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

The focus of this lecture

Huge!

Non-convex!

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

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

Unconstrained

Overview

- In this lecture, we will:
  - Go back to the initial discussion of non-convex optimization
  - We will provide generic convergence results for stochastic methods

    (More general case than whatever non-convex problem we considered so far)
  - 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**

Recall: Stochastic gradient descent

- SGD is used **almost everywhere**: training classical ML tasks (linear prediction, linear classification), training modern ML tasks (non-linear classification, neural networks)
- In simple math, it satisfies:

$$x_{t+1} = x_t - \eta \nabla f_{i_t}(x_t)$$

based on the objective: $\min_x \quad f(x) := \frac{1}{n} \sum_{i=1}^{n} f_i(x)$

Non-convex!

- 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

- 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
    - 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

- General observation: moving results from convex to non-convex settings is not straightforward in most cases

- Recall: GD vs Acc. GD

Strongly Convex

$$O\left(\boxed{\kappa}\log\frac{f(x_0)-f^\star}{\varepsilon}\right) \qquad O\left(\boxed{\sqrt{\kappa}}\log\frac{f(x_0)-f^\star}{\varepsilon}\right)$$

- GD vs Acc. GD

Non Convex

$$O\left(\tfrac{1}{\varepsilon^2}\right) \qquad O\left(\tfrac{1}{\varepsilon^{7/4}}\cdot\log(1/\varepsilon)\right)$$

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

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

Acceleration in SGD in non-convex scenaria

- General observation: moving results from convex to non-convex settings is not straightforward in most cases

- Recall:

	SGD	vs	Acc. SGD
Strongly Convex	$O\left(\frac{1}{\varepsilon}\right)$		(Results for specific cases – Still an open question in its most generality)
Non Convex	$O\left(\frac{1}{\varepsilon^2}\right)$		(Results for specific cases – Still an open question in its most generality)

(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

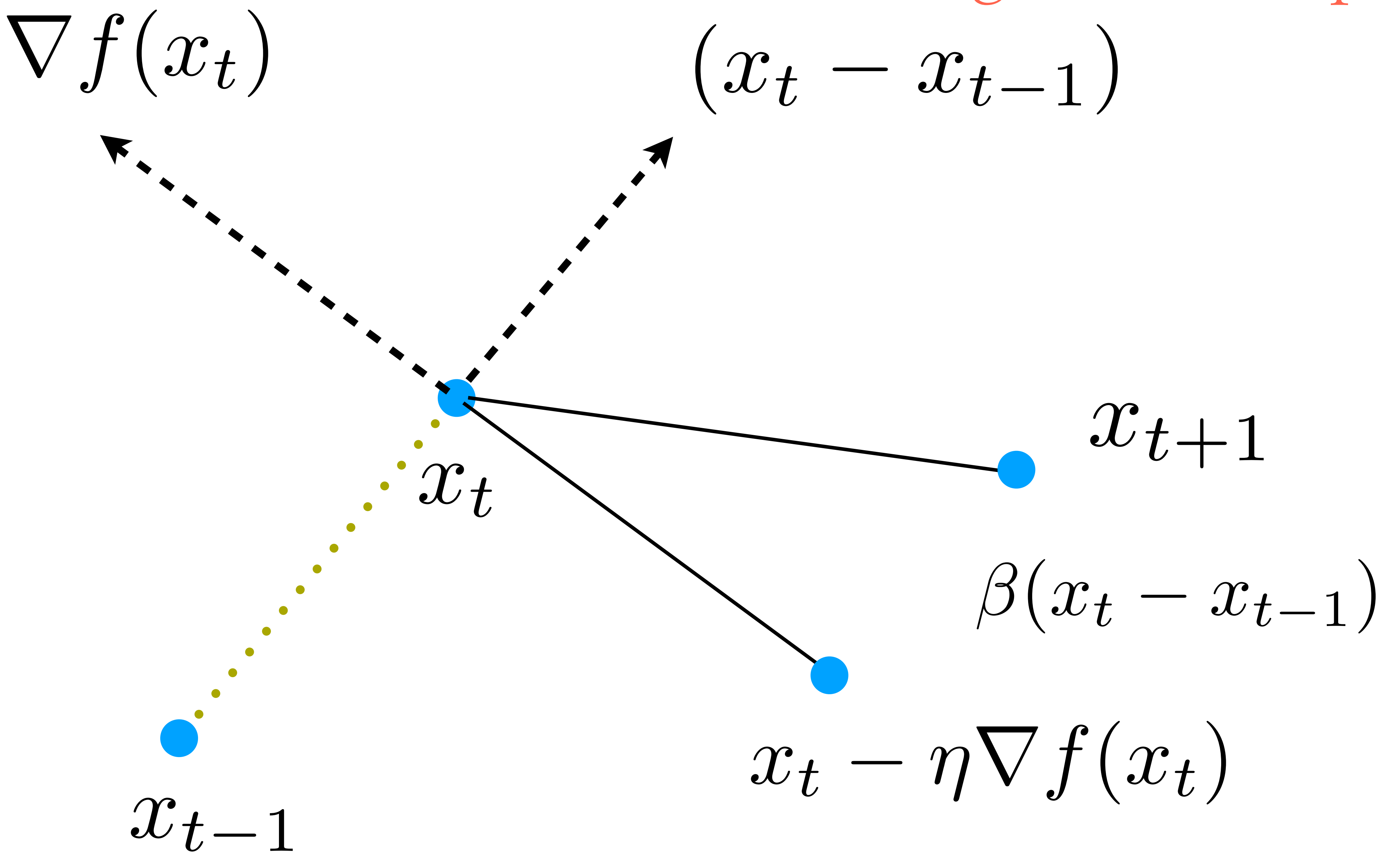
https://www.tensorflow.org/api_docs/python/tf/train/MomentumOptimizer

Recall: Momentum acceleration

Recall: Momentum acceleration

– Heavy ball method

$$x_{t+1} = \underbrace{x_t - \eta \nabla f(x_t)}_{\text{Standard gradient step}} + \underbrace{\beta(x_t - x_{t-1})}_{\text{Momentum step}}$$



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

Non−convex!

$$\min_{x \in \mathbb{R}^p} f(x)$$

"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:

$$\|x_{t+1} - x^\star\|_2 \leq \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}\right)^t \|x_0 - x^\star\|_2$$ *"*

AdaGrad algorithm

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

- Algorithms so far assume a common (and often fixed) step size for all components of x_t

- AdaGrad adapts the initial step size for each of the components:
  - Associates small step sizes to frequently occurring features
  - Associates large step sizes to rate occurring features

- What is the main idea? Consider $x_{t+1,i} = x_{t,i} - \eta \nabla f(x_t)_i$

Entrywise representation of GD

Then, practical version of AdaGrad does: $x_{t+1,i} = x_{t,i} - \frac{\eta}{\sqrt{\boxed{B_{t,ii}} + \epsilon}} \cdot \nabla f_{i_t}(x_t)_i$

What is this quantity?

AdaGrad algorithm

– AdaGrad is just another preconditioning algorithm:

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

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

where

$$B_t = \left(\sum_{j=1}^{t} \nabla f_{i_j}(x_j) \cdot \nabla f_{i_j}(x_j)^\top \right)^{1/2}$$

"Square root of the sum of gradient outer products, till current iteration"

Full matrix AdaGrad

– Compare this to the simpler (and practical version)

$$x_{t+1,i} = x_{t,i} - \frac{\eta}{\sqrt{B_{t,ii} + \boxed{\epsilon}}} \cdot \nabla f_{i_t}(x_t)_i$$

Avoids division with zero

AdaGrad algorithm

– "What is the intuition behind the form of B_t ?"

$$B_t = \left(\sum_{j=1}^{t} \nabla f_{i_j}(x_j) \cdot \nabla f_{i_j}(x_j)^\top \right)^{1/2}$$

Relates to the **Fisher Information matrix** (which is related to the expected Hessian) – outside our scope

– "What is the connection between full and diagonal preconditioner?"

Whiteboard

– "What are some properties of AdaGrad?"

1. Step size is automatically set – default values for initial step size is $\eta = 0.01$
2. The original version keeps accumulating squared gradients, which makes resulting step sizes really small.

– "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 $\{\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(m)}\}$ 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)

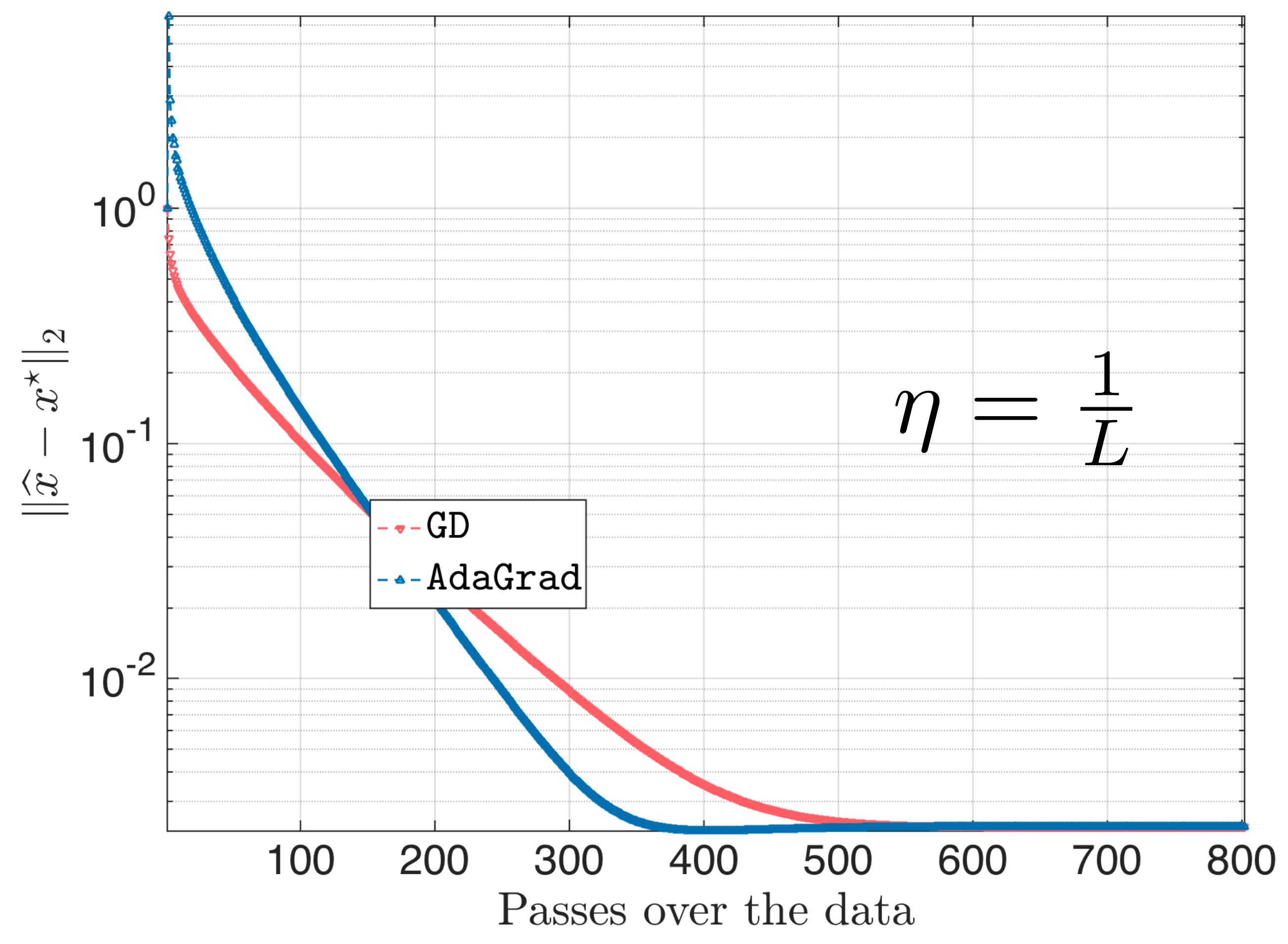
Apply update: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \Delta\boldsymbol{\theta}$

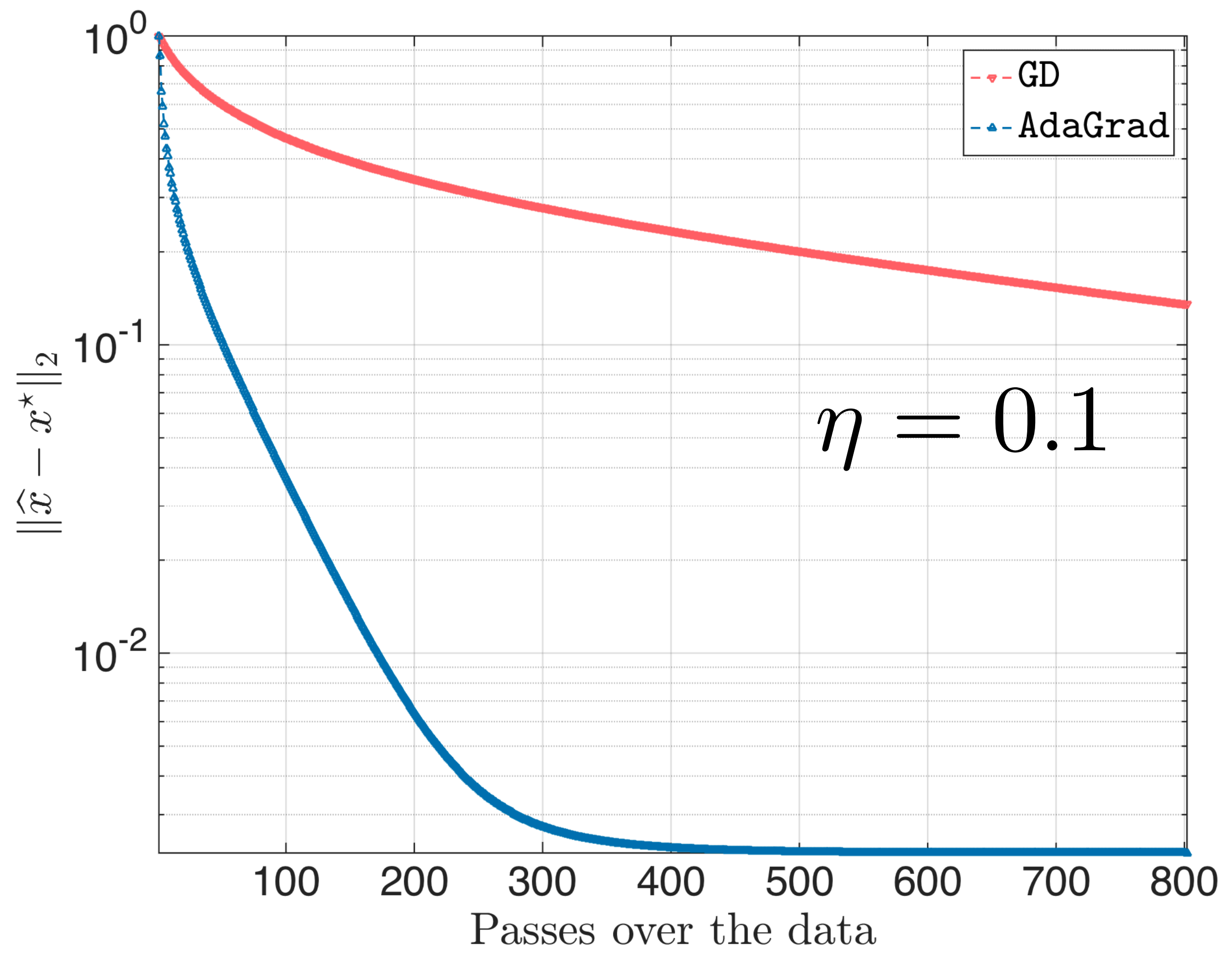
end while

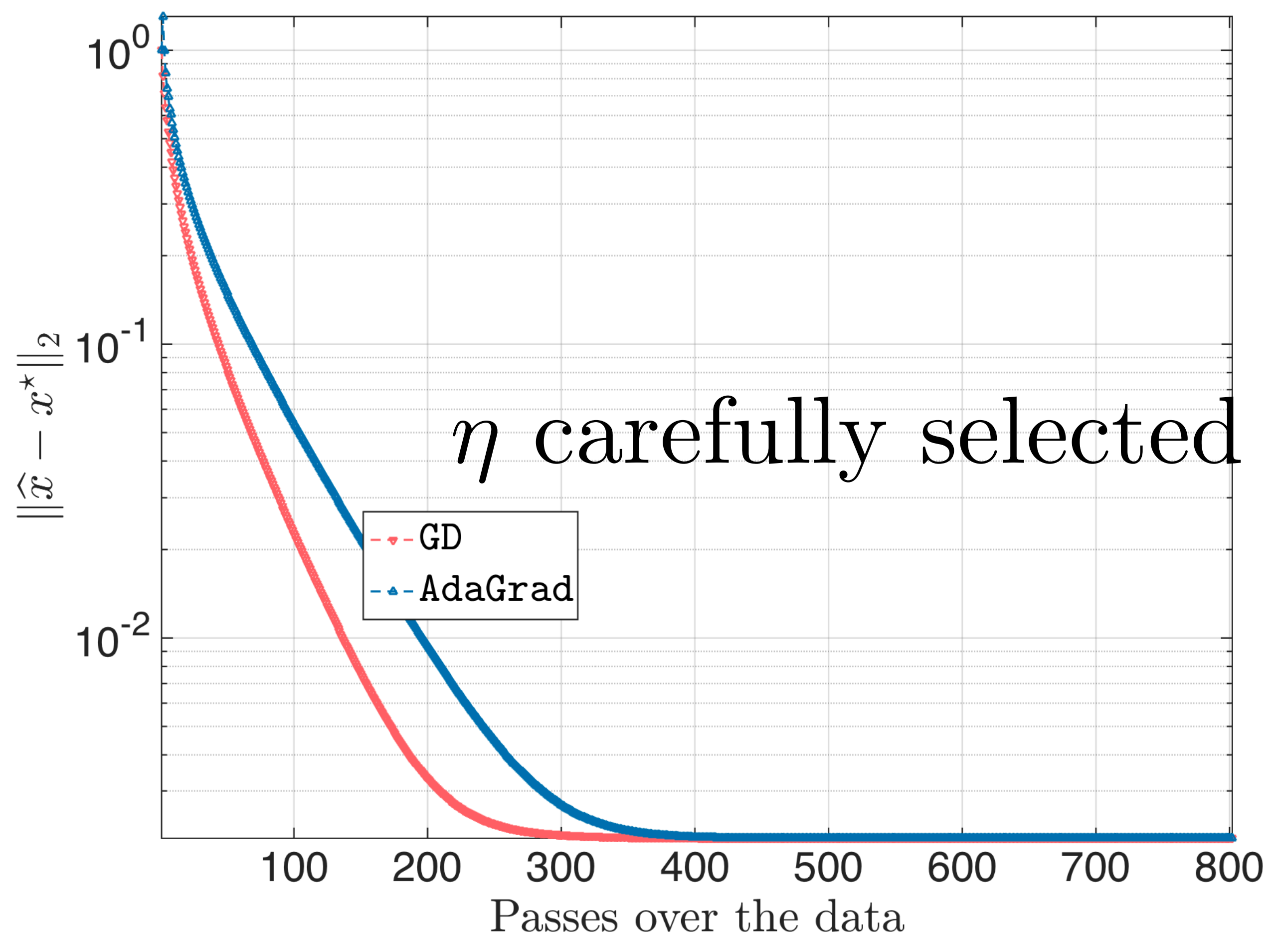
AdaGrad in practice

(Similar performance in logistic regression)

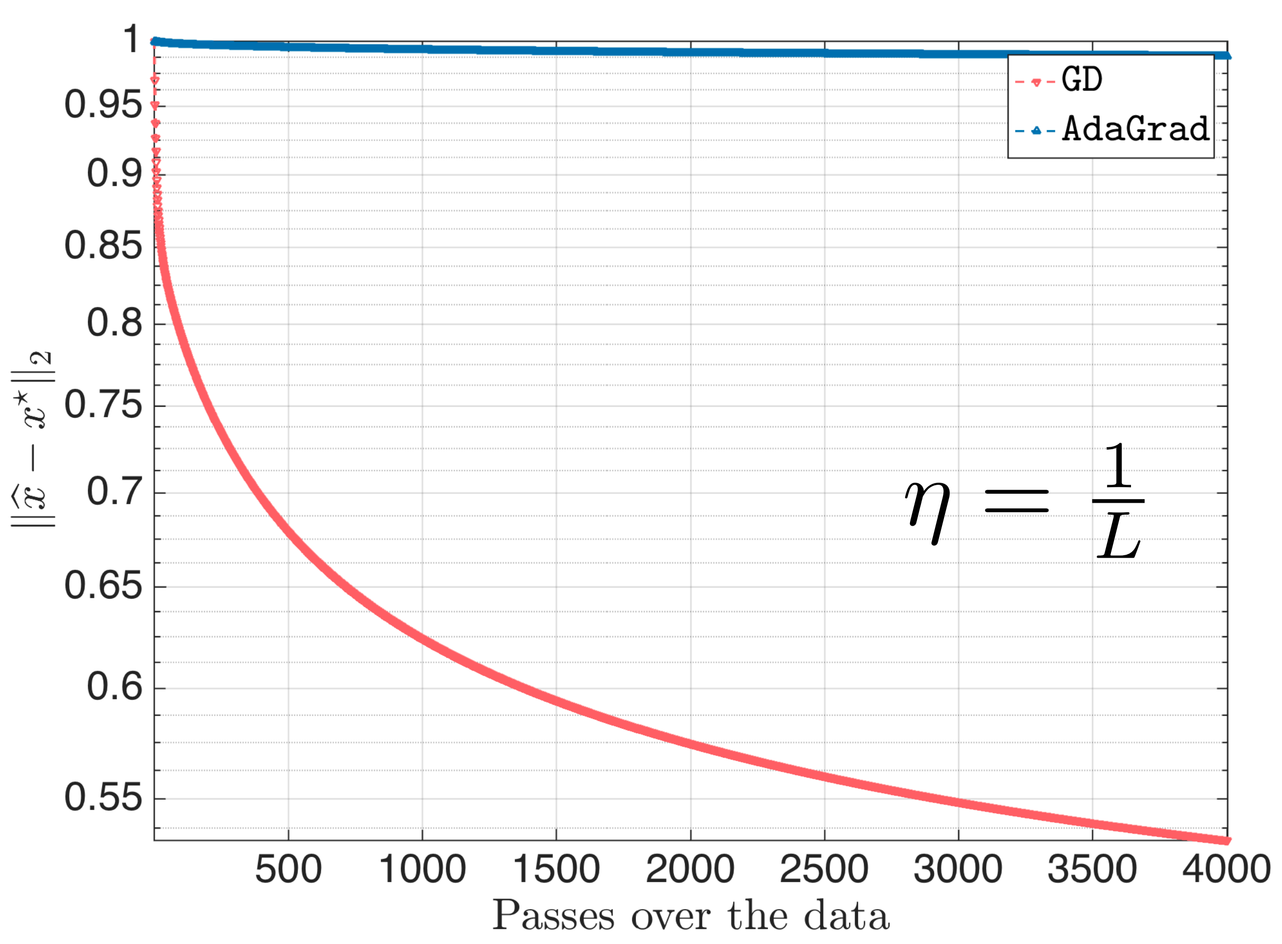
Well−conditioned linear regression

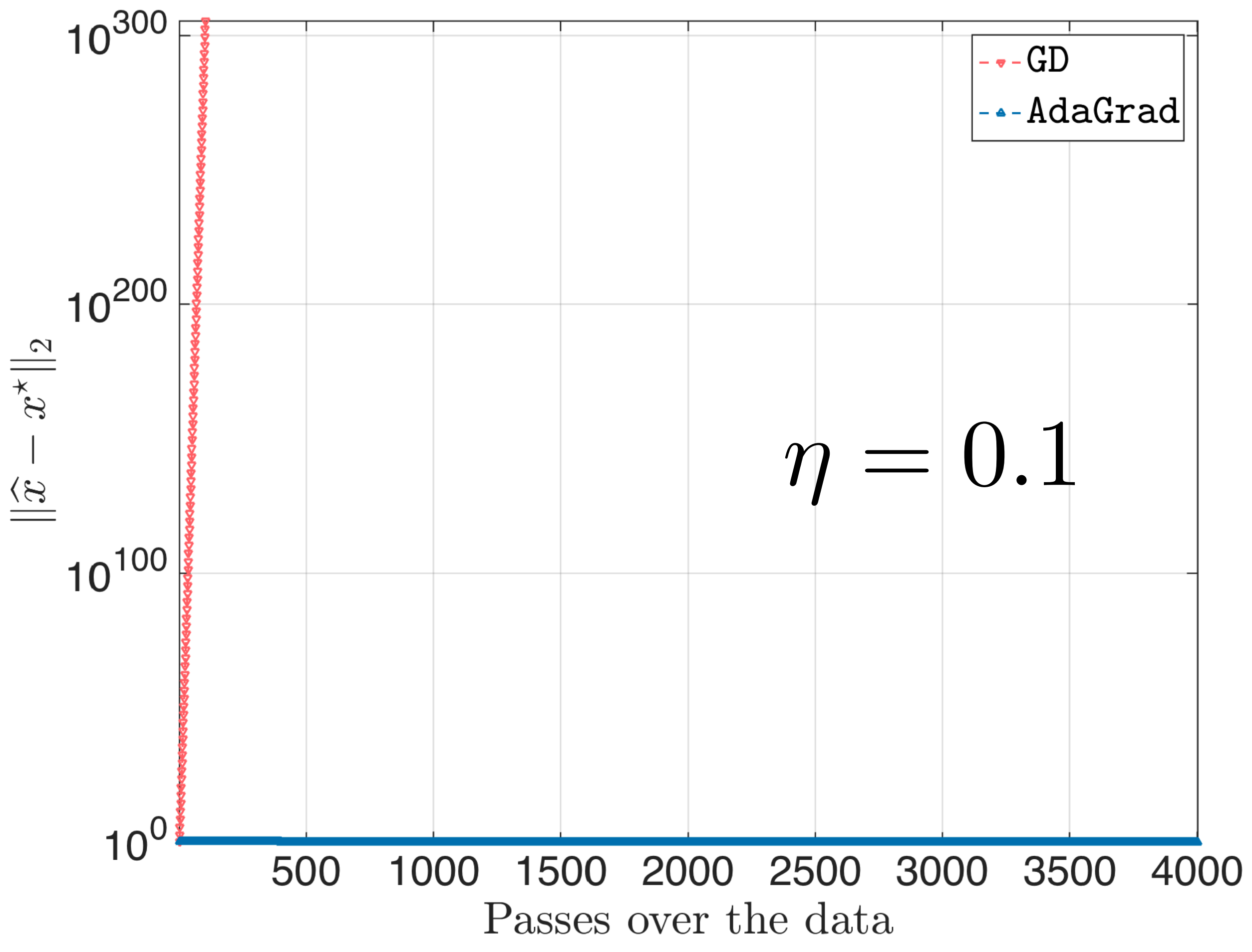


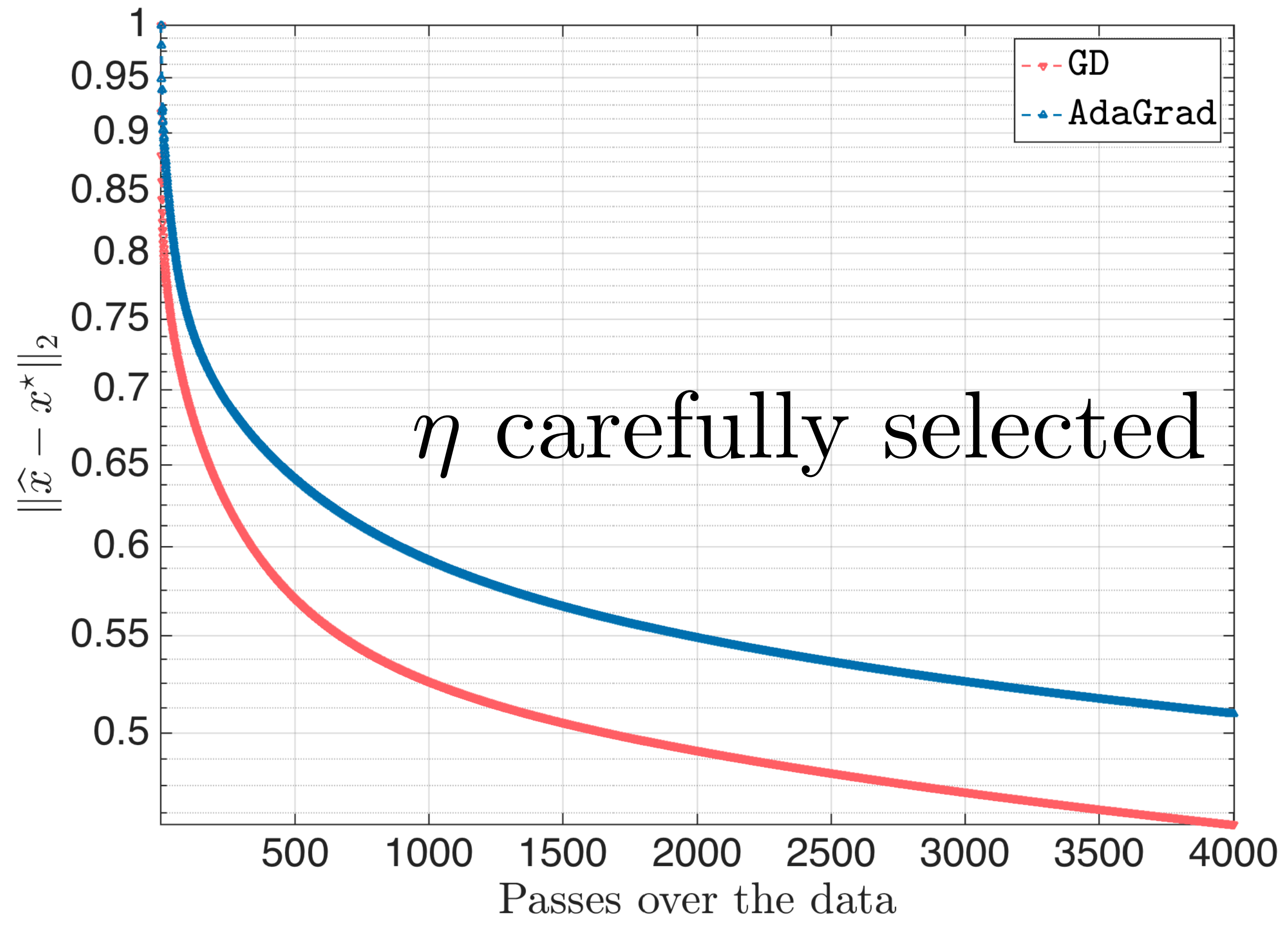




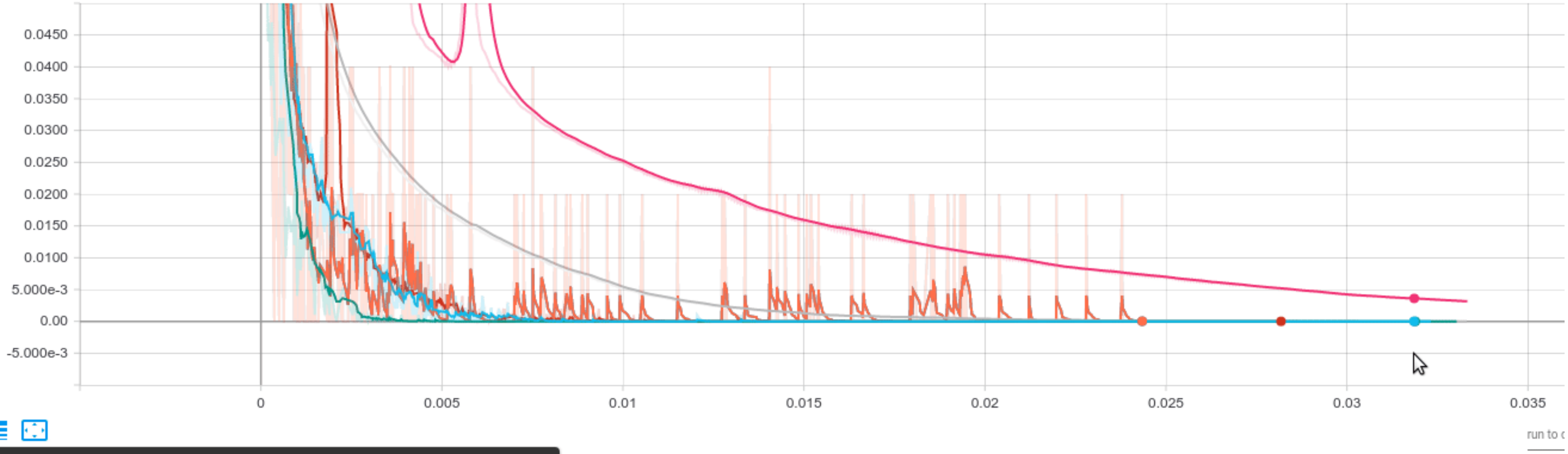
Ill−conditioned linear regression







AdaGrad in practice



Name	Smoothed	Value	Step	Time	Relative
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
SGD1/.	2.1986e-5	0.000	5.486k	Sun Dec 10, 15:01:31	1m 27s
SGD2	-1.1921e-7	-1.1921e-7	5.486k	Sun Dec 10, 15:03:13	1m 41s

Removing extended gradient accumulation: **RMSprop** algorithm

– Idea: keep AdaGrad as it is; except, use a weighted moving average for gradient accumulation

+ Diagonal AdaGrad rule: $\underbrace{\mathrm{diag}(B_t)}_{E[g^2]_t} = \underbrace{\mathrm{diag}(B_{t-1})}_{E[g^2]_{t-1}} + \underbrace{\mathrm{diag}\left(\nabla f_{i_t}(x_t) \circ \nabla f_{i_t}(x_t)\right)}_{g_t^2}$

+ RMSprop rule: $E[g^2]_t = \frac{9}{10} \cdot E[g^2]_{t-1} + \frac{1}{10} \cdot g_t^2$

``We always give weight 0.1 to the new information``

– Algorithm:

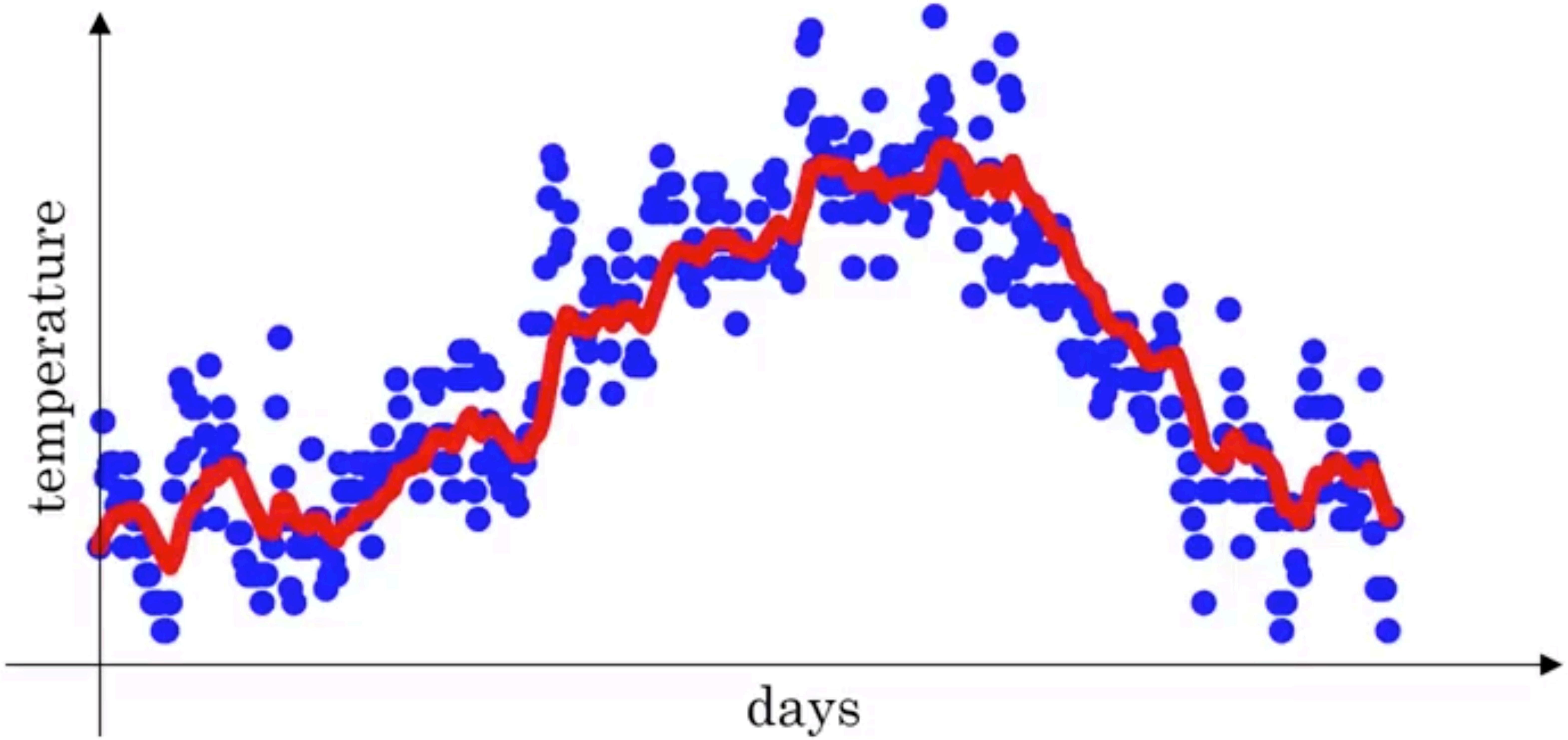
$$E[g^2]_t = \frac{9}{10} \cdot E[g^2]_{t-1} + \frac{1}{10} \cdot g_t^2$$

$$x_{t+1} = x_t - \frac{\eta}{\sqrt{E[g^2]_t + \epsilon}} \nabla f_{i_t}(x_t)$$

Introducing exponentially weighted averages

(Adapted from Ng's lectures)

- Toy example: temperature values over a year



- Computing trends: local averages and how they evolve

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

Introducing exponentially weighted averages

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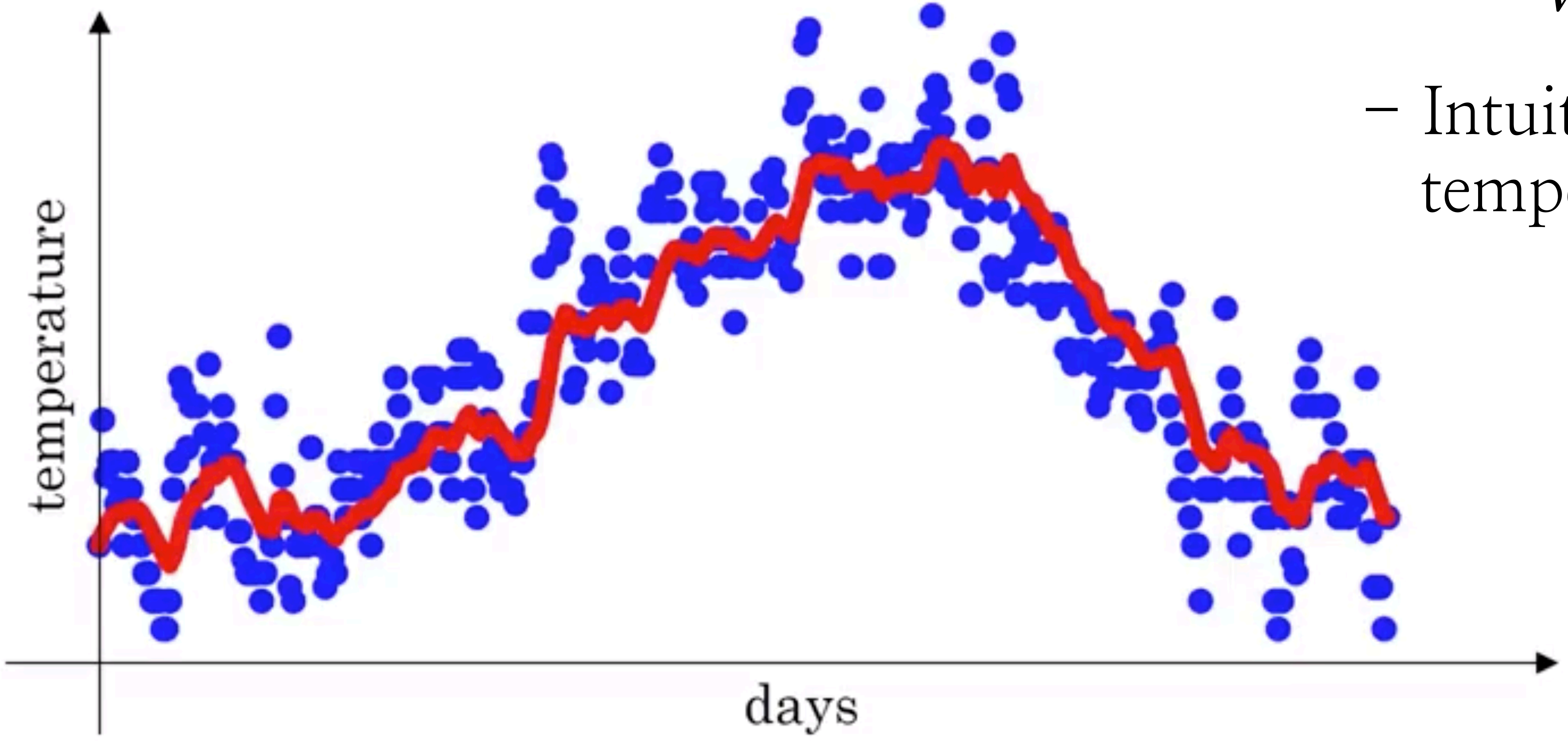
- Toy example: temperature values over a year



- General formula:

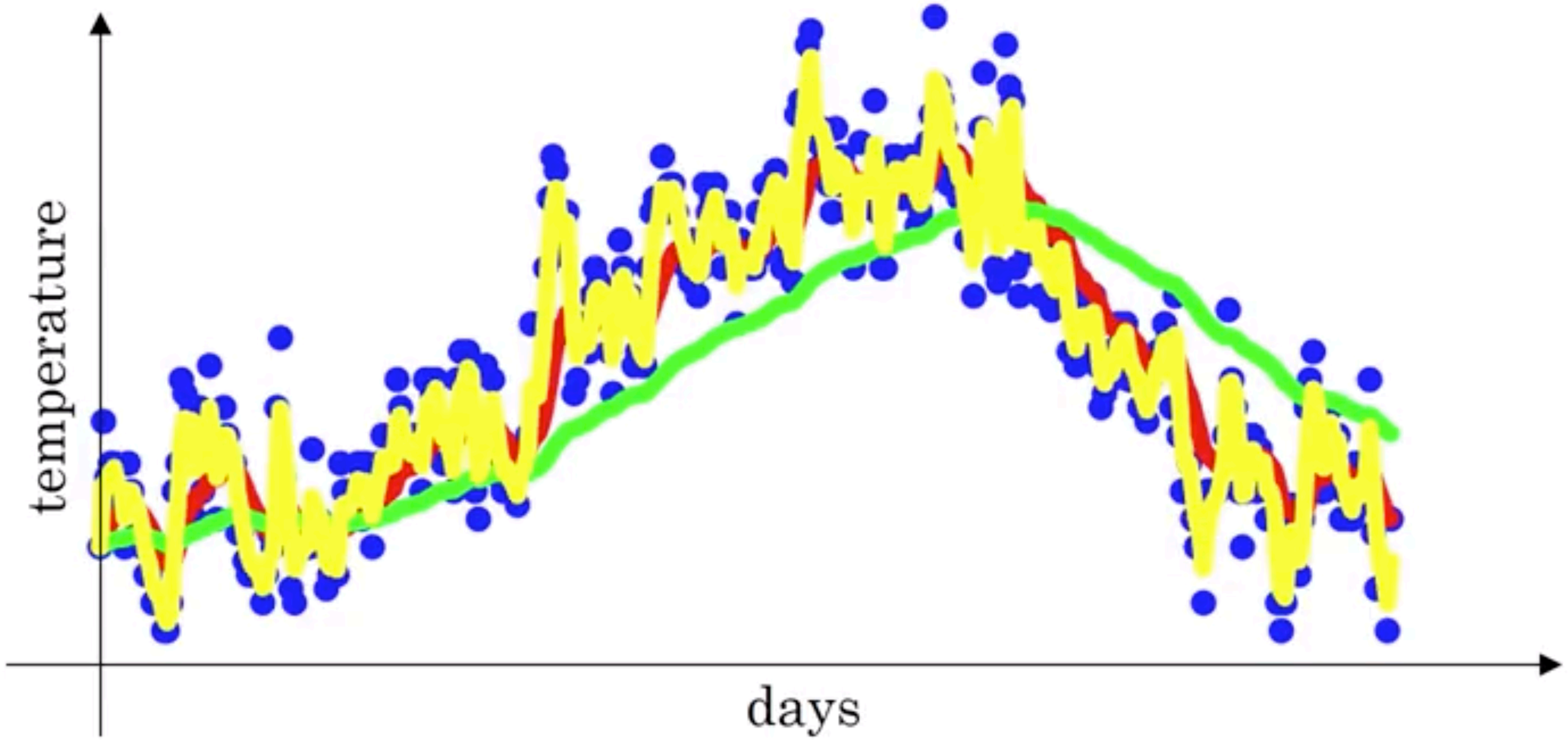
$$V_t = \beta V_{t-1} + (1-\beta)\theta_t$$

- Intuition: V_t approximates temperature over $\approx \dfrac{1}{1-\beta}$ days

Introducing exponentially weighted averages

(Adapted from Ng's lectures)

- Toy example: temperature values over a year



- Examples:

$\beta = 0.9 \rightarrow \quad \approx 10$ days

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

$\beta = 0.5 \rightarrow \quad \approx 2$ days

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

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"

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

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

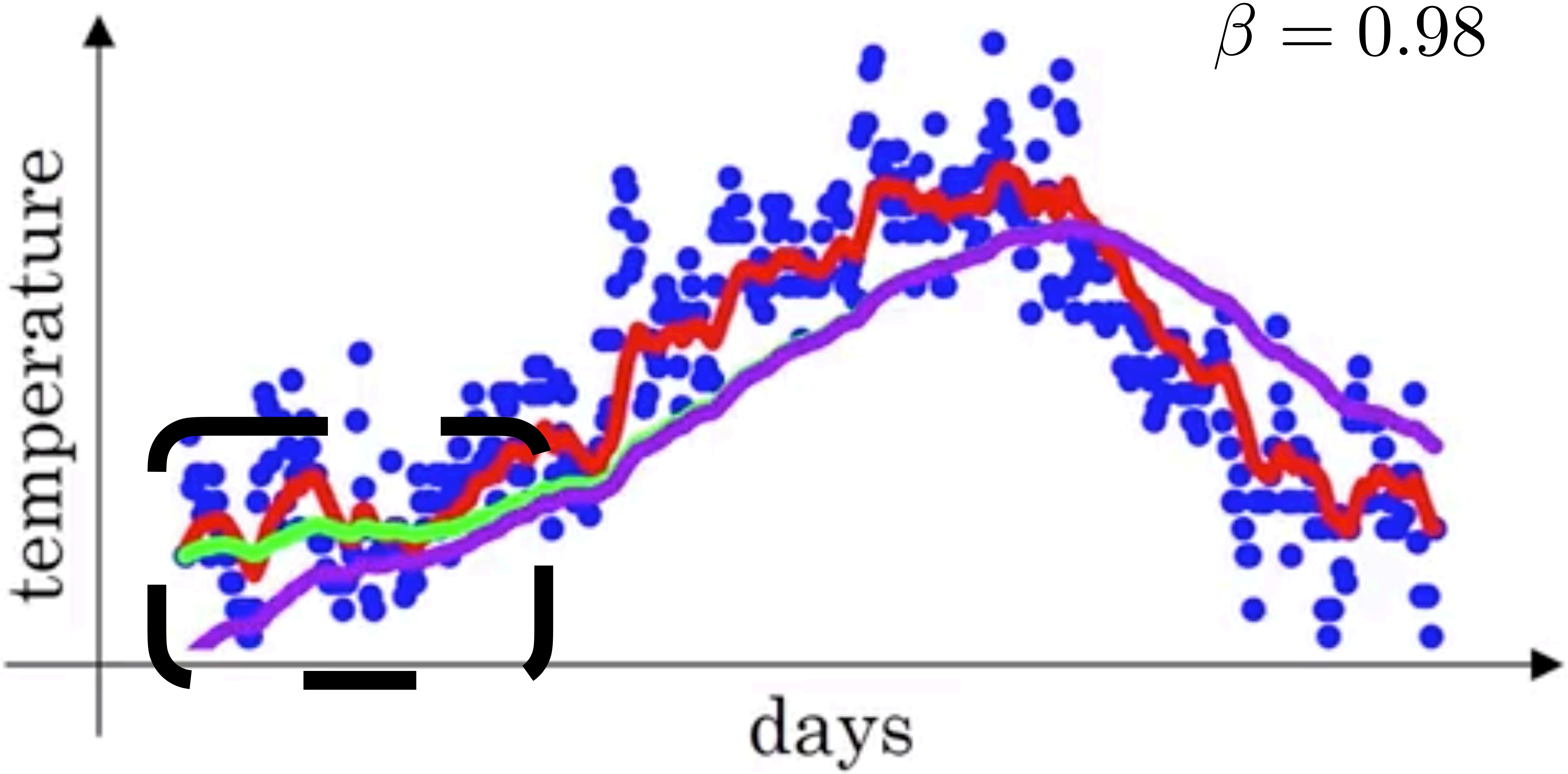
Bias correction in weighted averages

(Adapted from Ng's lectures)

– How to explain these "weird" denominators?

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

$\beta = 0.98$

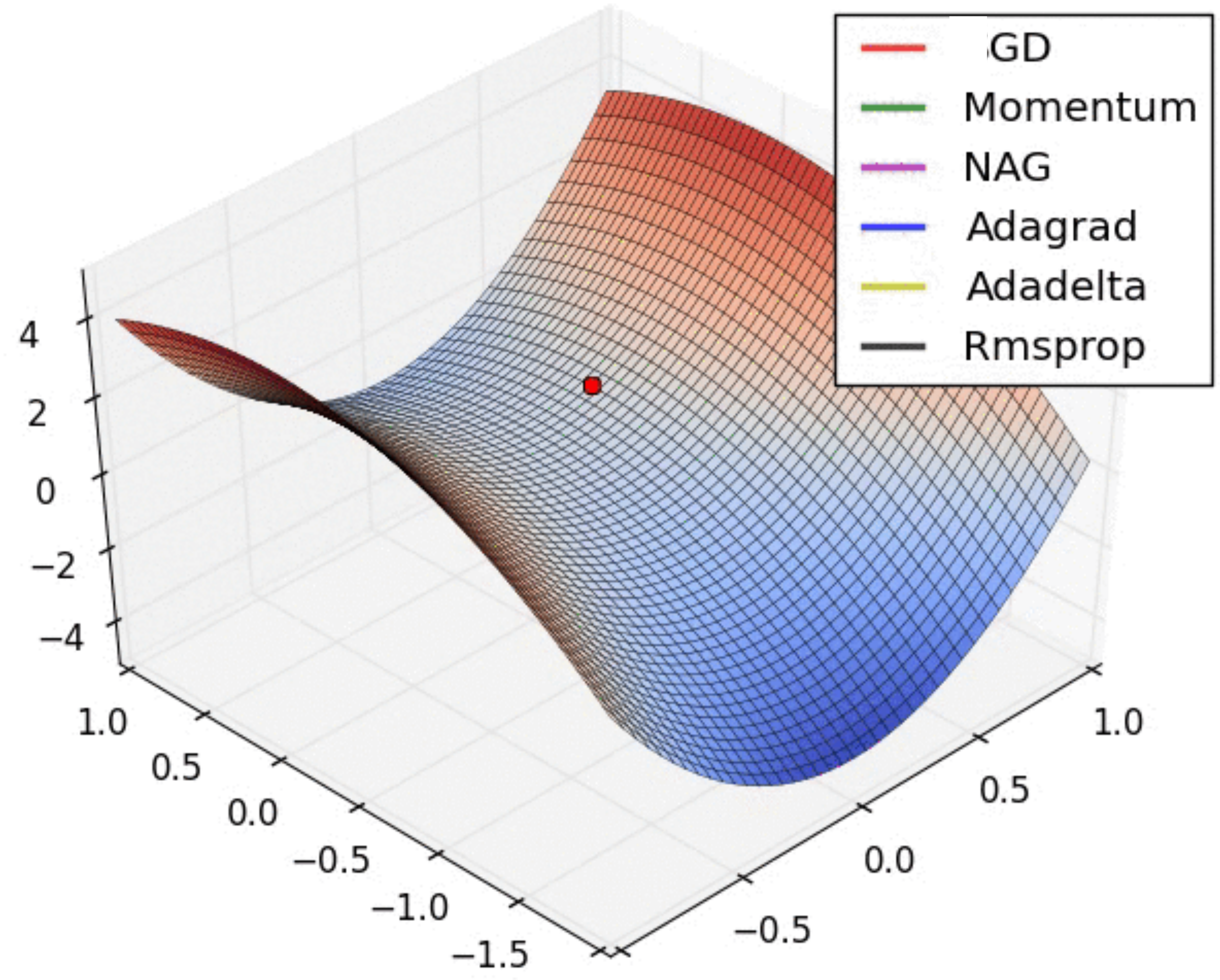


Other algorithms and sources

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

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

- Choosing the right algorithm: there is no consensus about it (see next slides)
- A visualization of their performance in toy examples:



GD
Momentum
NAG
Adagrad
Adadelta
Rmsprop
4
2
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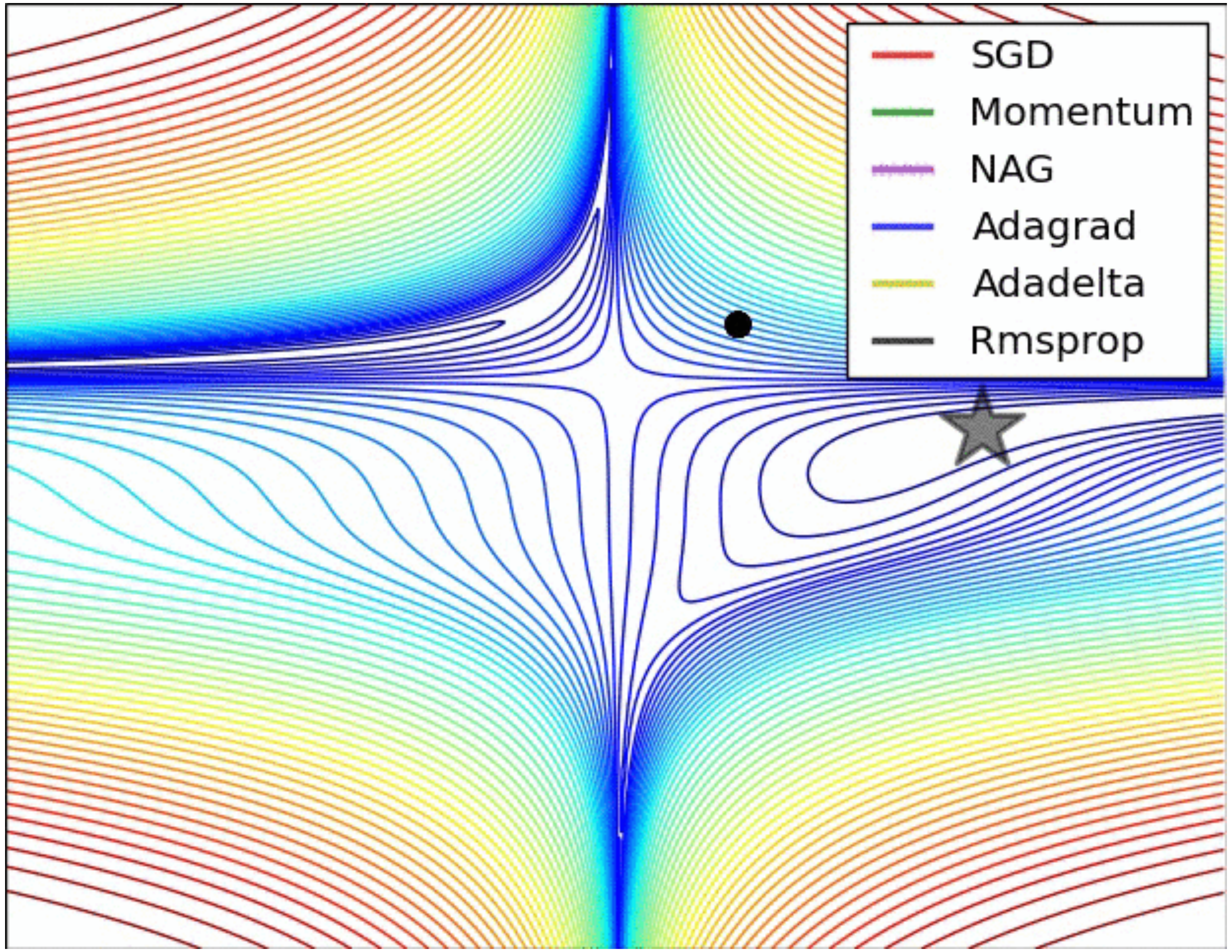

SGD
Momentum
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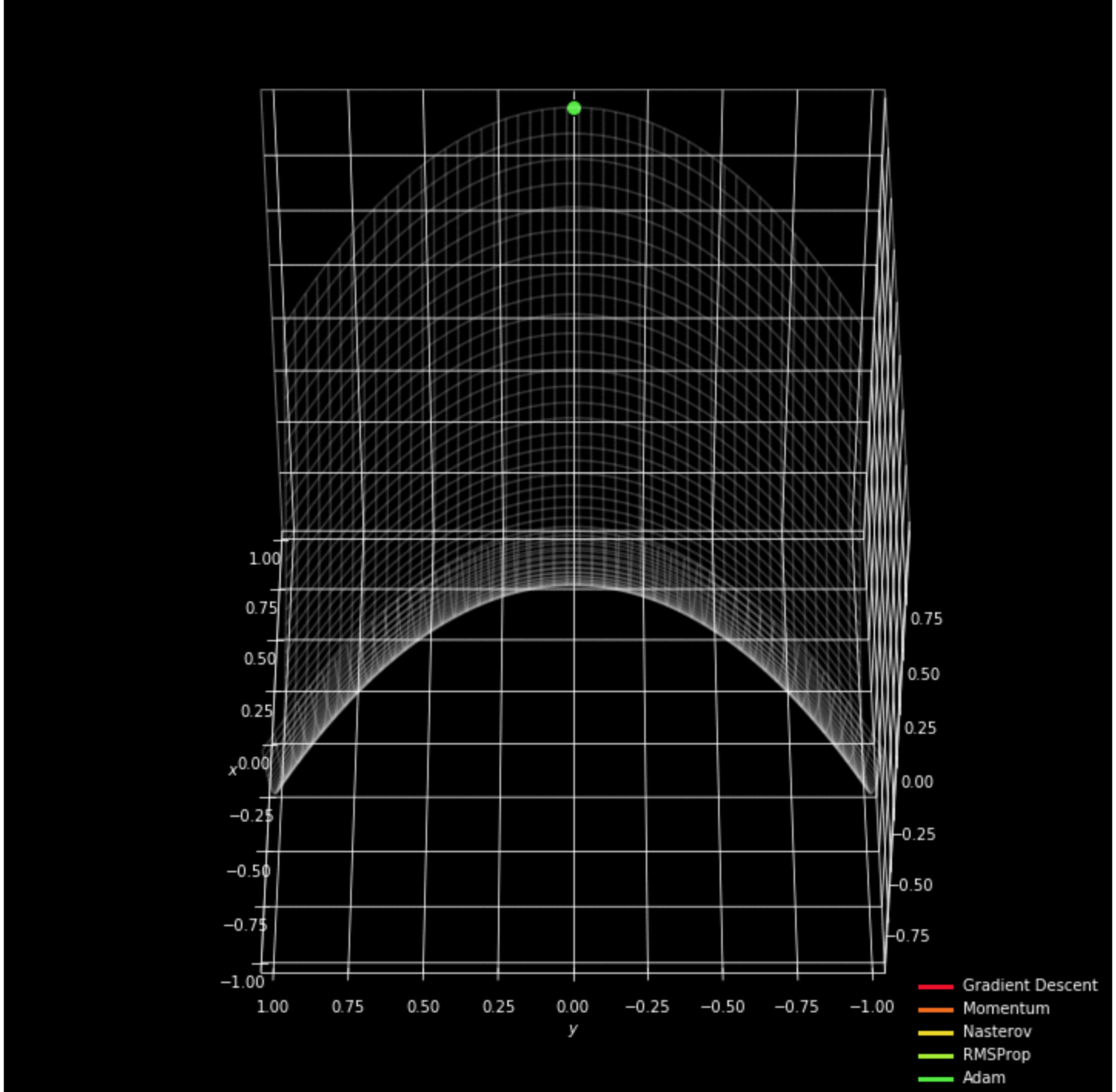
Adagrad
Adadelta
Rmsprop


1.00
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Gradient Descent
Momentum
Nasterov
RMSProp
Adam

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- A visualization of their performance in toy examples:

- Bonus discussion: **The marginal value of adaptive methods**

(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)