CS-568 Deep Learning

Momentum-based Gradient Descent

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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

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

- 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 $\hat{w}.$

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

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.

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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

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

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

- ▶ Root-mean-squared (RMS) value $\sqrt{\bar{v}_i^{\tau}} + \epsilon$ 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.

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

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.

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

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

ADAM RMSprop+Momentum

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

$$ar{m}_i^{ au} = \delta ar{m}_i^{ au-1} + (1-\delta) rac{\partial L}{\partial w_i}$$

- 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[x²].
 - Average of the square of a centered random variable is also called its 2nd statistical moment E[(x μ)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.

$$ar{m}_i^ au = rac{ar{m}_i^ au}{1-\delta^ au} ext{ and } ar{v}_i^ au = rac{ar{v}_i^ au}{1-\gamma^ au}$$

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.