

CS-453 Machine Learning

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Momentum-based Gradient Descent

So far ...

- ▶ Neural Networks are universal approximators.
- ▶ Backpropagation allows computation of derivatives in hidden layers.
- ▶ Gradient descent finds weights corresponding to local minimum of loss surface.
- ▶ 1st- and 2nd-order variants of gradient descent can be faster and better.
- ▶ In this lecture:
 - ▶ Momentum-based first-order methods
 - ▶ Momentum
 - ▶ Nesterov Accelerated Gradient
 - ▶ RMSprop
 - ▶ ADAM

Momentum Updates

Basic idea

- ▶ Keep track of oscillating directions.
- ▶ Increase learning rate in directions that converge smoothly.
- ▶ Decrease learning rate in directions that overshoot and oscillate.

Steps

1. Compute gradient step $-\eta \nabla_{\mathbf{w}} L|_{\mathbf{w}^\tau}$ at the current location \mathbf{w}^τ .
2. Add the scaled previous step $\beta \Delta \mathbf{w}^\tau$ to obtain a running average of the step

$$\Delta \mathbf{w}^{\tau+1} = \beta \Delta \mathbf{w}^\tau - \eta \nabla_{\mathbf{w}} L|_{\mathbf{w}^\tau}$$

Typically $\beta = 0.9$.

3. Update parameters by the running average of the step

$$\mathbf{w}^{\tau+1} = \mathbf{w}^\tau + \Delta \mathbf{w}^{\tau+1}$$

Why does momentum work?

- ▶ Directions that oscillate will cancel each other out in the running average.
 - ▶ So the running average will be small in magnitude.
 - ▶ So the steps for oscillating directions will be smaller.
- ▶ Directions that are consistently converging will be reinforced.
 - ▶ So the running average will be large in magnitude.
 - ▶ So those directions will gain *momentum* by having larger and larger steps.

Nesterov Accelerated Gradient

Same idea as momentum updates *but with steps 1 and 2 swapped*.

1. Extend the previous scaled step.

$$\hat{\mathbf{w}} = \mathbf{w}^\tau + \beta \Delta \mathbf{w}^\tau$$

2. Compute gradient step at resultant location $\hat{\mathbf{w}}$.

$$-\eta \nabla_{\mathbf{w}} L|_{\hat{\mathbf{w}}}$$

3. Add previous scaled step and new gradient step to obtain the running average of the step

$$\Delta \mathbf{w}^{\tau+1} = \beta \Delta \mathbf{w}^\tau - \eta \nabla_{\mathbf{w}} L|_{\hat{\mathbf{w}}}$$

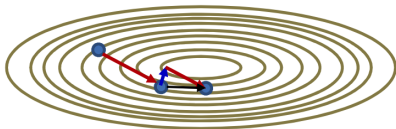
4. Update parameters by the running average of the step

$$\mathbf{w}^{\tau+1} = \mathbf{w}^\tau + \Delta \mathbf{w}^{\tau+1}$$

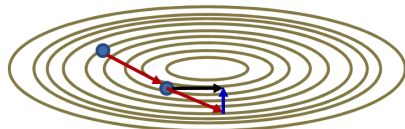
Nesterov's method has been shown to converge faster than momentum updates.

Momentum vs. Nesterov Momentum

Momentum



Nestorov



Nesterov – Sometimes it is better to make a correction after making an error.

Source: Bhiksha Raj

RMSprop

- ▶ Decouple each direction.
- ▶ We can compute the running average of the *squared* 1st-derivative in direction i as

$$\bar{v}_i^T = \gamma \bar{v}_i^{T-1} + (1 - \gamma) \left(\frac{\partial L}{\partial w_i} \right)^2$$

with initialization $\bar{v}_i^0 = 0$.

- ▶ Root-mean-squared (RMS) value $\sqrt{\bar{v}_i^T} + \epsilon$ represents average magnitude of 1st-derivative for direction i .
 - ▶ High value indicates oscillating derivatives. So reduce learning rate.
 - ▶ Low value indicates flat region. So increase learning rate.
- ▶ So divide learning rate by this average before performing gradient descent.

$$w_i^T = w_i^{T-1} - \frac{\eta}{\sqrt{\bar{v}_i^T} + \epsilon} \frac{\partial L}{\partial w_i}$$

Rprop vs RMSprop

Rprop

Multiplicatively increase learning rate when derivative retains its sign.

$$\eta \leftarrow \alpha \eta$$

Multiplicatively decrease learning rate when derivative oscillates.

$$\eta \leftarrow \beta \eta$$

RMSprop

Multiplicatively increase/decrease learning rate when average derivative magnitude decreases/increases.

$$\eta \leftarrow \frac{\eta_0}{\sqrt{\bar{v}} + \epsilon}$$

Fixed multiplicative factors α and β in Rprop are replaced by *adaptive* factor $\frac{1}{\sqrt{\bar{v}} + \epsilon}$ in RMSprop.

ADAM

RMSprop+Momentum

- ▶ RMSprop uses the current derivative.
- ▶ ADAM¹ replaces current derivative by its running average.

$$\bar{m}_i^\tau = \delta \bar{m}_i^{\tau-1} + (1 - \delta) \frac{\partial L}{\partial w_i}$$

- ▶ *Currently the most popular flavor of gradient descent.*
- ▶ Statistics terminology:
 - ▶ Average of random variable x is also called its 1st statistical moment $E[x]$.
 - ▶ Average of the square of a random variable is also called its 2nd *uncentered* statistical moment $E[x^2]$.
 - ▶ Average of the square of a centered random variable is also called its 2nd statistical moment $E[(x - \mu)^2]$ or variance.

¹Kingma and Ba, 'ADAM: A Method for Stochastic Optimization'.

ADAM

RMSprop+Momentum

- ▶ Initialize moments $\bar{m}_i^0 = 0$ and $\bar{v}_i^0 = 0$.
- ▶ Compute 1st moment and 2nd uncentered moment of derivative

$$\bar{m}_i^\tau = \delta \bar{m}_i^{\tau-1} + (1 - \delta) \frac{\partial L}{\partial w_i}$$
$$\bar{v}_i^\tau = \gamma \bar{v}_i^{\tau-1} + (1 - \gamma) \left(\frac{\partial L}{\partial w_i} \right)^2$$

- ▶ Correct for bias of initial moments (= 0) by scaling up in early iterations.

$$\bar{m}_i^\tau = \frac{\bar{m}_i^\tau}{1 - \delta^\tau} \text{ and } \bar{v}_i^\tau = \frac{\bar{v}_i^\tau}{1 - \gamma^\tau}$$

- ▶ Perform update

$$w_i^\tau = w_i^{\tau-1} - \frac{\eta}{\sqrt{\bar{v}_i^\tau} + \epsilon} \bar{m}_i^\tau$$

- ▶ Proposed hyperparameter values: $\eta = 10^{-3}$, $\delta = 0.9$, $\gamma = 0.999$, $\epsilon = 10^{-8}$.

Summary

- ▶ For complex and non-convex loss functions of deep networks, vanilla gradient descent can get stuck in poor local minima and saddle points.
- ▶ It can also converge very slowly.
- ▶ Different directions require different learning rates.
- ▶ Adaptive learning rates are very important.
- ▶ Most useful technique is to adapt learning rate based on *recent trend* of 1st-derivative.