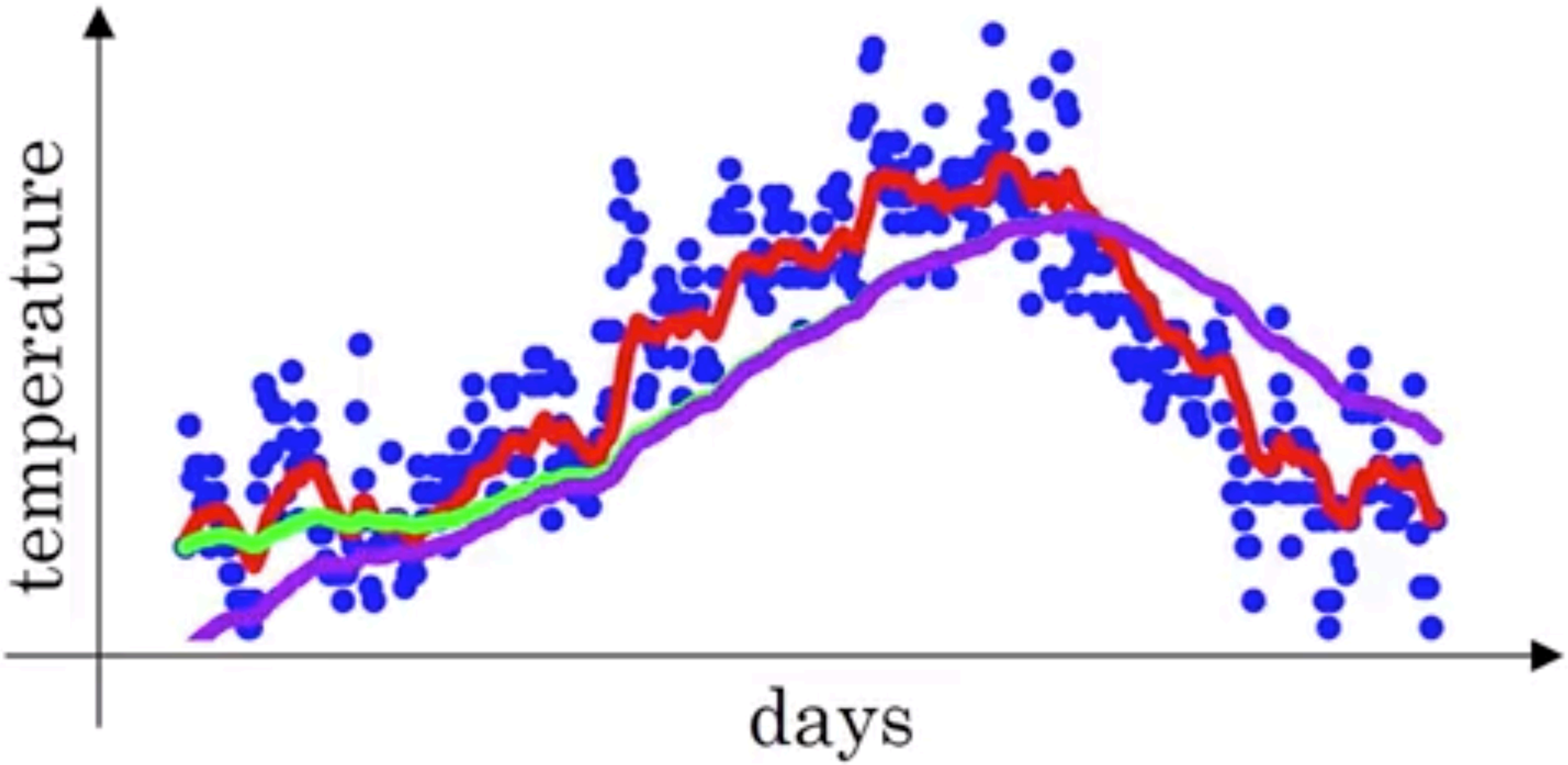
- How to explain these ``weird`` denominators?

$$V_t = \beta V_{t-1} + (1-\beta)\theta_t$$



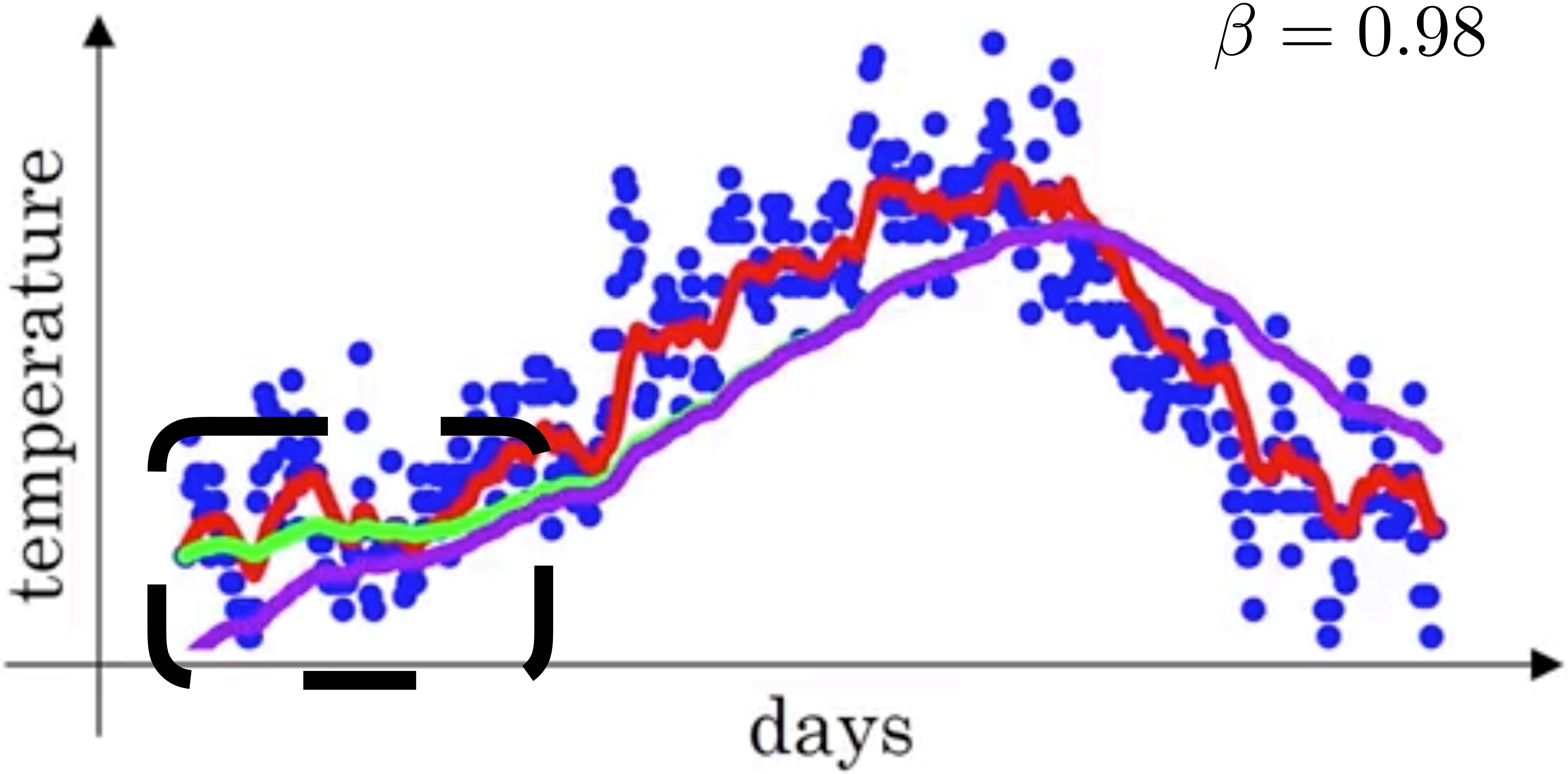
Bias correction in weighted averages

(Adapted from Ng's lectures)

- How to explain these "weird" denominators?

$$V_t = \beta V_{t-1} + (1-\beta)\theta_t$$

$\beta = 0.98$



Other algorithms and sources

- Not a complete list: **AdaMax, Nadam, AMSGrad**, ..
- A nice blog post on the matter:

http://ruder.io/optimizing-gradient-descent/

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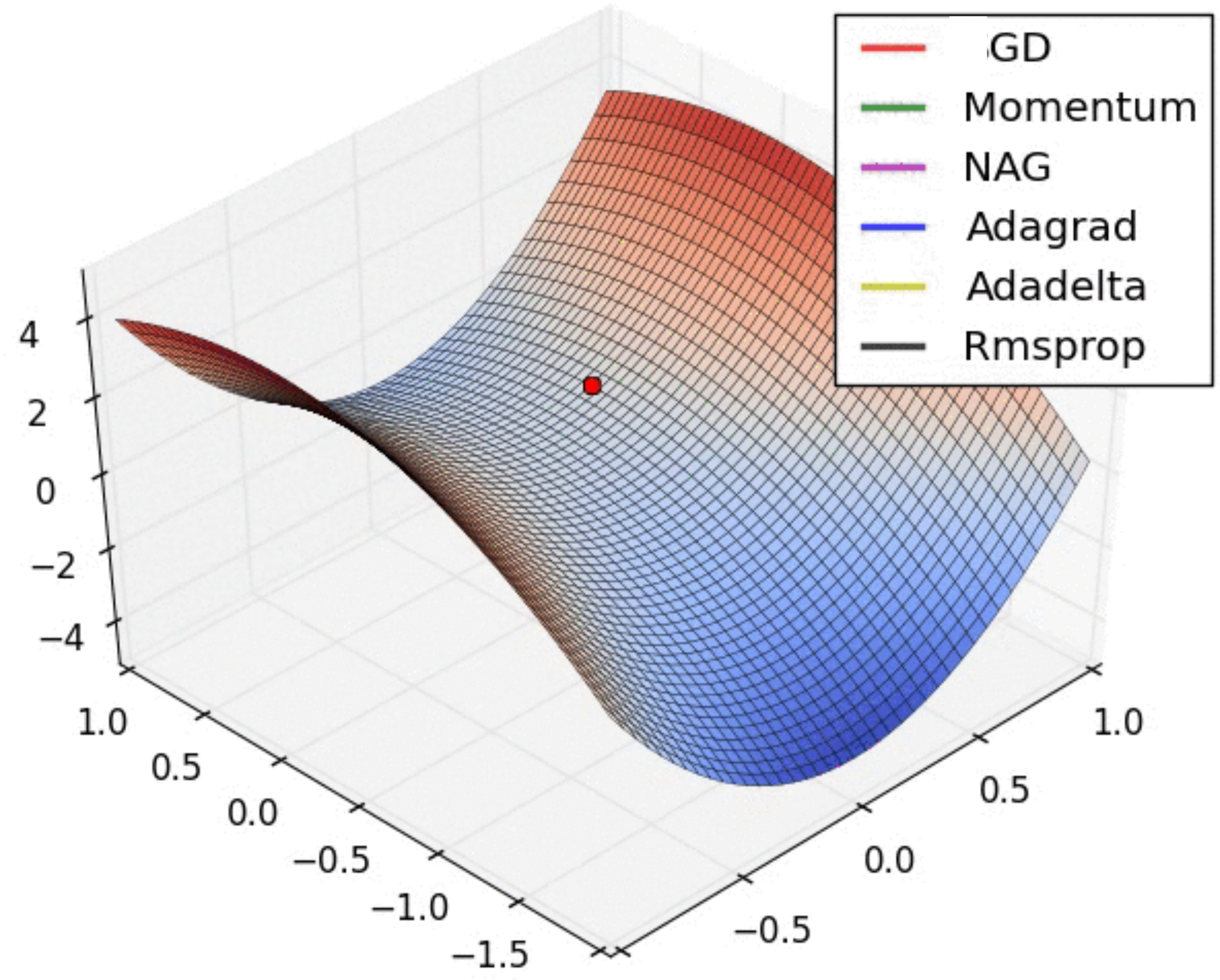
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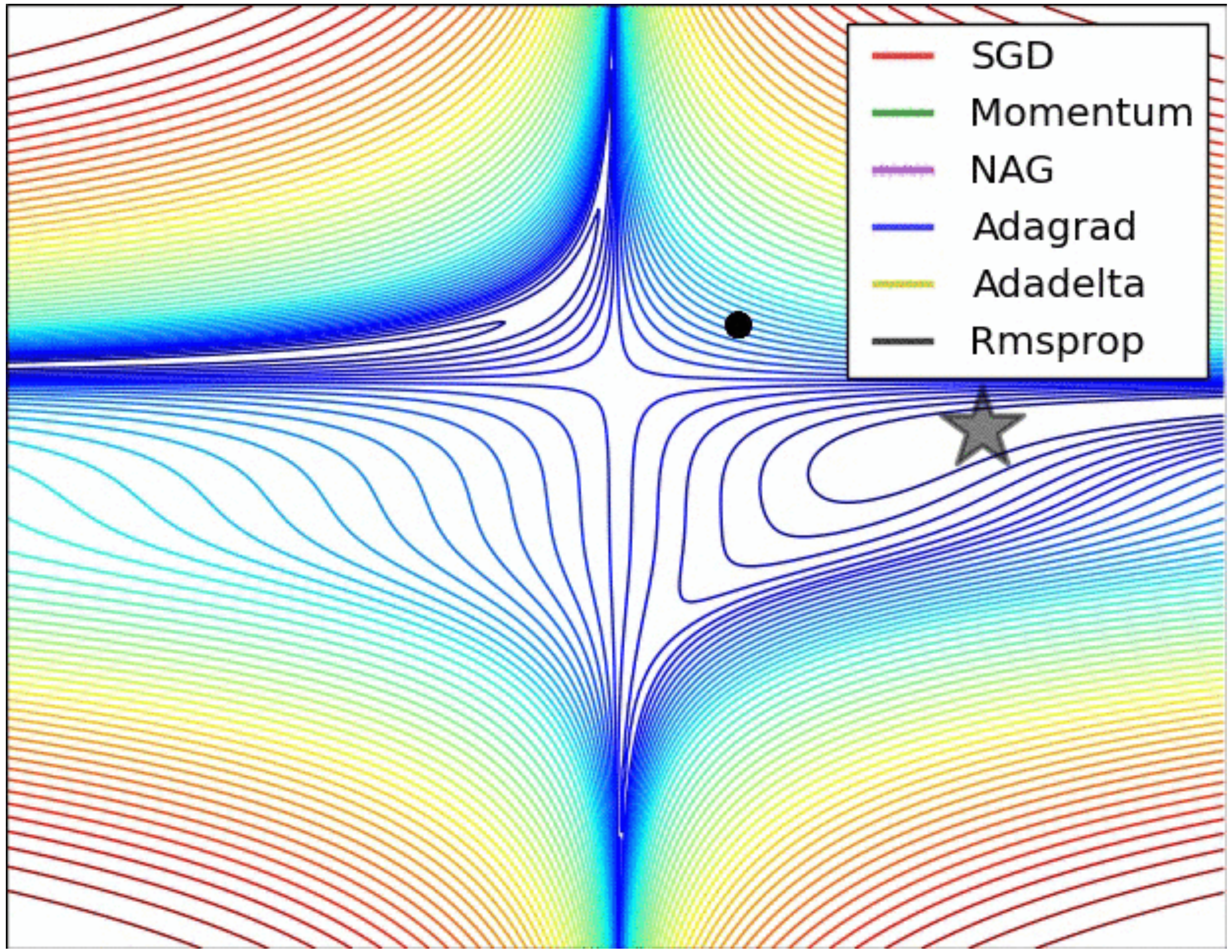
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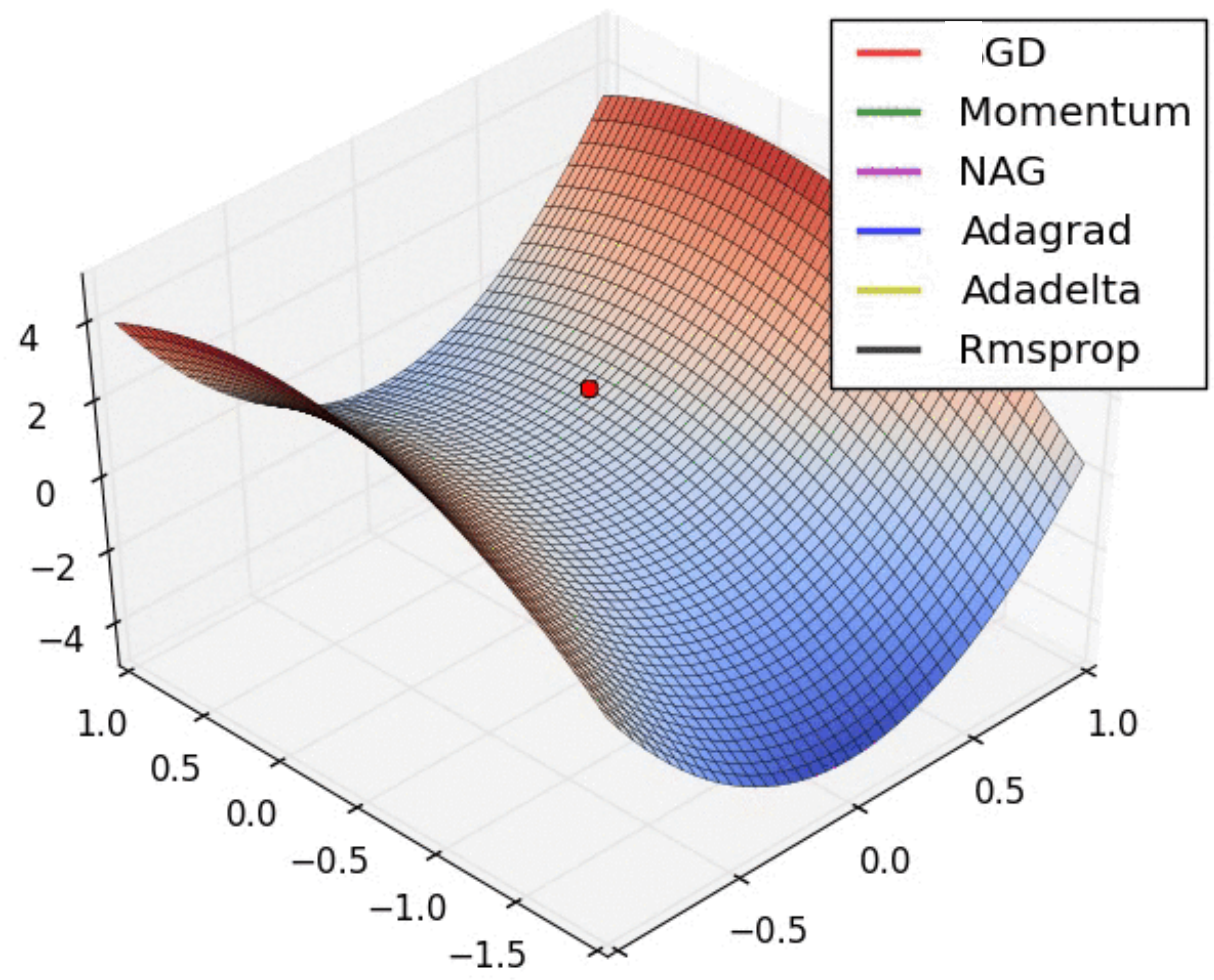
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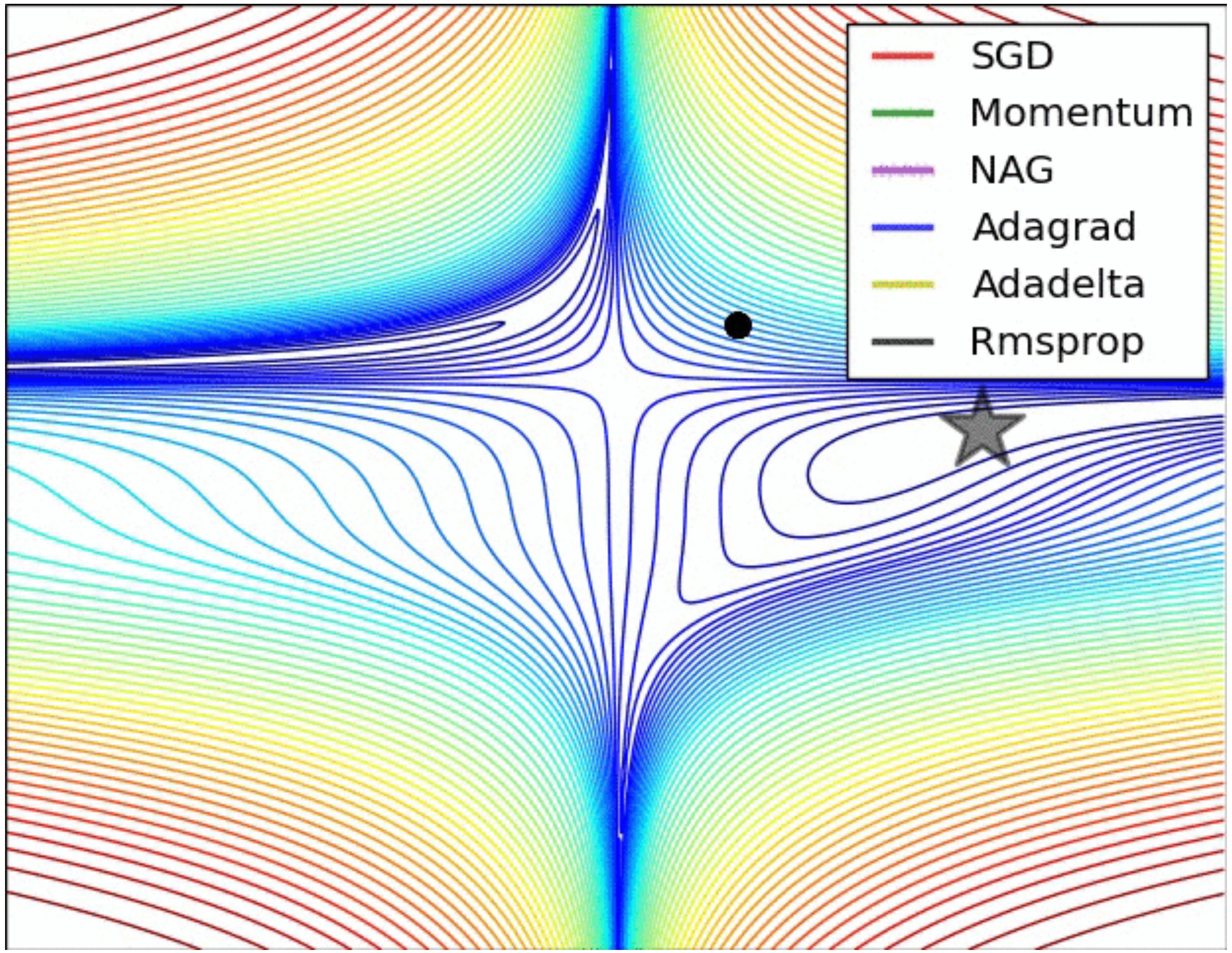
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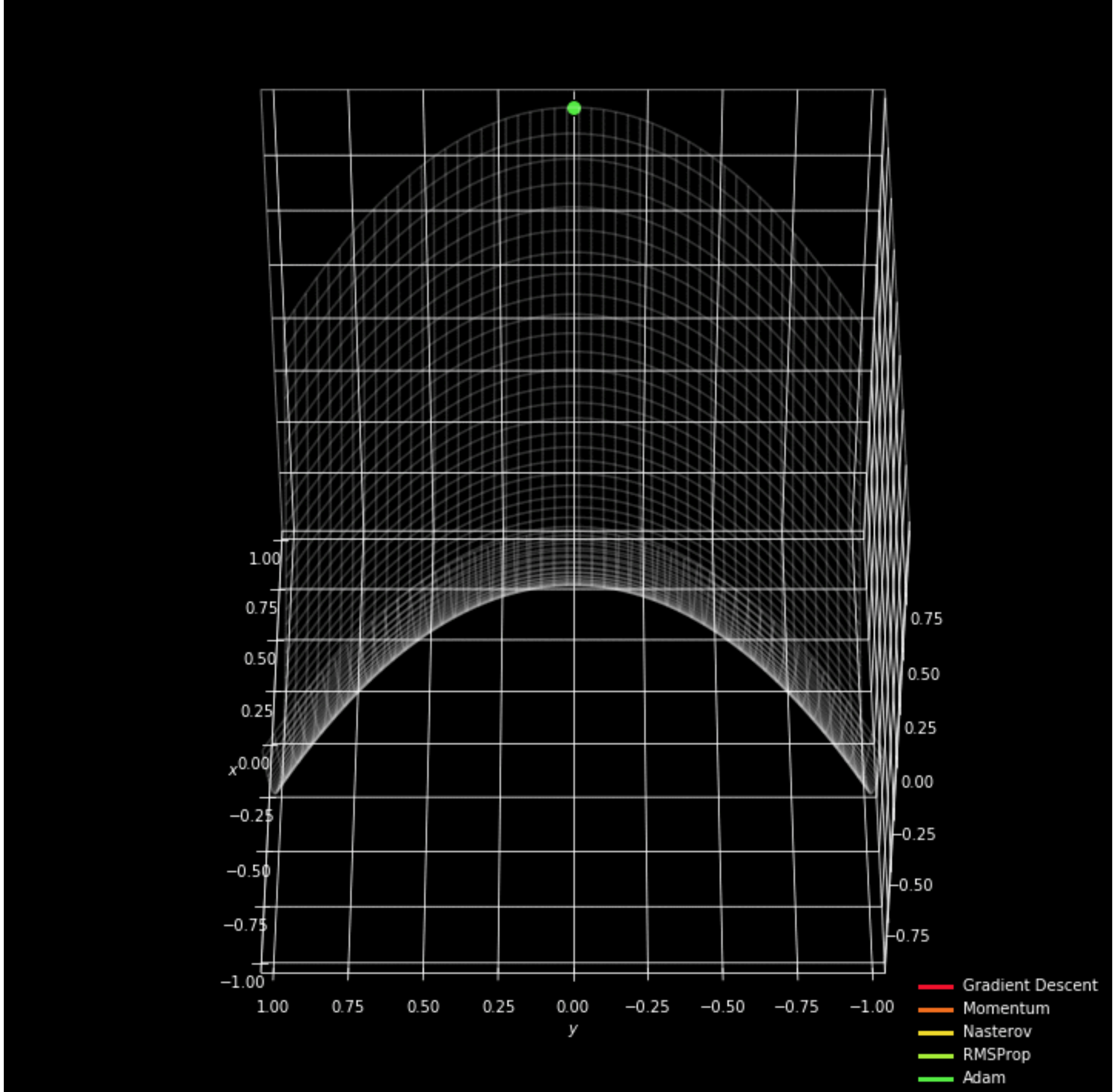

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y
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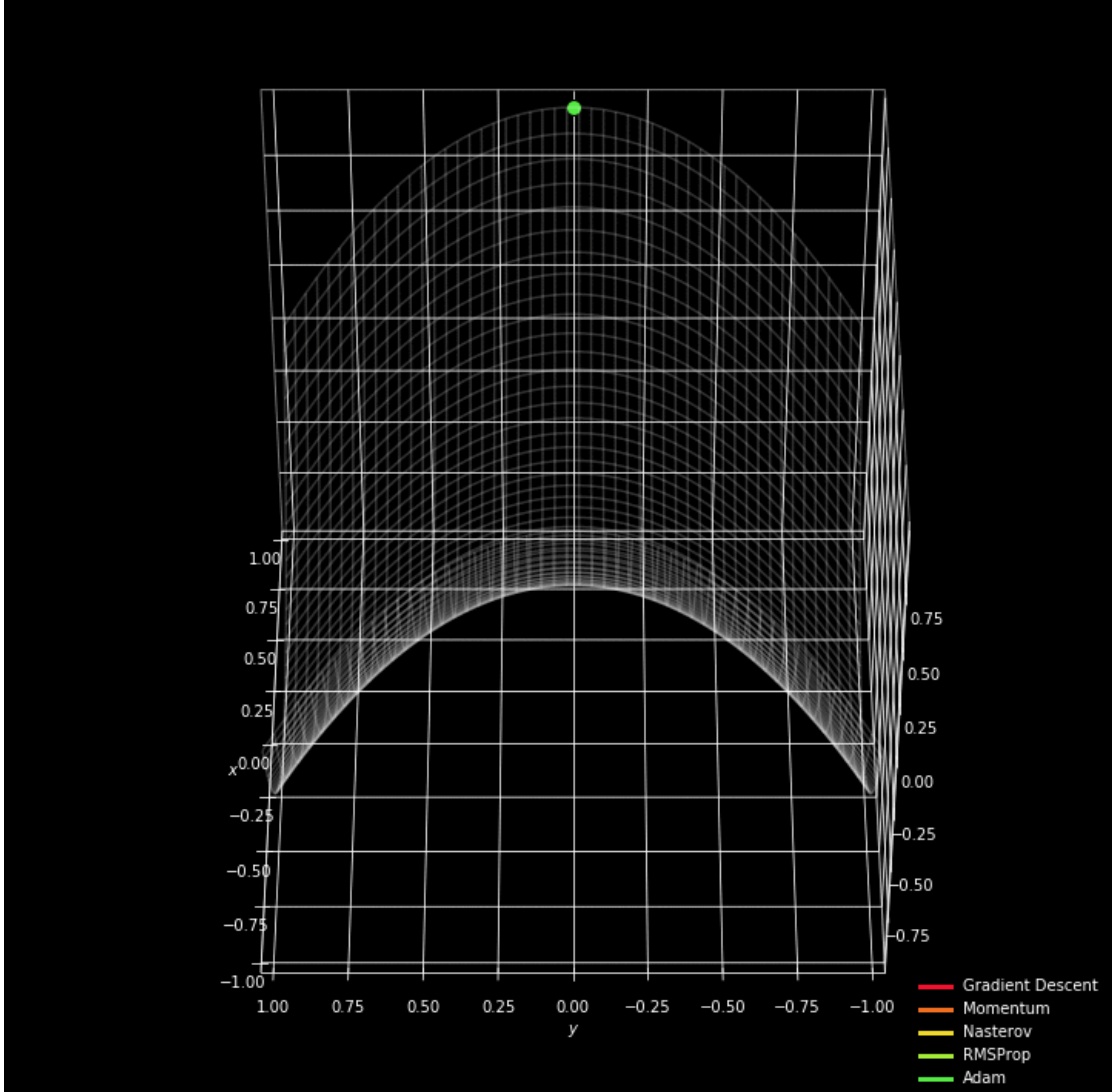
Gradient Descent
Momentum
Nasterov
RMSProp
Adam



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(Switch presentations)

Conclusion

- There are various algorithms for modern machine learning
- The most successful of them are gradient based; however, there are variations that make difference in practice (acceleration helps, adaptive learning rates work for most applications, etc).
- Which algorithm to use depends on the problem and the resources at hand
- These topics are highly attractive (research-wise): the idea is to devise new algorithms that achieve practical acceleration (with minimal tuning effort)