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

Overview

- In the last lecture, we:
 - Talked about a bit of second-order methods and their approximations
 - In theory, they break lower bounds of gradient descent
 - They come with a computational cost + often do not work in all cases

(open problem: generalizability of second order methods in NNs)

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 - Talked about a bit of second-order methods and their approximations
 - In theory, they break lower bounds of gradient descent
 - They come with a computational cost + often do not work in all cases (open problem: generalizability of second order methods in NNs)
- In this lecture, we will:
 - Discuss gradient descent versions that somehow accelerate convergence
 - Discuss techniques that do not accelerate in analytical complexity but help in iteration complexity

From previous lecture: lower bounds

- For objectives with Lipschitz continuous gradients:

$$f(x_t) - f(x^*) \ge \frac{3L||x_0 - x^*||_2^2}{32(t+1)^2}$$

(Under these assumptions, and using only gradients, we cannot achieve better than $O\left(\frac{1}{t^2}\right)$)

- In addition, for objectives that are strongly convex:

$$||x_t - x^*||_2^2 \ge \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}\right)^{2t} ||x_0 - x^*||_2^2 \qquad \qquad \kappa := \frac{L}{\mu}$$

(The case we described has near optimal exponent, but does not involve the square root of κ)

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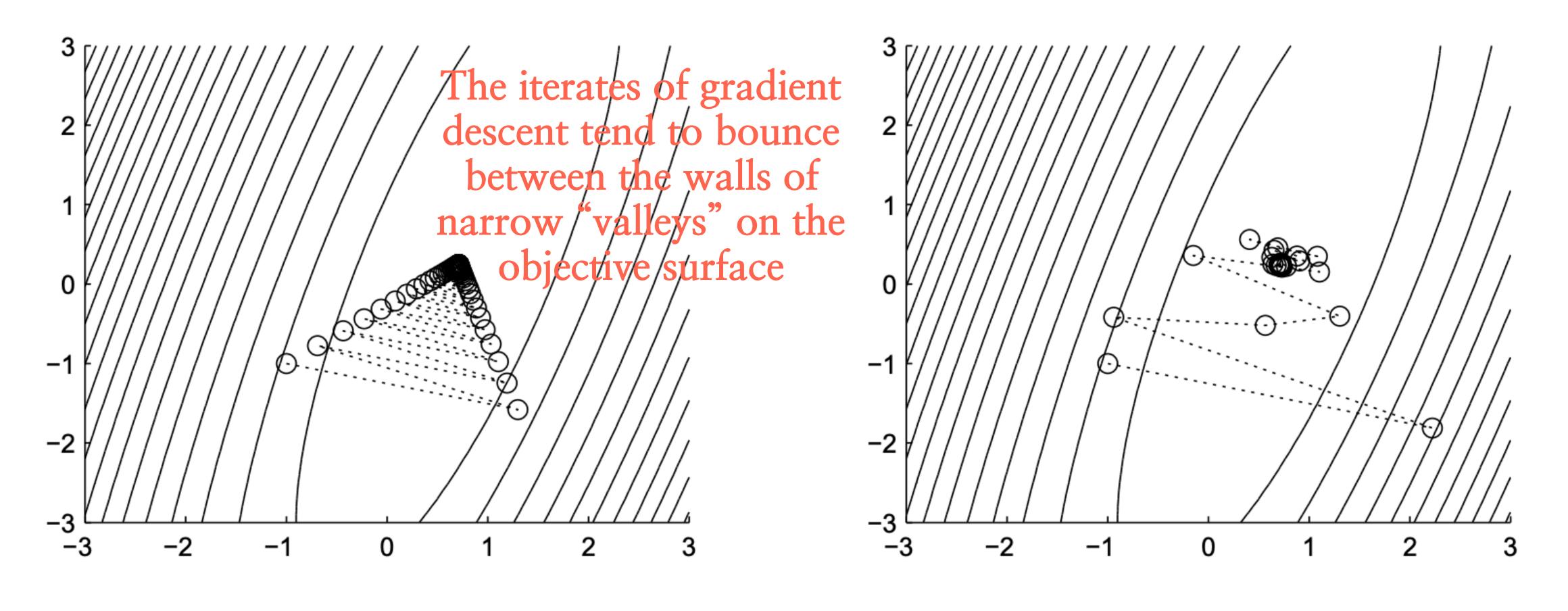
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Can we do better if we use more information?

"Can we accelerate having as our basis the standard gradient descent?"



Gradient descent

Extrapolating previous directions





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

- Heavy ball method

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

Standard gradient step

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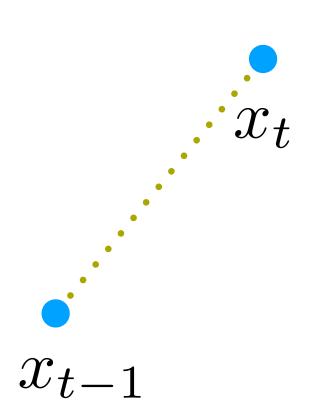
Momentum step

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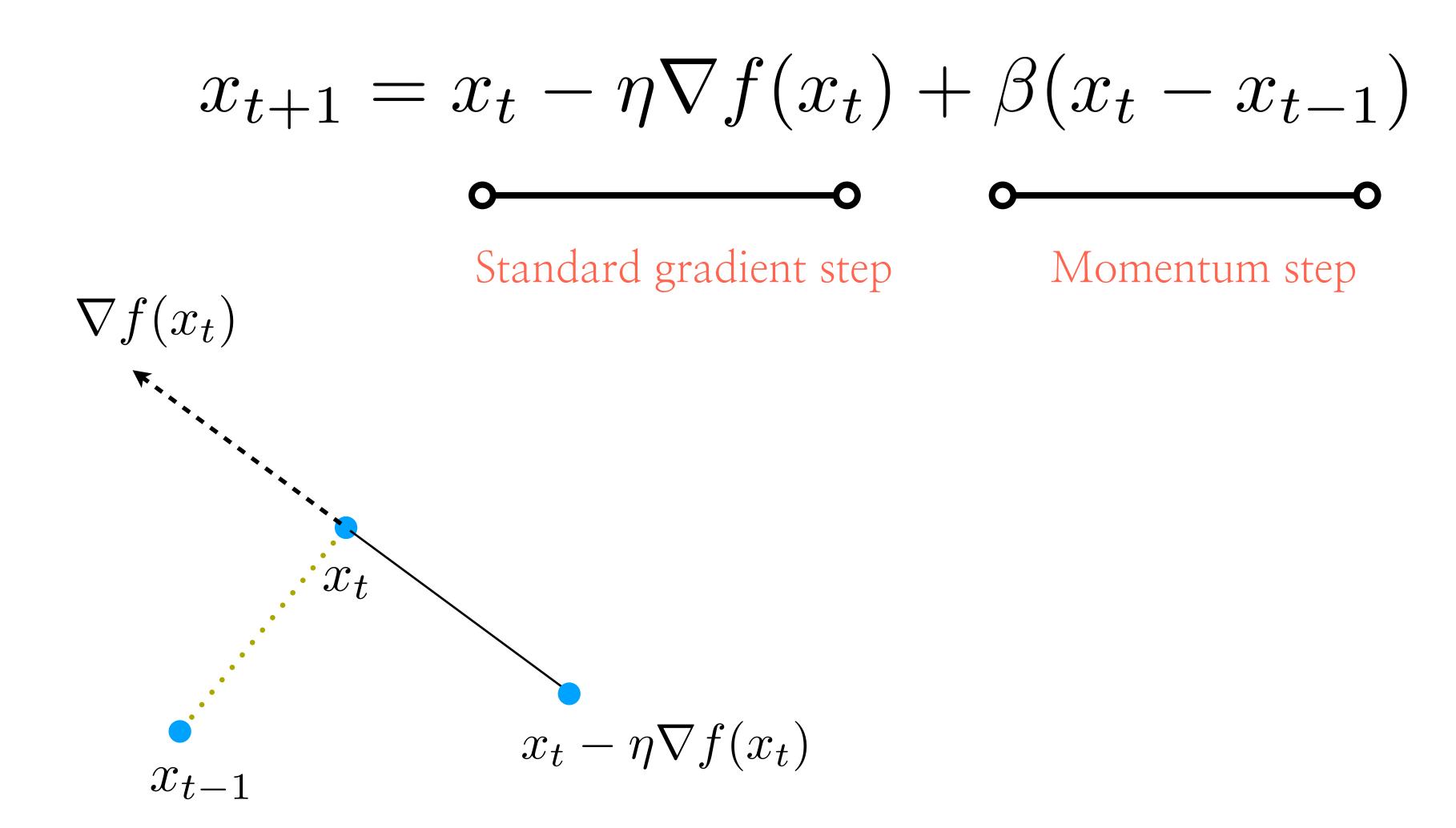


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$$x_{t+1} = x_t - \eta \nabla f(x_t) + \beta (x_t - x_{t-1})$$
Standard gradient step

Momentum step

 $abla f(x_t)$ $abla x_t$ $abla x_{t-1}$



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

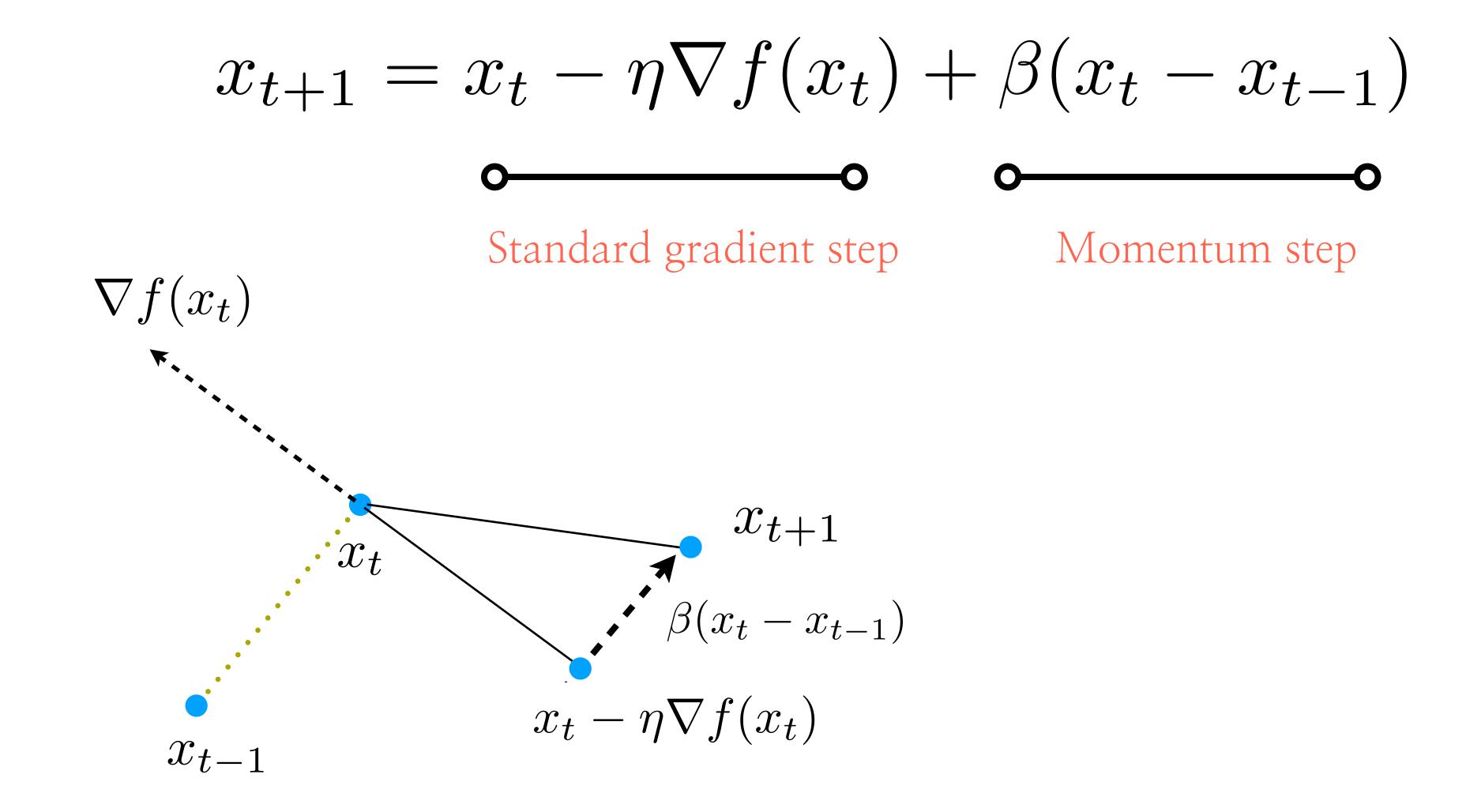
$$x_{t+1} = x_t - \eta \nabla f(x_t) + \beta(x_t - x_{t-1})$$
Standard gradient step $(x_t - x_{t-1})$

$$x_t - \eta \nabla f(x_t)$$

$$x_{t-1}$$
Momentum step

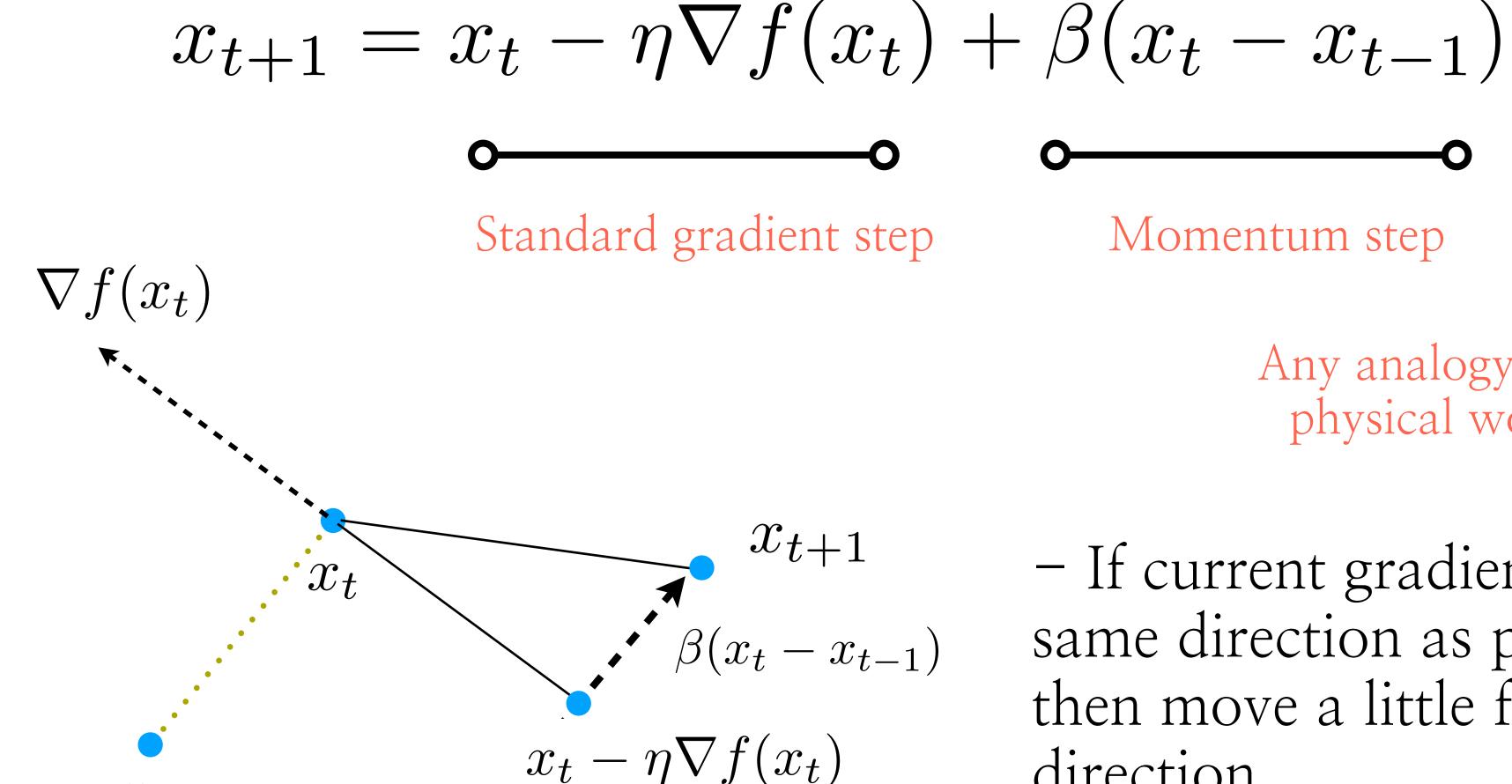
$$x_{t+1} = x_t - \eta \nabla f(x_t) + \beta(x_t - x_{t-1})$$
Standard gradient step
$$\nabla f(x_t)$$
Momentum step
$$x_t - \eta \nabla f(x_t)$$

$$x_t - \eta \nabla f(x_t)$$



- Heavy ball method

 x_{t-1}



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

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

"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
$$\eta = \frac{4}{\sqrt{L} + \sqrt{L}}$$

for
$$\eta = \frac{4}{\sqrt{L} + \sqrt{\mu}}$$
 and $\beta = \max\{|1 - \sqrt{\eta \mu}|, |1 - \sqrt{\eta L}|\}^2$

converges linearly according to:

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

Whiteboard

- It achieves the lower bound for strongly convex cases!

$$||x_t - x^*||_2^2 \ge \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}\right)^{2t} ||x_0 - x^*||_2^2 \qquad \qquad \kappa := \frac{L}{\mu}$$

- It achieves the lower bound for strongly convex cases!

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- In comparison with simple gradient descent:

$$O\left(\kappa \log \frac{1}{\varepsilon}\right)$$
 vs $O\left(\sqrt{\kappa} \log \frac{1}{\varepsilon}\right)$

Performance of Heavy Ball method

Demo

- Nesterov's work: a collection of acceleration methods

Constant Step Scheme, I

- **0.** Choose $x_0 \in \mathbb{R}^n$ and $\gamma_0 > 0$. Set $v_0 = x_0$.
- 1. kth iteration $(k \ge 0)$.
 - a). Compute $\alpha_k \in (0,1)$ from the equation

$$L\alpha_k^2 = (1 - \alpha_k)\gamma_k + \alpha_k\mu.$$

Set $\gamma_{k+1} = (1 - \alpha_k)\gamma_k + \alpha_k \mu$.

b). Choose $y_k = \frac{\alpha_k \gamma_k v_k + \gamma_{k+1} x_k}{\gamma_k + \alpha_k \mu}$. Compute $f(y_k)$ and $f'(y_k)$.

c). Set $x_{k+1} = y_k - \frac{1}{L}f'(y_k)$ and

$$v_{k+1} = \frac{1}{\gamma_{k+1}} [(1 - \alpha_k)\gamma_k v_k + \alpha_k \mu y_k - \alpha_k f'(y_k)].$$

Constant Step Scheme, II

- **0.** Choose $x_0 \in \mathbb{R}^n$ and $\alpha_0 \in (0,1)$. Set $y_0 = x_0$ and $q = \frac{\mu}{L}$.
- 1. kth iteration $(k \ge 0)$.
 - a). Compute $f(y_k)$ and $f'(y_k)$. Set

$$x_{k+1} = y_k - \frac{1}{L}f'(y_k).$$

b). Compute $\alpha_{k+1} \in (0,1)$ from equation

$$\alpha_{k+1}^2 = (1 - \alpha_{k+1})\alpha_k^2 + q\alpha_{k+1}$$

and set
$$\beta_k = \frac{\alpha_k(1-\alpha_k)}{\alpha_k^2+\alpha_{k+1}}$$
,

$$y_{k+1} = x_{k+1} + \beta_k (x_{k+1} - x_k)$$

Constant step scheme, III

- **0.** Choose $y_0 = x_0 \in \mathbb{R}^n$.
- **1.** kth iteration $(k \ge 0)$.

$$x_{k+1} = y_k - \frac{1}{L}f'(y_k),$$

$$y_{k+1} = x_{k+1} + \frac{\sqrt{L} - \sqrt{\mu}}{\sqrt{L} + \sqrt{\mu}} (x_{k+1} - x_k).$$

- Nesterov's work: a collection of acceleration methods

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

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

$$\vdots$$

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

$$x_{t+1} = \widetilde{x} + \beta(x_t - x_{t-1})$$

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Evaluate gradient at current point

- Nesterov's work: a collection of acceleration methods

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$$x_{t+1} = \widetilde{x} + \beta(x_t - x_{t-1})$$
Evaluate gradient at current point

What if we evaluate the gradient at the point we end up?

$$\widetilde{x} = x_t - \eta \nabla f(x_t + \beta(x_t - x_{t-1}))$$

$$x_{t+1} = \widetilde{x} + \beta(x_t - x_{t-1})$$

- Nesterov's work: a collection of acceleration methods

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

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$$\widetilde{x} = x_t - \eta \nabla f(x_t)$$
Evaluate gradient at current point

$$x_{t+1} = \tilde{x} + \beta(x_t - x_{t-1})$$

What if we evaluate the gradient at the point we end up?

• • •

Nesterov's acceleration (1/2)

$$\widetilde{x} = x_t - \eta \nabla f(x_t + \beta(x_t - x_{t-1}))$$

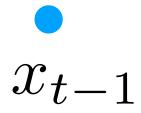
$$x_{t+1} = \widetilde{x} + \beta(x_t - x_{t-1})$$

$$x_{t+1} = y_t - \eta \nabla f(y_t)$$

$$y_{t+1} = x_{t+1} + \beta(x_{t+1} - x_t)$$

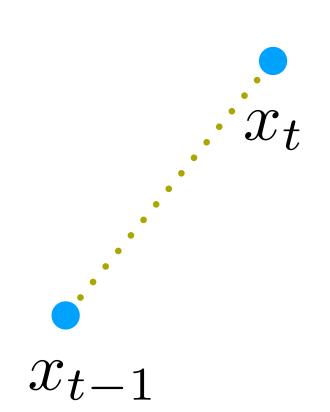
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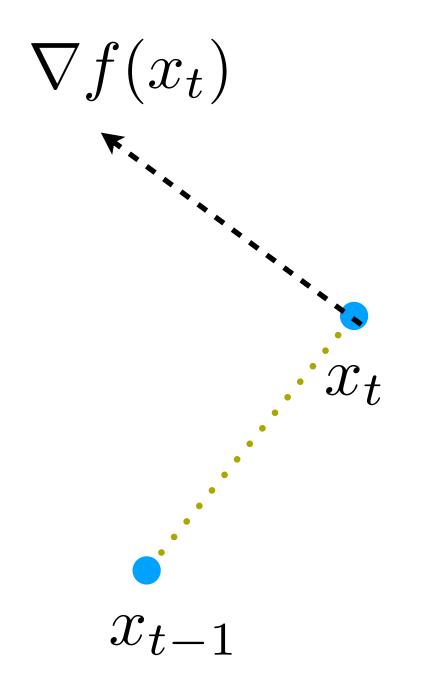
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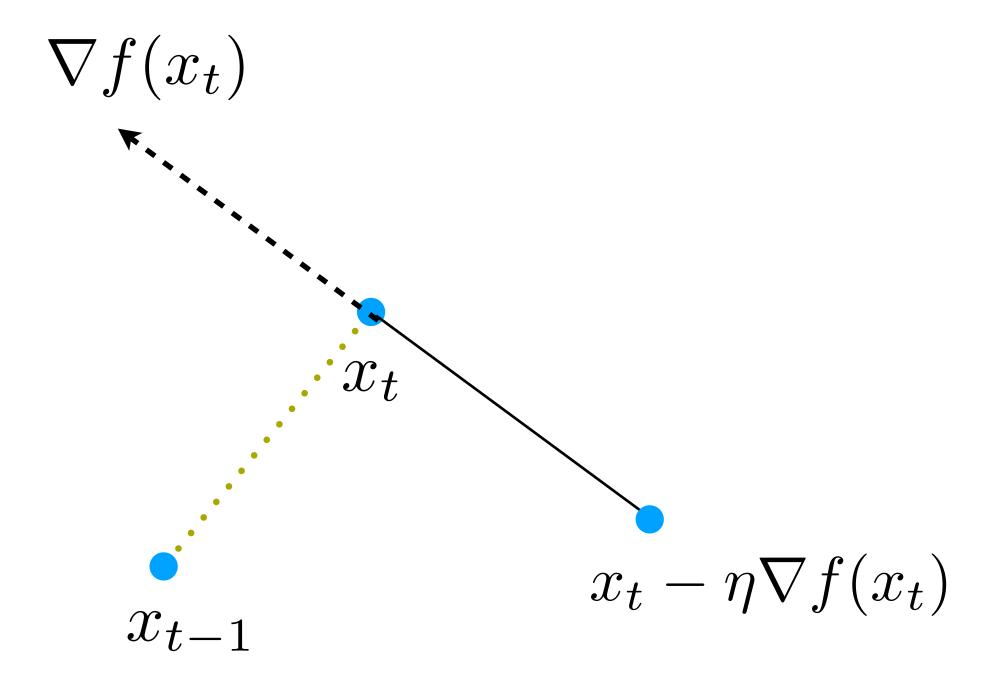
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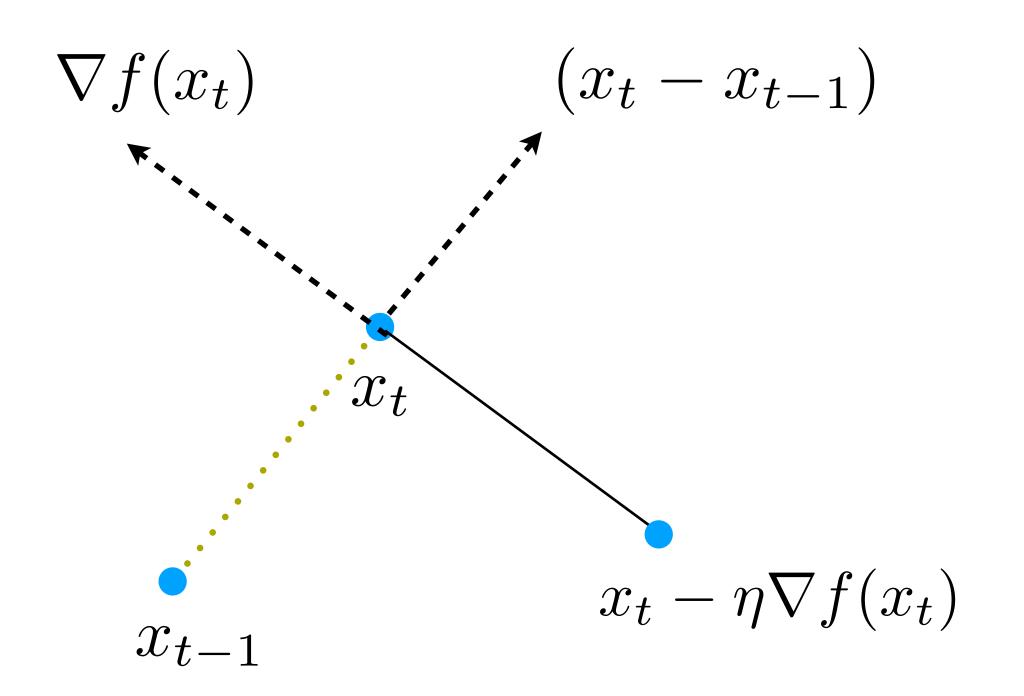
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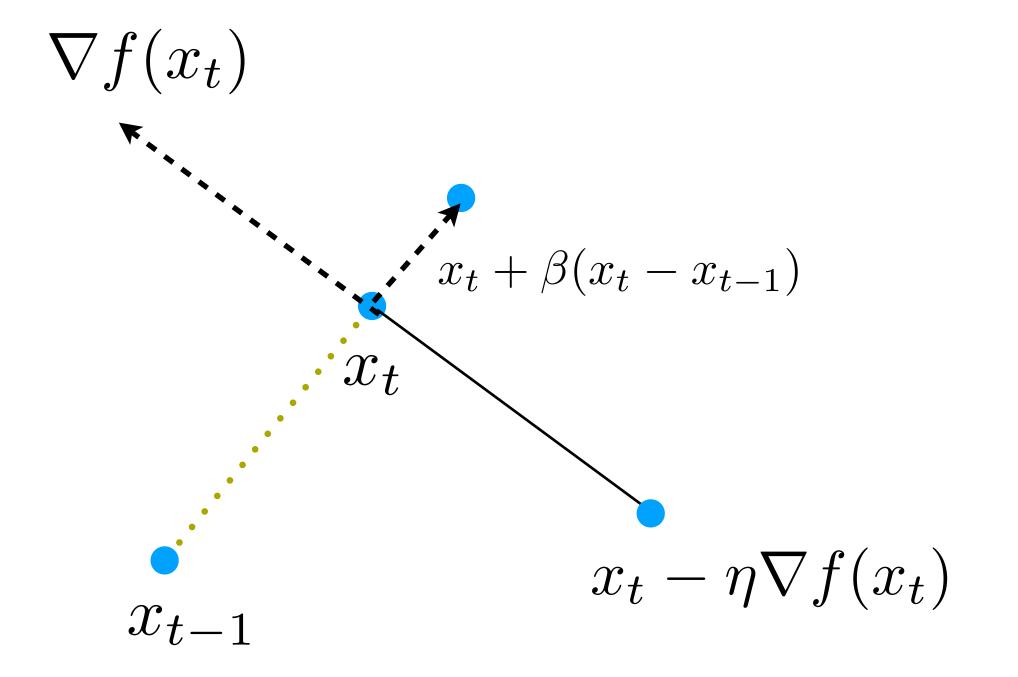
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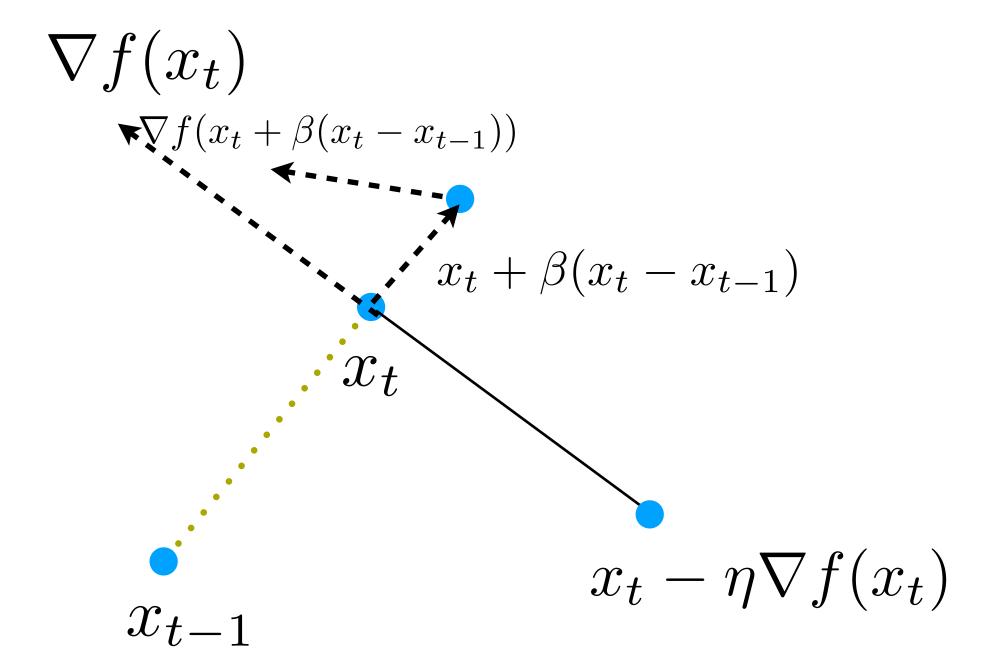
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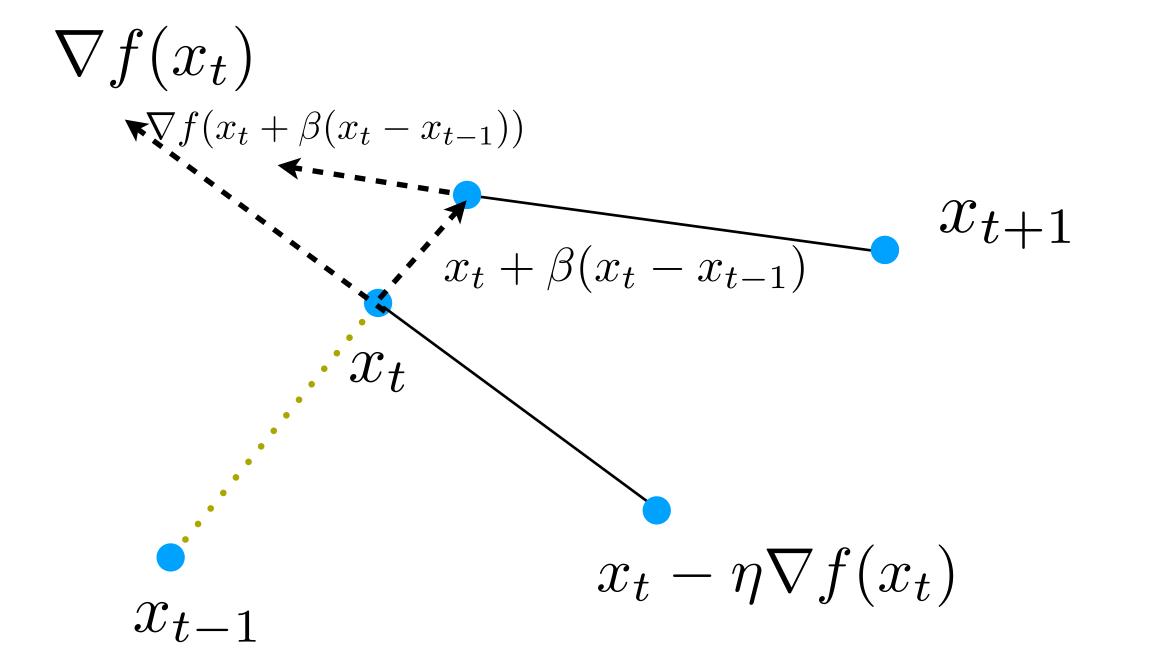
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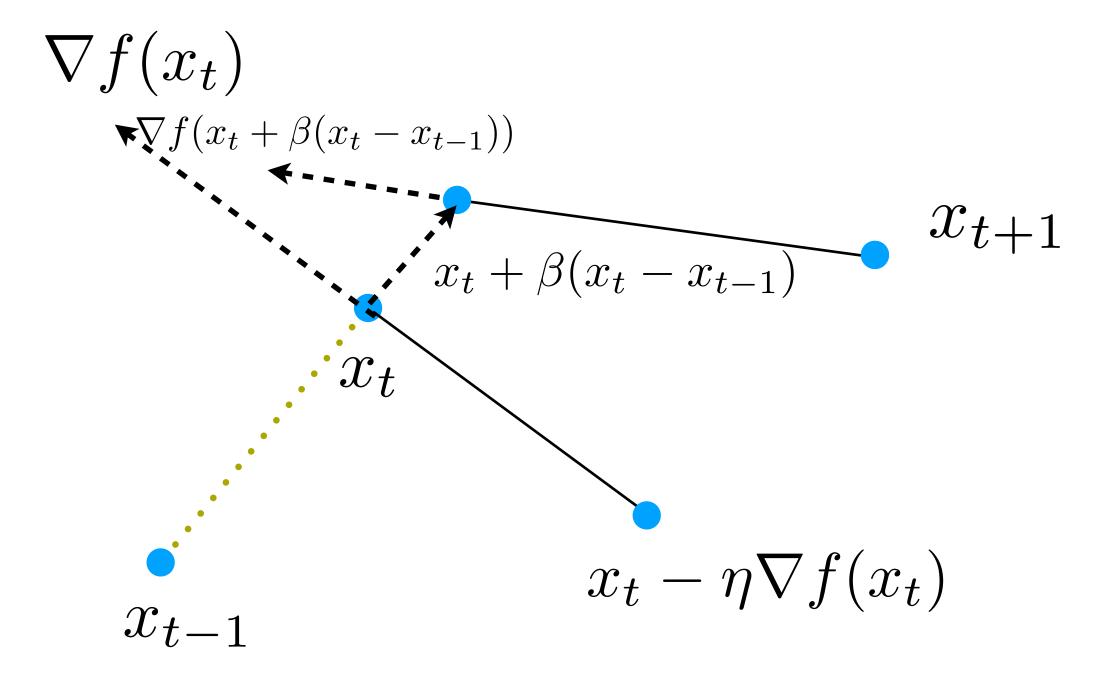
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- Nesterov's work: most famous version

$$x_{t+1} = y_t - \eta \nabla f(y_t)$$

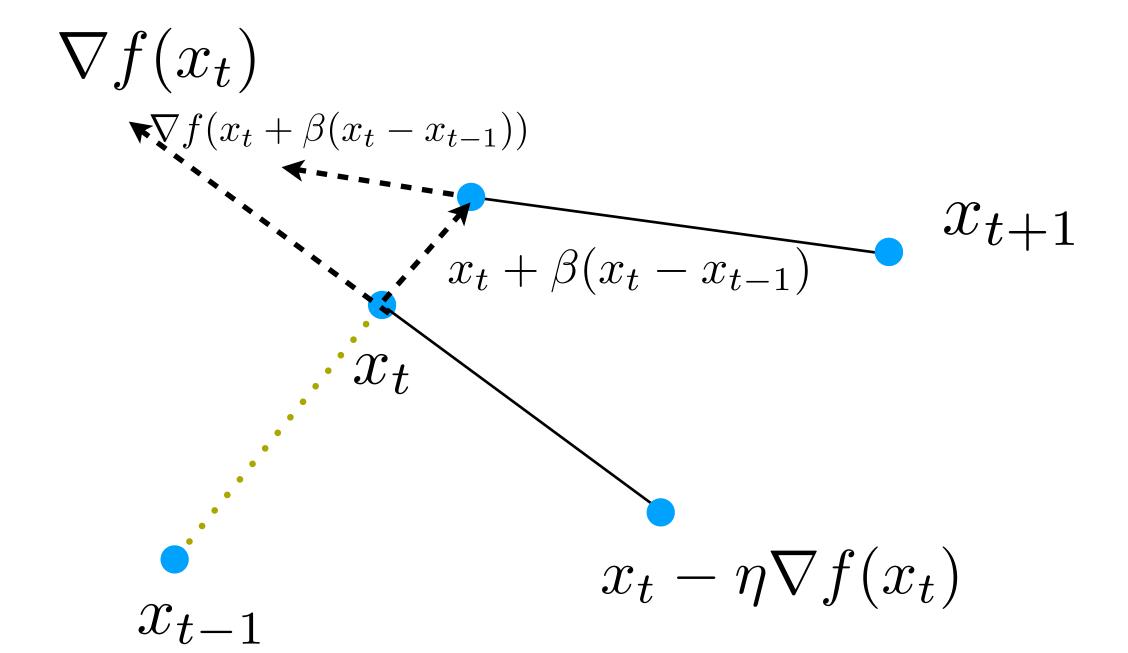
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- Main difference: the point that x_{t+1} we are calculating the gradient at.

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- Main difference: the point that we are calculating the gradient at.
- Heavy ball can fail converging in cases where Nesterov's scheme still succeeds

$$x_{t+1} = y_t - \eta \nabla f(y_t)$$

$$y_{t+1} = x_{t+1} + \beta(x_{t+1} - x_t)$$

$$x_{t+1} = y_t - \eta \nabla f(y_t)$$

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1.
$$\beta = \frac{\theta_t - 1}{\theta_{t+1}}$$
 where $\theta_0 = 1$, $\theta_{t+1} = \frac{1 + \sqrt{1 + 4\theta_t^2}}{2}$

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3.
$$\beta = 0.9$$

- Nesterov's work: how do we set up the momentum parameter?

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One of the mysteries of optimization..

Performance of Nesterov's acceleration

Demo

(No theory but willing to provide – Gradient descent in the absence of strong convexity links for whoever is interested)

$$f(x_t) - f(x^*) \le \frac{2L||x_0 - x^*||_2^2}{t + 4}$$

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- Nesterov's acceleration (with momentum similarly set up as in previous slide)

$$f(x_t) - f(x^*) \le \frac{4L||x_0 - x^*||_2^2}{(t+2)^2}$$

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- Reminder of lower bounds for Lipschitz continuous gradients:

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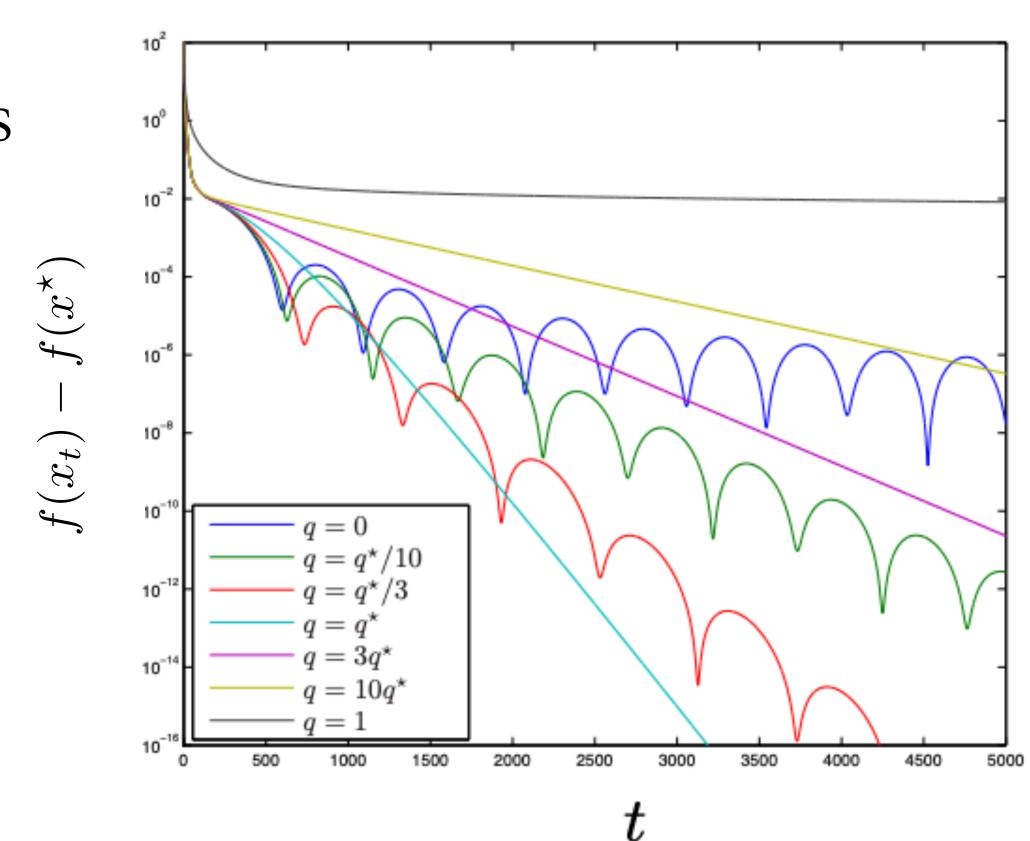
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Notes on Nesterov's acceleration

- The original paper of 1983 does not converge linearly for strongly convex functions, but there is a fix to this
- It is a common observation to see ripples
- There are heuristics for resetting the momentum term to zero that improves the convergence rate.
- Often used even in cases where it is not guaranteed to work: deep learning

