Optimization for Training I

First-Order Methods Training algorithm

OPTIMIZATION METHODS

Topics: Types of optimization methods.

- Practical optimization methods breakdown into two categories:
    1. First-order methods
    2. Second-order methods

$$\hat{J}(\boldsymbol{\theta}) = J(\boldsymbol{a}) + \nabla_{\boldsymbol{\theta}} J(\boldsymbol{a})(\boldsymbol{\theta} - \boldsymbol{a}) + \frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{a})^\top \boldsymbol{H}(\boldsymbol{\theta} - \boldsymbol{a})$$

- Today we will focus on first-order methods

STOCHASTIC GRADIENT DESCENT

- Vanilla SGD is still probably the most popular method of training deep learning models.
- (+) Works on a single example or a mini-batch / (-) Can converge slowly.

Algorithm 1 Stochastic gradient descent (SGD) update at training iteration k

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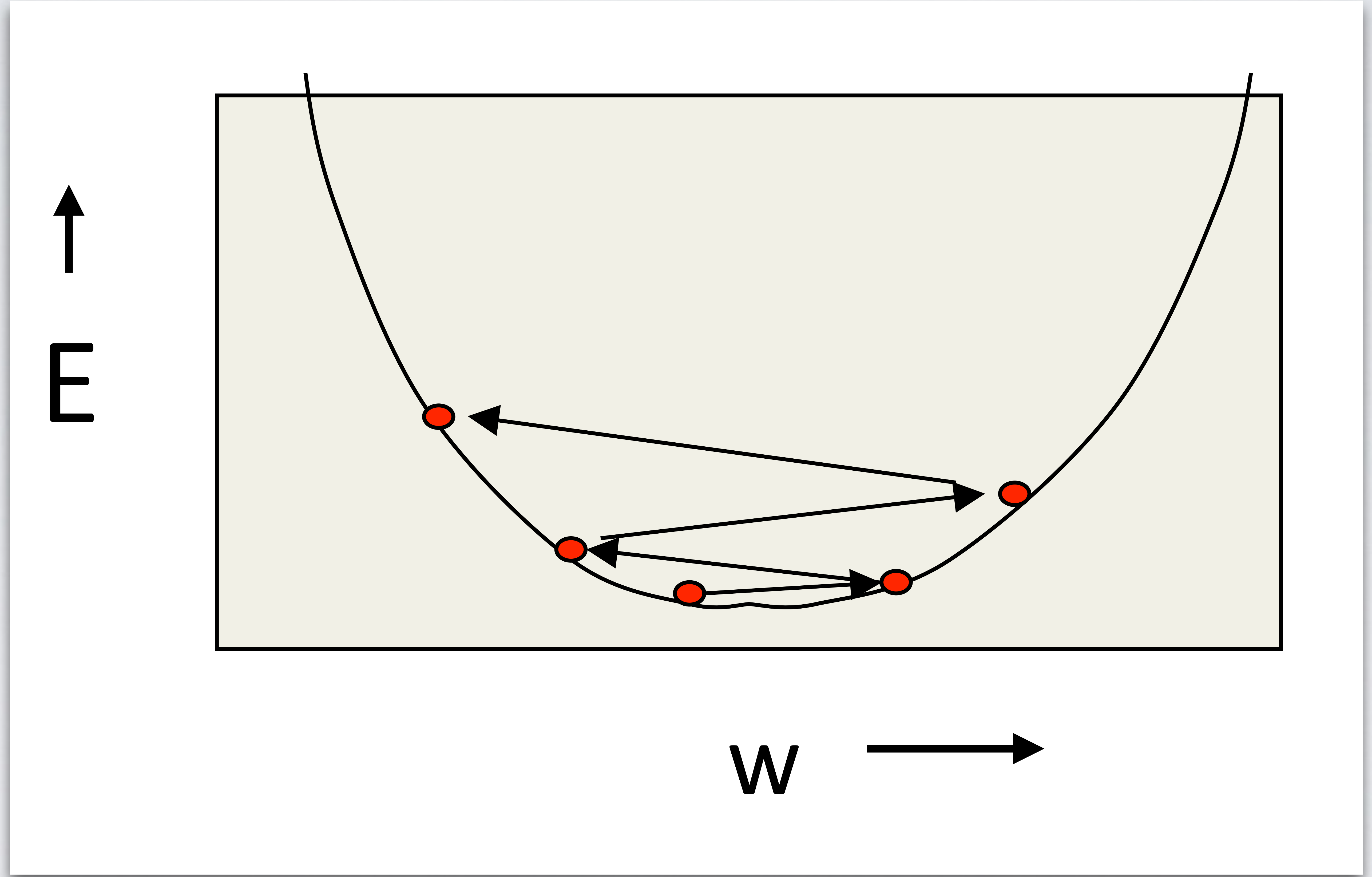
Require: Learning rate ϵ_k.
Require: Initial parameter $\boldsymbol{\theta}$
  while stopping criterion not met **do**
    Sample a minibatch of m examples from the training set $\{\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(m)}\}$ with corresponding targets $\boldsymbol{y}^{(i)}$.
    Compute gradient estimate: $\hat{\boldsymbol{h}} \leftarrow +\frac{1}{m} \nabla_{\boldsymbol{\theta}} \sum_i L(f(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}), \boldsymbol{y}^{(i)})$
    Apply update: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \epsilon \hat{\boldsymbol{h}}$
  end while

STOCHASTIC GRADIENT DESCENT



MOMENTUM METHOD

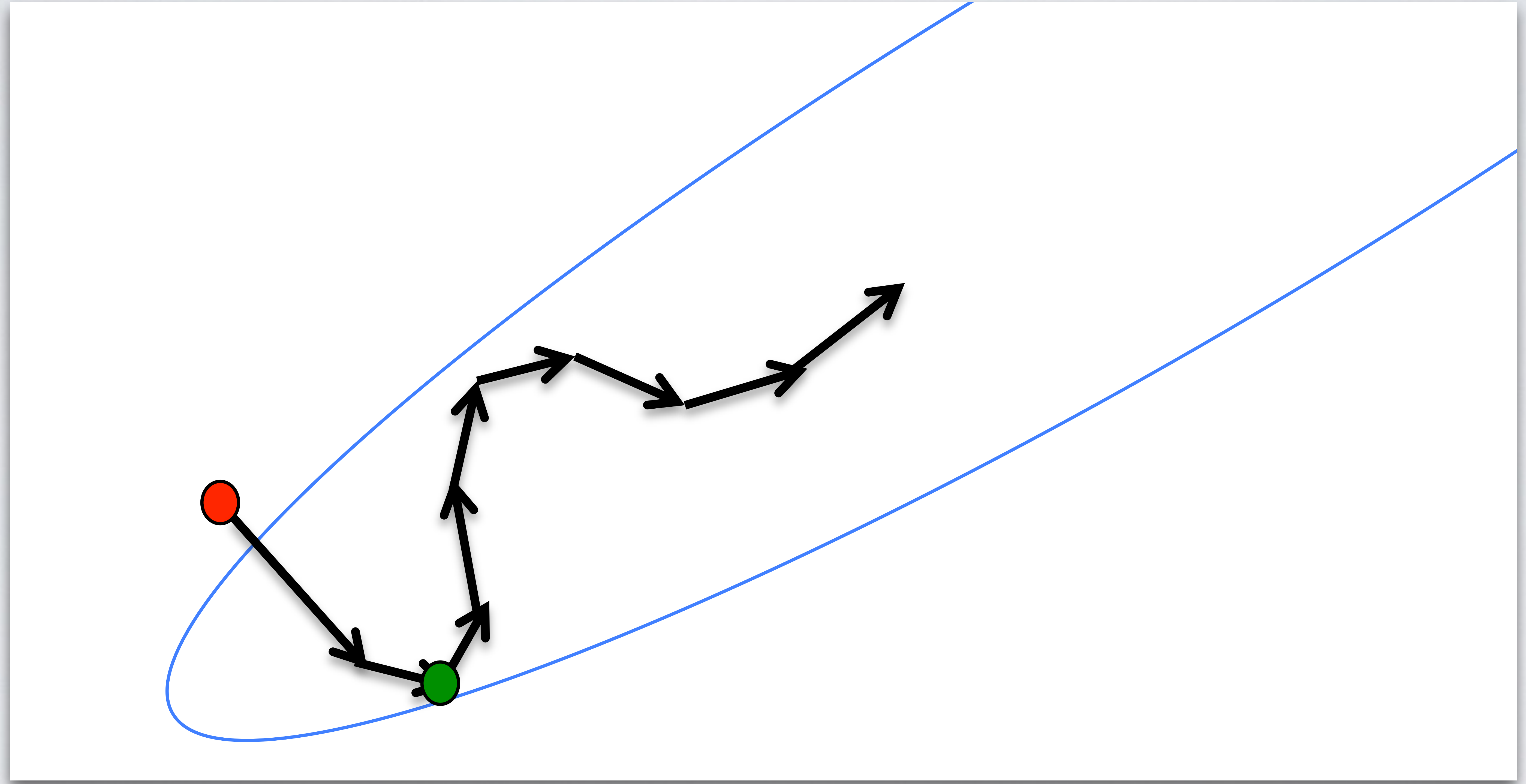
- Designed to accelerate learning, especially with small consistent gradients.
- Inspired from physical interpretation of the optimization process: Imagine you have a small ball rolling on a surface defined by the loss function.

MOMENTUM METHOD

Algorithm 1 Stochastic gradient descent (SGD) with momentum

Require: Learning rate ϵ, momentum parameter α.
Require: Initial parameter $\boldsymbol{\theta}$, initial velocity $\boldsymbol{v}$.
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 estimate: $\boldsymbol{h} \leftarrow \frac{1}{m}\nabla_{\boldsymbol{\theta}} \sum_i L(f(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}), \boldsymbol{y}^{(i)})$
  Compute velocity update: $\boldsymbol{v} \leftarrow \alpha \boldsymbol{v} - \epsilon \boldsymbol{h}$
  Apply update: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \boldsymbol{v}$
end while

MOMENTUM METHOD



NESTEROV MOMENTUM

- Sutskever et al (ICML 2013) presented a modified version of momentum they called Nesterov momentum.
- **Basic idea**: apply the gradient "correction" after the velocity term is applied.

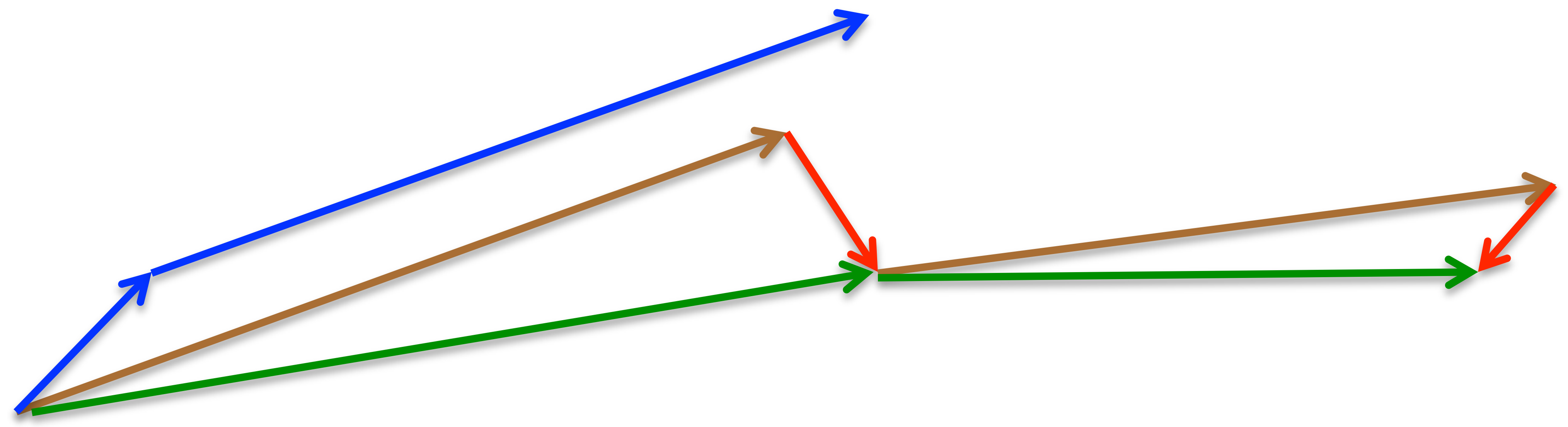
NESTEROV MOMENTUM

Algorithm 1 Stochastic gradient descent (SGD) with Nesterov momentum

Require: Learning rate ϵ, momentum parameter α.
Require: Initial parameter $\boldsymbol{\theta}$, initial velocity $\boldsymbol{v}$.
  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 labels $\boldsymbol{y}^{(i)}$.
    Apply interim update: $\tilde{\boldsymbol{\theta}} \leftarrow \boldsymbol{\theta} + \alpha \boldsymbol{v}$
    Compute gradient (at interim point): $\boldsymbol{h} \leftarrow \frac{1}{m} \nabla_{\tilde{\boldsymbol{\theta}}} \sum_i L(f(\boldsymbol{x}^{(i)}; \tilde{\boldsymbol{\theta}}), \boldsymbol{y}^{(i)})$
    Compute velocity update: $\boldsymbol{v} \leftarrow \alpha \boldsymbol{v} - \epsilon \boldsymbol{h}$
    Apply update: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \boldsymbol{v}$
  end while

NESTEROV MOMENTUM

- First make a big jump in the direction of the previous accumulated gradient.
- Then measure the gradient where you end up and make a correction.



brown vector = jump, red vector = correction, green vector = accumulated gradient

blue vectors = standard momentum

Slide from Hinton's Coursera course.

ADAGRAD

- Adagrad (Duchi et al, COLT 2010) is a method of adapting the learning rate.

- (+) Can adapt independent learning rates for all parameters
- (-) Accumulating gradients from the start makes later learning very slow.

ADAGRAD

Algorithm 1 The AdaGrad algorithm

Require: Global learning rate ϵ

Require: Initial parameter $\boldsymbol{\theta}$

Require: Small constant δ, perhaps 10^{-7}, for numerical stability

Initialize gradient accumulation variable $\boldsymbol{r} = \mathbf{0}$

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

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

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

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

end while

RMSPROP

Algorithm 1 The RMSProp algorithm

Require: Global learning rate ϵ, decay rate ρ.
Require: Initial parameter $\boldsymbol{\theta}$
Require: Small constant δ, usually 10^{-6}, used to stabilize division by small numbers.

Initialize accumulation variables $\boldsymbol{r} = 0$
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: $\boldsymbol{h} \leftarrow \frac{1}{m} \nabla_{\boldsymbol{\theta}} \sum_i L(f(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}), \boldsymbol{y}^{(i)})$
Accumulate squared gradient: $\boldsymbol{r} \leftarrow \rho \boldsymbol{r} + (1 - \rho) \boldsymbol{h} \odot \boldsymbol{h}$
Compute parameter update: $\Delta \boldsymbol{\theta} = -\frac{\epsilon}{\sqrt{\delta + \boldsymbol{r}}} \odot \boldsymbol{h}$. $\quad$ ($\frac{1}{\sqrt{\delta + \boldsymbol{r}}}$ applied elem-wise)
Apply update: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \Delta \boldsymbol{\theta}$
end while

RMSPROP+MOMENTUM

Algorithm 1 RMSProp algorithm with Nesterov momentum

Require: Global learning rate ϵ, decay rate ρ, momentum coefficient α.

Require: Initial parameter $\boldsymbol{\theta}$, initial velocity $\boldsymbol{v}$.

Initialize accumulation variable $\boldsymbol{r} = \mathbf{0}$

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 interim update: $\tilde{\boldsymbol{\theta}} \leftarrow \boldsymbol{\theta} + \alpha \boldsymbol{v}$

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

Accumulate gradient: $\boldsymbol{r} \leftarrow \rho \boldsymbol{r} + (1 - \rho) \boldsymbol{h} \odot \boldsymbol{h}$

Compute velocity update: $\boldsymbol{v} \leftarrow \alpha \boldsymbol{v} - \frac{\epsilon}{\sqrt{\boldsymbol{r}}} \odot \boldsymbol{h}$. ($\frac{1}{\sqrt{\boldsymbol{r}}}$ applied element-wise)

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

end while

ADAM

- ``Adam'' derives from the phrase ``adaptive moments.''
- Variant of RMSProp + momentum with a few important distinctions:
  1. Momentum is incorporated directly as an estimate of the first order moment (with exponential weighting) of the gradient.
  2. Includes bias corrections to the estimates of both the first-order moments (the momentum term) and the (uncentered) second-order moments to account for their initialization at the origin.
- To date, Adam has largely become the default optimization algorithm for training deep learning systems.

ADAM:

Algorithm 1 The Adam algorithm

Require: Step size ϵ (Suggested default: 0.001)
Require: Exponential decay rates for moment estimates, ρ_1 and ρ_2 in $[0, 1)$. (Suggested defaults: 0.9 and 0.999 respectively)
Require: Small constant δ used for numerical stabilization. (Suggestion: 10^{-8})
Require: Initial parameters $\boldsymbol{\theta}$

Initialize 1st and 2nd moment variables $\boldsymbol{s} = \boldsymbol{0}$, $\boldsymbol{r} = \boldsymbol{0}$
Initialize time step $t = 0$
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: $\boldsymbol{h} \leftarrow \frac{1}{m} \nabla_{\boldsymbol{\theta}} \sum_i L(f(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}), \boldsymbol{y}^{(i)})$
  $t \leftarrow t + 1$
  Update biased first moment estimate: $\boldsymbol{s} \leftarrow \rho_1 \boldsymbol{s} + (1 - \rho_1)\boldsymbol{h}$
  Update biased second moment estimate: $\boldsymbol{r} \leftarrow \rho_2 \boldsymbol{r} + (1 - \rho_2)\boldsymbol{h} \odot \boldsymbol{h}$
  Correct bias in first moment: $\hat{\boldsymbol{s}} \leftarrow \frac{\boldsymbol{s}}{1-\rho_1^t}$
  Correct bias in second moment: $\hat{\boldsymbol{r}} \leftarrow \frac{\boldsymbol{r}}{1-\rho_2^t}$
  Compute update: $\Delta\boldsymbol{\theta} = -\epsilon \frac{\hat{\boldsymbol{s}}}{\sqrt{\hat{\boldsymbol{r}}}+\delta}$ (operations applied element-wise)
  Apply update: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \Delta\boldsymbol{\theta}$
end while