Statistical Machine Learning (BE4M33SSU)
Lecture 7a: Stochastic Gradient Descent

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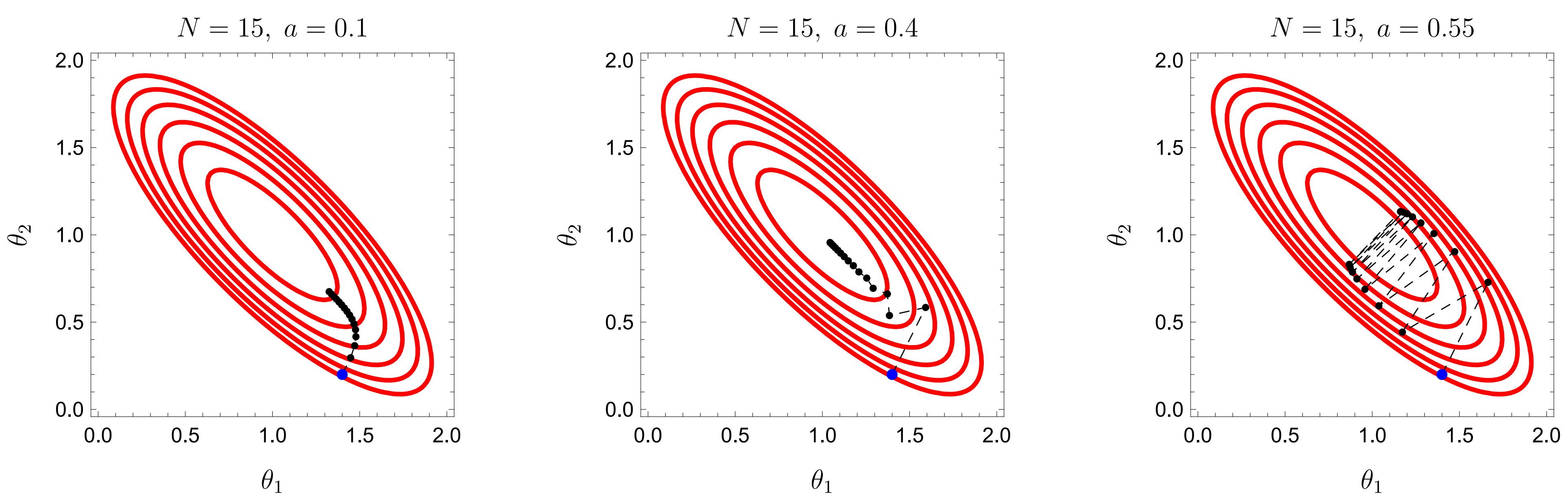
Gradient Descent (GD)

- **Task**: find parameters which minimize loss over the training dataset:

$$\boldsymbol{\theta}^* = \operatorname*{argmin}_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\theta})$$

where $\boldsymbol{\theta}$ is a set of all parameters defining the ANN

- Gradient descent: $\boldsymbol{\theta}_{k+1} = \boldsymbol{\theta}_k - \alpha_k \nabla \mathcal{L}(\boldsymbol{\theta}_k)$
where $\alpha_k > 0$ is the **learning rate** or **stepsize** at iteration k



Stochastic Gradient Descent (SGD): Motivation

- The loss has typically an additive structure, hence:

$$\nabla \mathcal{L}(\boldsymbol{\theta}) = \frac{1}{m} \sum_{i=1}^{m} \nabla \ell(y_i, h_{\boldsymbol{\theta}}(\boldsymbol{x}_i))$$

- Evaluation of $\nabla \mathcal{L}(\boldsymbol{\theta})$ takes $\mathcal{O}(m)$ time
- What if we have duplicate samples in $\mathcal{T}_m$?
- Online learning?
- Use a single sample or a *mini-batch* instead of the *full-batch* approach $\Rightarrow$ Stochastic Gradient Descent (SGD)
- The following is based on *Bottou, Curtis and Nocedal: Optimization Methods for Large-Scale Machine Learning, 2018*

Simplifying the Notation

- Let's simplify and generalize the notation
- The gradient of loss (empirical risk) is

$$\nabla \mathcal{L}(\boldsymbol{\theta}) = \frac{1}{m} \sum_{i=1}^{m} \nabla \ell(y_i, h_{\boldsymbol{\theta}}(\boldsymbol{x}_i))$$

- Represent a sample (or a set of samples) by a *seed* s, meaning the realization of s is either an input-output pair (x, y) or a set of pairs $\{(x_i, y_i)\}_{i \in \mathcal{S}}$, $\mathcal{S} \subseteq \{1, \ldots, m\}$
- Define f to be a composite of ℓ and prediction h
- As an example, for GD above we can define $s_i \triangleq (x_i, y_i) \in \mathcal{T}^m$ and write

$$\nabla \mathcal{L}(\boldsymbol{\theta}) = \frac{1}{m} \sum_{i=1}^{m} \nabla f(\theta, s_i)$$

SGD Algorithm

- Stochastic Gradient Descent

1 Choose an initial iterate $\boldsymbol{\theta}_1$
2 **for** $k = 1, 2, \ldots$
3 Generate a realization of the random variable s_k
4 Compute a stochastic gradient estimate vector $g(\boldsymbol{\theta}_k, s_k)$
5 Choose a stepsize $\alpha_k > 0$
6 Set the new iterate as $\boldsymbol{\theta}_{k+1} \leftarrow \boldsymbol{\theta}_k - \alpha_k \, g(\boldsymbol{\theta}_k, s_k)$

- Possible options of a stochastic vector

$$g(\boldsymbol{\theta}_k, s_k) = \begin{cases} \nabla f(\boldsymbol{\theta}_k, s_k) & \text{single sample, online learning} \\ \frac{1}{m_k} \sum_{i=1}^{m_k} \nabla f(\boldsymbol{\theta}_k, s_{k,i}) & \text{batch/mini-batch} \\ H_k \, \frac{1}{n_k} \sum_{i=1}^{n_k} \nabla f(\boldsymbol{\theta}_k, s_{k,i}) & \text{Newton/quasi-Newton direction} \end{cases}$$

- Holds for picking samples of $\mathcal{T}_m$ *with replacement*, for picking *without replacement* it holds only until dataset gets exhausted in general
- We consider the elements of the random sequence $\{s_k\}$ independent

SGD Convergence Theorem: Overview

- The main theorem shows that the *expected optimality gap*

$$\mathbb{E}[\mathcal{L}(\boldsymbol{\theta}_k) - \mathcal{L}_*] \xrightarrow{k \to \infty} 0$$

where $\mathcal{L}_*$ is the optimal (minimal) loss

- Assumptions:

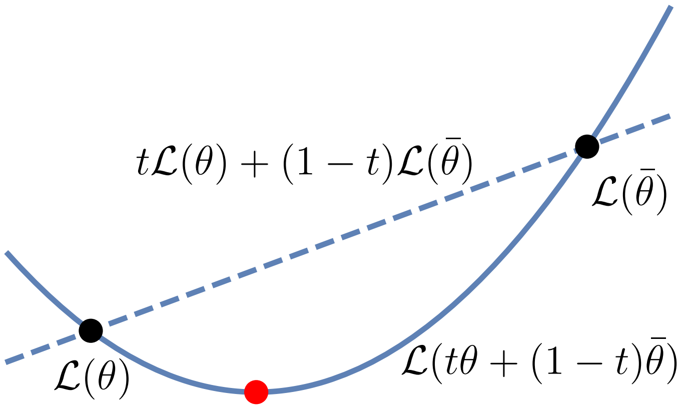
1. Strong convexity of $\mathcal{L}$
2. Lipschitz continuous gradient $\nabla\mathcal{L}$
3. Bounds on $\mathcal{L}$ and $g(\boldsymbol{\theta}_k, s_k)$:
    - $\mathcal{L}$ is bounded below by a scalar $\mathcal{L}_{inf}$,
    - directions of $g(\boldsymbol{\theta}_k, s_k)$ and $\nabla\mathcal{L}(\boldsymbol{\theta}_k)$ *similar*,
    - their norms are also *similar*

Convexity

- Convex function definition:

$$\mathcal{L}(t\boldsymbol{\theta} + (1-t)\bar{\boldsymbol{\theta}}) \le t\mathcal{L}(\boldsymbol{\theta}) + (1-t)\mathcal{L}(\bar{\boldsymbol{\theta}})$$

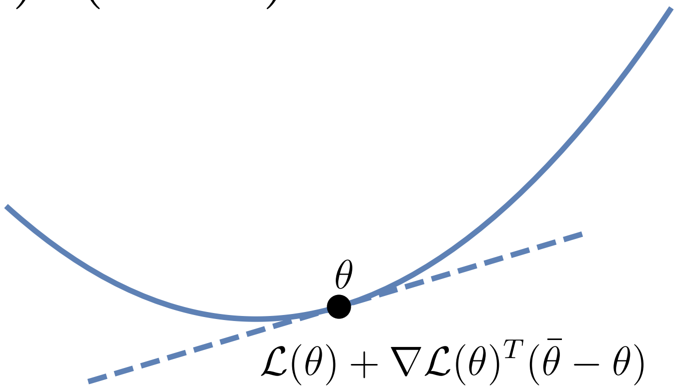
for all $(\boldsymbol{\theta}, \bar{\boldsymbol{\theta}}) \in \mathbb{R}^d \times \mathbb{R}^d$



- Equivalently (first-order condition):

$$\mathcal{L}(\bar{\boldsymbol{\theta}}) \ge \mathcal{L}(\boldsymbol{\theta}) + \nabla\mathcal{L}(\boldsymbol{\theta})^T(\bar{\boldsymbol{\theta}} - \boldsymbol{\theta})$$

the function lies above all its tangents



- See A4B33OPT
- But we need a stronger assumption...

Assumption 1: Strong Convexity

- The loss function $\mathcal{L} : \mathbb{R}^d \to \mathbb{R}$ is strongly convex if there exists constant $c > 0$ such that

$$\mathcal{L}(\bar{\boldsymbol{\theta}}) \geq \mathcal{L}(\boldsymbol{\theta}) + \nabla \mathcal{L}(\boldsymbol{\theta})^T (\bar{\boldsymbol{\theta}} - \boldsymbol{\theta}) + \frac{1}{2} c \left\| \bar{\boldsymbol{\theta}} - \boldsymbol{\theta} \right\|_2^2$$

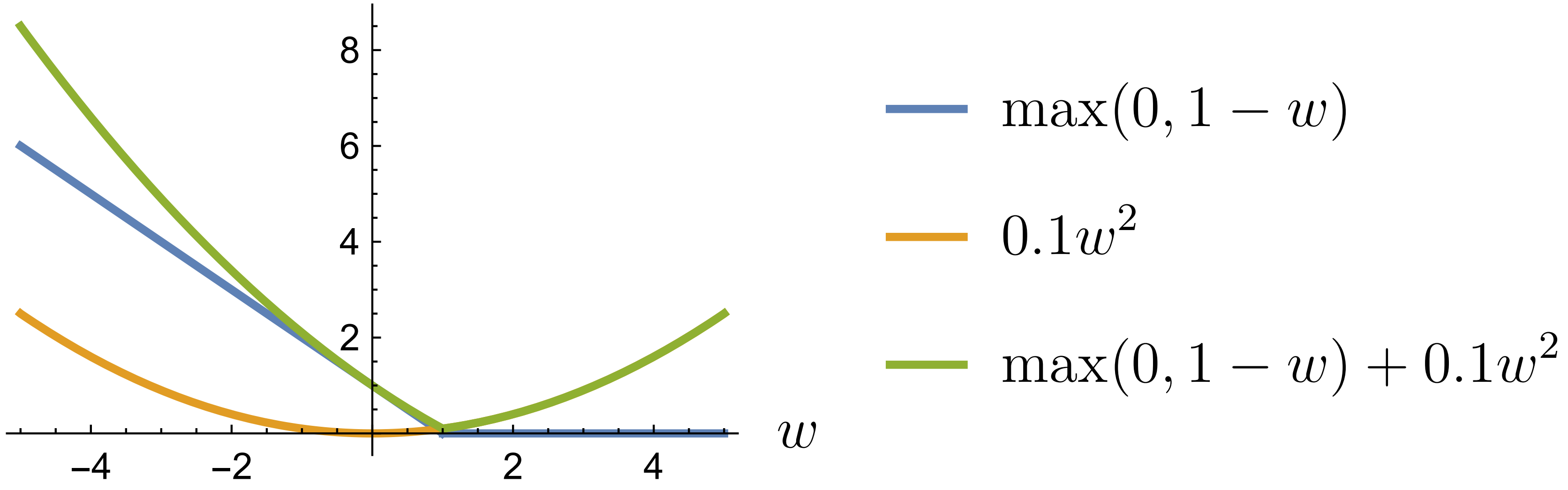
  for all $(\boldsymbol{\theta}, \bar{\boldsymbol{\theta}}) \in \mathbb{R}^d \times \mathbb{R}^d$

- *Intuition*: quadratic lower bound on function growth

Strong Convexity Example

- Example (SVM objective): $\max(0, 1 - y(\boldsymbol{w}^T\boldsymbol{x} + b)) + \frac{\lambda}{2}\|\boldsymbol{w}\|_2^2$
- Here, simplified to 1D
- Hinge loss is linear and constant in part: it is convex
- w^2 is strongly convex, easily show equality for $c = 2$:

$$\bar{w}^2 \geq w^2 + 2w(\bar{w} - w) + (\bar{w} - w)^2$$
$$\bar{w}^2 \geq w^2 + 2w(\bar{w} - w) + \bar{w}^2 - 2\bar{w} \cdot w + w^2$$
$$0 \geq 2w^2 + 2w \cdot \bar{w} - 2w^2 - 2\bar{w} \cdot w = 0$$



Assumption 2: Lipschitz Continuous Gradient

- The loss function is continuously differentiable and the gradient is *Lipschitz continuous* with *Lipschitz constant* $L > 0$:

$$\left\|\nabla\mathcal{L}(\boldsymbol{\theta}) - \nabla\mathcal{L}(\bar{\boldsymbol{\theta}})\right\|_2 \leq L \left\|\boldsymbol{\theta} - \bar{\boldsymbol{\theta}}\right\|_2, \text{ for all } (\boldsymbol{\theta}, \bar{\boldsymbol{\theta}}) \in \mathbb{R}^d \times \mathbb{R}^d$$

- *Intuition:* the gradient does not change too quickly w.r.t. $\boldsymbol{\theta}$
- Provides an indicator for how far to move to decrease $\mathcal{L}$
- Lemma (see Bottou et al. for the proof):

$$\mathcal{L}(\bar{\boldsymbol{\theta}}) \leq \mathcal{L}(\boldsymbol{\theta}) + \nabla\mathcal{L}(\boldsymbol{\theta})^T(\bar{\boldsymbol{\theta}} - \boldsymbol{\theta}) + \frac{1}{2}L\left\|\bar{\boldsymbol{\theta}} - \boldsymbol{\theta}\right\|_2^2$$

Assumptions 1 & 2: Summary

- We have the strong convexity:

$$\mathcal{L}(\bar{\boldsymbol{\theta}}) \geq \mathcal{L}(\boldsymbol{\theta}) + \nabla\mathcal{L}(\boldsymbol{\theta})^T(\bar{\boldsymbol{\theta}} - \boldsymbol{\theta}) + \frac{1}{2}c\left\|\bar{\boldsymbol{\theta}} - \boldsymbol{\theta}\right\|_2^2$$

  and the Lipschitz continuous gradient:

$$\mathcal{L}(\bar{\boldsymbol{\theta}}) \leq \mathcal{L}(\boldsymbol{\theta}) + \nabla\mathcal{L}(\boldsymbol{\theta})^T(\bar{\boldsymbol{\theta}} - \boldsymbol{\theta}) + \frac{1}{2}L\left\|\bar{\boldsymbol{\theta}} - \boldsymbol{\theta}\right\|_2^2$$

  hence $c \leq L$ holds

- Quadratic lower and upper bounds on $\mathcal{L}(\bar{\boldsymbol{\theta}})$ growth

Assumptions Summary

constant	description	higher value means
$c > 0$	strong convexity (lower bound)	"more convex"
$L > 0$	Lipschitz continuous gradient (upper bound)	higher gradient change allowed
$\mathcal{L} \geq \mathcal{L}_{inf}$	lower bound on loss	
$\mu > 0$	$g(\boldsymbol{\theta}_k, s_k)$ direction comparable to $\nabla\mathcal{L}(\boldsymbol{\theta}_k)$	smaller angular difference between $\mathbb{E}_{s_k}[g(\boldsymbol{\theta}_k, s_k)]$ and $\nabla\mathcal{L}(\boldsymbol{\theta}_k)$
$M \geq 0$	limits expected *scalar variance* of $g(\boldsymbol{\theta}_k, s_k)$	higher variance of $g(\boldsymbol{\theta}_k, s_k)$ allowed
$M_G \geq \mu^2$	limits expected squared norm of $g(\boldsymbol{\theta}_k, s_k)$ w.r.t. the $\|\nabla\mathcal{L}(\boldsymbol{\theta}_k)\|_2$	higher expected ratio of $\mathbb{E}_{s_k}[g(\boldsymbol{\theta}_k, s_k)]$ and $\nabla\mathcal{L}(\boldsymbol{\theta}_k)$ norms allowed

SGD Convergence: Strongly Convex $\mathcal{L}$, Fixed Stepsize

- **Theorem:** assuming Lipschitz continuity, the Bounds and strong convexity of $\mathcal{L}$, the SGD is run with a fixed stepsize $\alpha_k = \alpha$ for all $k \in \mathbb{N}$, where $0 < \alpha \leq \frac{\mu}{LM_G}$. Then the *expected optimality gap* satisfies the following for all k:

$$\mathbb{E}[\mathcal{L}(\boldsymbol{\theta}_k) - \mathcal{L}_*] \leq \frac{\alpha LM}{2c\mu} + (1 - \alpha c\mu)^{k-1} \left(\mathcal{L}(\boldsymbol{\theta}_1) - \mathcal{L}_* - \frac{\alpha LM}{2c\mu} \right)$$
$$\xrightarrow{k\to\infty} \frac{\alpha LM}{2c\mu}$$

- Note: $(1 - \alpha c\mu)^{k-1} \xrightarrow{k\to\infty} 0$ as $0 < \alpha c\mu \leq \frac{c\mu^2}{LM_G} \leq \frac{c\mu^2}{L\mu^2} = \frac{c}{L} \leq 1$
- In general, for the fixed stepsize, the *optimality gap* tends to zero, but converges to $\frac{\alpha LM}{2c\mu} \geq 0$

Full-Batch Gradient Descent

- How does the theorem apply to the full-batch setting (GD)?
- The $g(\boldsymbol{\theta}_k, s_k)$ is an unbiased estimate of $\nabla\mathcal{L}(\boldsymbol{\theta}_k)$:

$$\mathbb{E}_{s_k}[g(\boldsymbol{\theta}_k, s_k)] = \nabla\mathcal{L}(\boldsymbol{\theta}_k)$$

- Zero variance implies $M = 0$
- The optimality gap simplifies to:

$$\epsilon_k = \mathbb{E}[\mathcal{L}(\boldsymbol{\theta}_k) - \mathcal{L}_*] \leq (1 - \alpha c\mu)^{k-1} (\mathcal{L}(\boldsymbol{\theta}_1) - \mathcal{L}_*) \xrightarrow{k\to\infty} 0$$

- Asymptotically we have $\epsilon_k \leq \mathcal{O}(\rho^k)$, $\rho \in [0, 1)$
- For a given gap ϵ, the number of iterations k is proportional to $\log(1/\epsilon)$ in the worst case.

SGD Convergence: Strongly Convex $\mathcal{L}$, Diminishing Stepsize

- **Theorem:** assuming the strong convexity of $\mathcal{L}$ the Lipschitz continuity of $\nabla\mathcal{L}$ and the Bounds, the SGD is run with a stepsize such that, for all k

$$\alpha_k = \frac{\beta}{\gamma + k} \text{ for some } \beta > \frac{1}{c\mu} > 0 \text{ and } \gamma > 0 \text{ such that } \alpha_1 \leq \frac{\mu}{LM_G}$$

Then the *expected optimality gap* satisfies the following for all k:

$$\mathbb{E}[\mathcal{L}(\boldsymbol{\theta}_k) - \mathcal{L}_*] \leq \frac{v}{\gamma + k}$$

where v is a constant

- Now we have $\mathbb{E}[\mathcal{L}(\boldsymbol{\theta}_k) - \mathcal{L}_*] \xrightarrow{k\to\infty} 0$
- Asymptotically the gap is $\epsilon_k \leq \mathcal{O}(1/k)$ which means that the number of iterations k is proportional to $1/\epsilon$ in the worst case

GD vs SGD

	GD	**SGD**
time per iteration	m	1
iterations for accuracy ϵ	$\log(1/\epsilon)$	$1/\epsilon$
time for accuracy ϵ	$m\log(1/\epsilon)$	$1/\epsilon$

- SGD time does not depend on dataset size (if not exhausted)
- For large-scale problems (large m) SGD is faster
- It is harder to tune stepsize schedule for SGD, but you can experiment on a small representative subset of the dataset
- In practise *mini-batches* are used to leverage optmization/parallelization on CPU/GPU

SGD for Nonconvex Objectives

- Corresponding theorems can be proven for nonconvex objectives
- For assumptions similar to the theorem for the diminishing stepsizes (and excluding the strong convexity) we get:

$$\lim_{k \to \infty} \mathbb{E}\left[\|\nabla \mathcal{L}(\boldsymbol{\theta}_k)\|_2^2\right] = 0$$

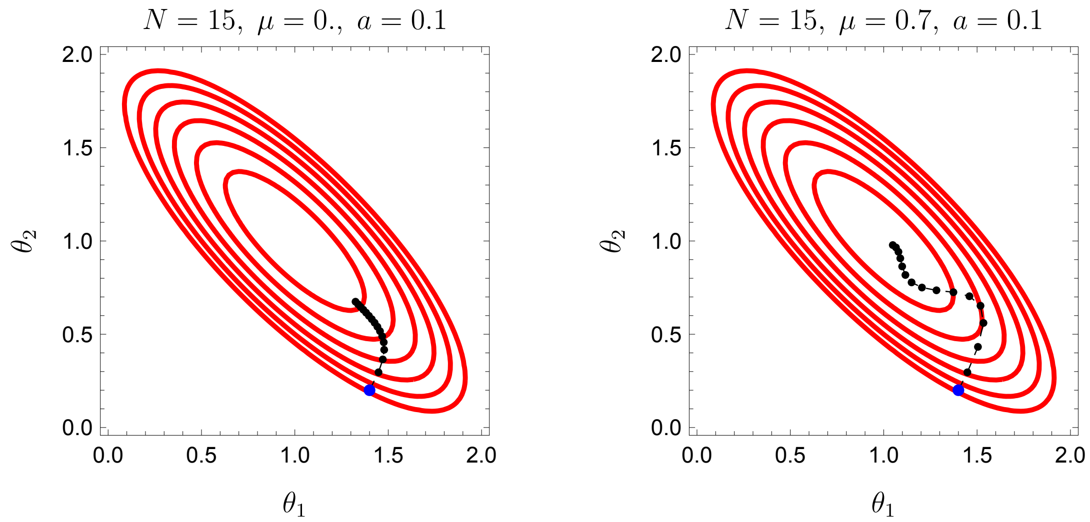
Momentum

- Simulate inertia to overcome plateaus in the error landscape:

$$\boldsymbol{v}_{k+1} \leftarrow \mu \boldsymbol{v}_k - \alpha_k \, g(\boldsymbol{\theta}_k, s_k)$$
$$\boldsymbol{\theta}_{k+1} \leftarrow \boldsymbol{\theta}_k + \boldsymbol{v}_{k+1}$$

where $\mu \in [0,1]$ is the *momentum parameter*

- Momentum damps oscillations in directions of high curvature
- It builds velocity in directions with consistent (possibly small) gradient



Adagrad

- Adaptive Gradient method (Duchi, Hazan and Singer, 2011)
- *Motivation:* a magnitude of gradient differs a lot for different parameters
- *Idea:* reduce learning rates for parameters having high values of gradient

$$G_{k+1,i} \leftarrow G_{k,i} + [g(\boldsymbol{\theta}_k, s_k)]_i^2$$
$$\theta_{k+1,i} \leftarrow \theta_{k,i} - \frac{\alpha}{\sqrt{G_{k+1,i}} + \epsilon} \cdot [g(\boldsymbol{\theta}_k, s_k)]_i$$

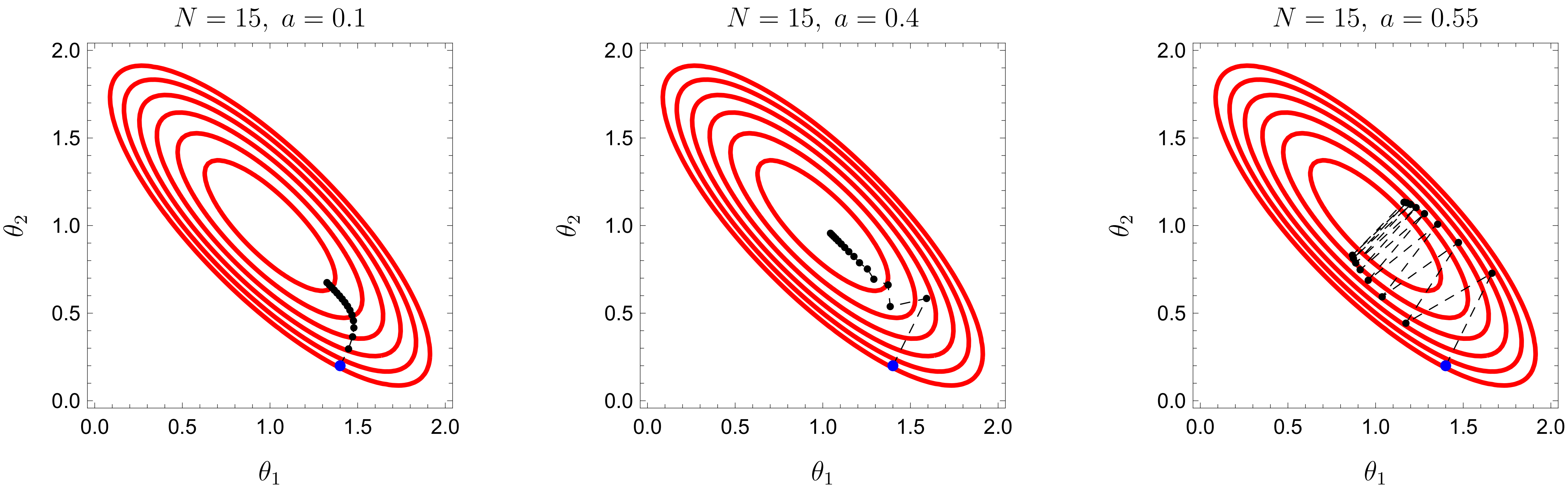
- $G_{k,i}$ accumulates squared partial derivative approximations w.r.t. to the parameter $\theta_{k,i}$
- ϵ is a small positive number to prevent division by zero
- *Weakness:* ever increasing G_i leads to slow convergence eventually

RMSProp

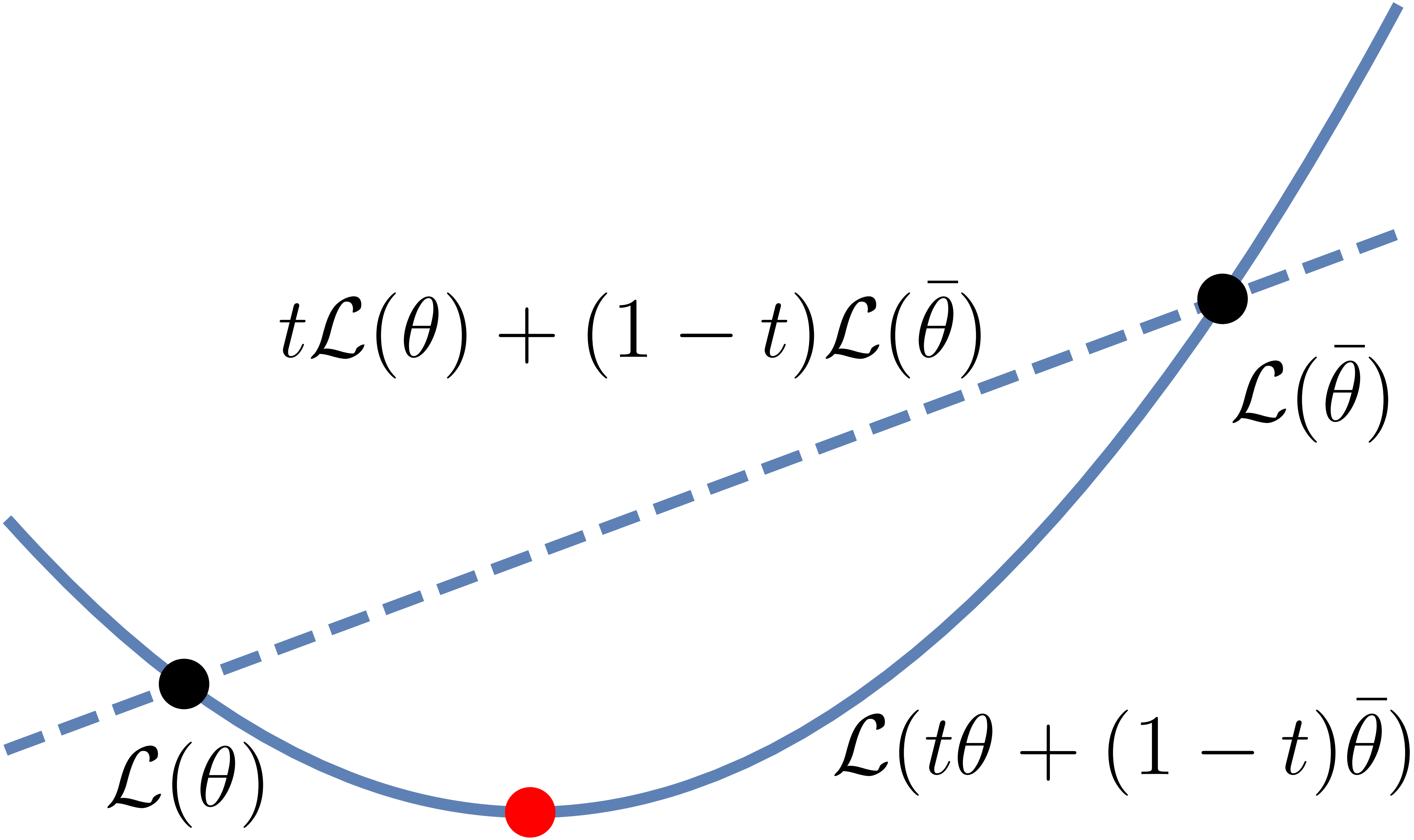
- Similar to Adagrad but employs a moving average:

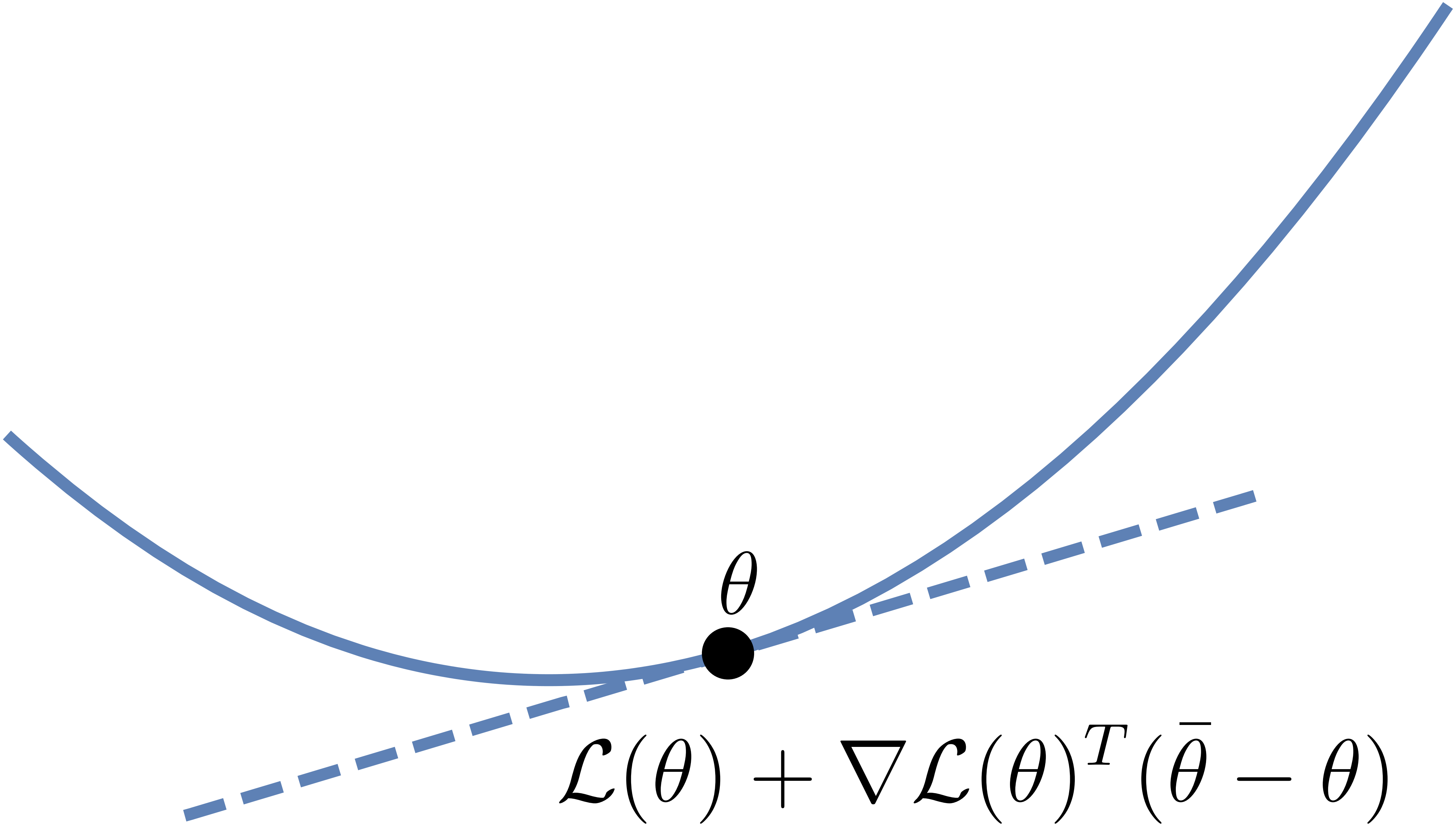
$$G_{k+1,i} = \gamma G_{k,i} + (1-\gamma)\left[g(\boldsymbol{\theta}_k, s_k)\right]_i^2$$

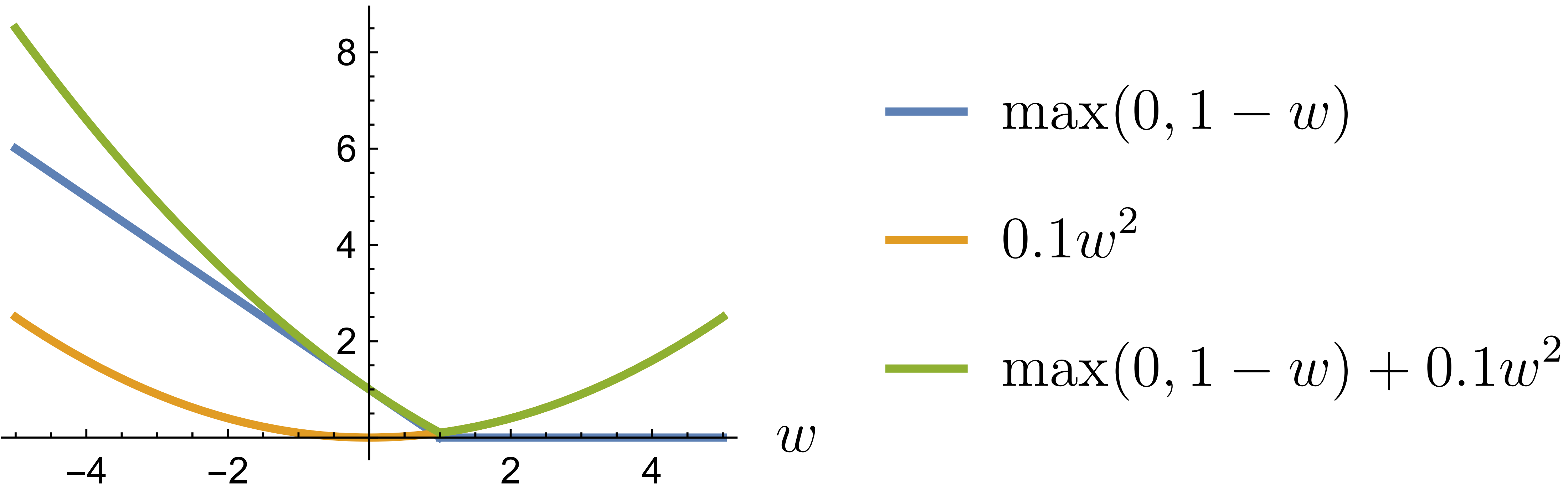
- γ is a *decay* parameter (typical value $\gamma = 0.9$)
- Unlike for Adagrad updates do not get infinitesimally small



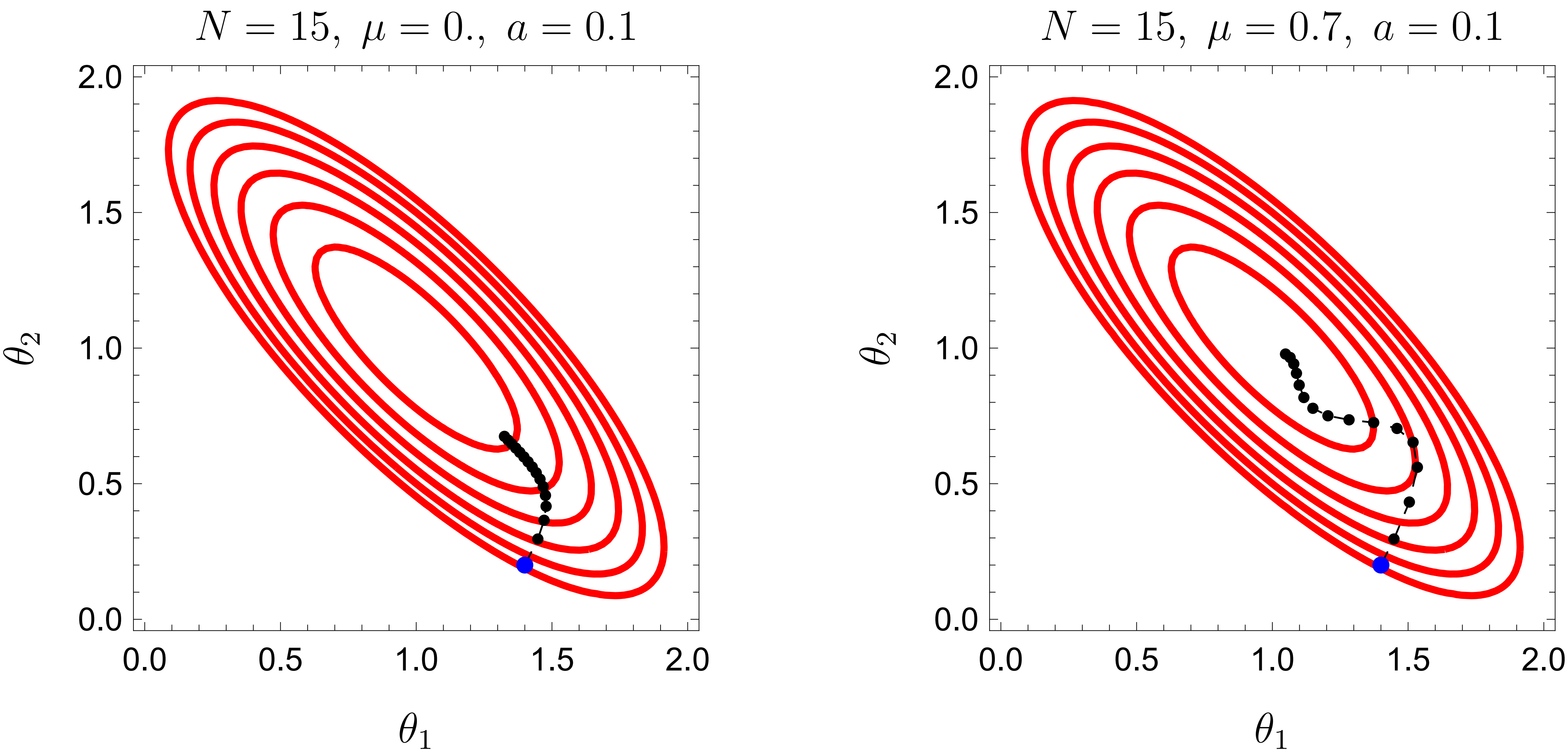
$N = 15,\ a = 0.1$
$N = 15,\ a = 0.4$
$N = 15,\ a = 0.55$
θ_2
θ_1
0.0
0.5
1.0
1.5
2.0


$t\mathcal{L}(\theta) + (1-t)\mathcal{L}(\bar{\theta})$
$\mathcal{L}(\bar{\theta})$
$\mathcal{L}(\theta)$
$\mathcal{L}(t\theta + (1-t)\bar{\theta})$


θ
$\mathcal{L}(\theta) + \nabla\mathcal{L}(\theta)^T(\bar{\theta} - \theta)$



8
6
4
2
−4
−2
2
4
w
$\max(0, 1 - w)$
$0.1w^2$
$\max(0, 1 - w) + 0.1w^2$



$N = 15,\ \mu = 0.,\ a = 0.1$
$N = 15,\ \mu = 0.7,\ a = 0.1$
θ_2
θ_1
0.0
0.5
1.0
1.5
2.0