CPEN 455: Deep Learning

Lecture 4: Backpropagation II

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Outline

- Learning Algorithm for Feedforward Neural Networks:
  - Backpropagation
  - Weight Initialization
  - Learning Rate & Momentum & Adam
  - Weight Decay & Early Stopping

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Backpropagation (BP)

Now we know how to compute gradients, let us see how to perform gradient-based learning (e.g., SGD)

Algorithm 1 SGD

Input: step T, learning Rate η, initial W^0, batch size B
For $t = 1, \cdots, T$
    Get mini-batch data (X^t, Y^t)
    $L(W^{t-1}, X^t, Y^t) = \frac{1}{B} \sum_{i=1}^{B} \ell(f(W^{t-1}, X^t[i]), Y^t[i])$
    $W^t = W^{t-1} - \eta \frac{\partial L(W^{t-1}, X^t, Y^t)}{\partial W}$
Return W^T

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Forward pass

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4: $L(W^{t-1}, X^t, Y^t) = \frac{1}{B}\sum_{i=1}^{B} \ell(f(W^{t-1}, X^t[i]), Y^t[i])$ — Forward pass: $f(W^{t-1}, X^t[i])$
5: $W^t = W^{t-1} - \eta \frac{\partial L(W^{t-1}, X^t, Y^t)}{\partial W}$ — Backward pass: $\frac{\partial L(W^{t-1}, X^t, Y^t)}{\partial W}$
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SGD has trouble navigating ravines, i.e. areas where the surface curves much more steeply in one dimension than in another [1, 2].

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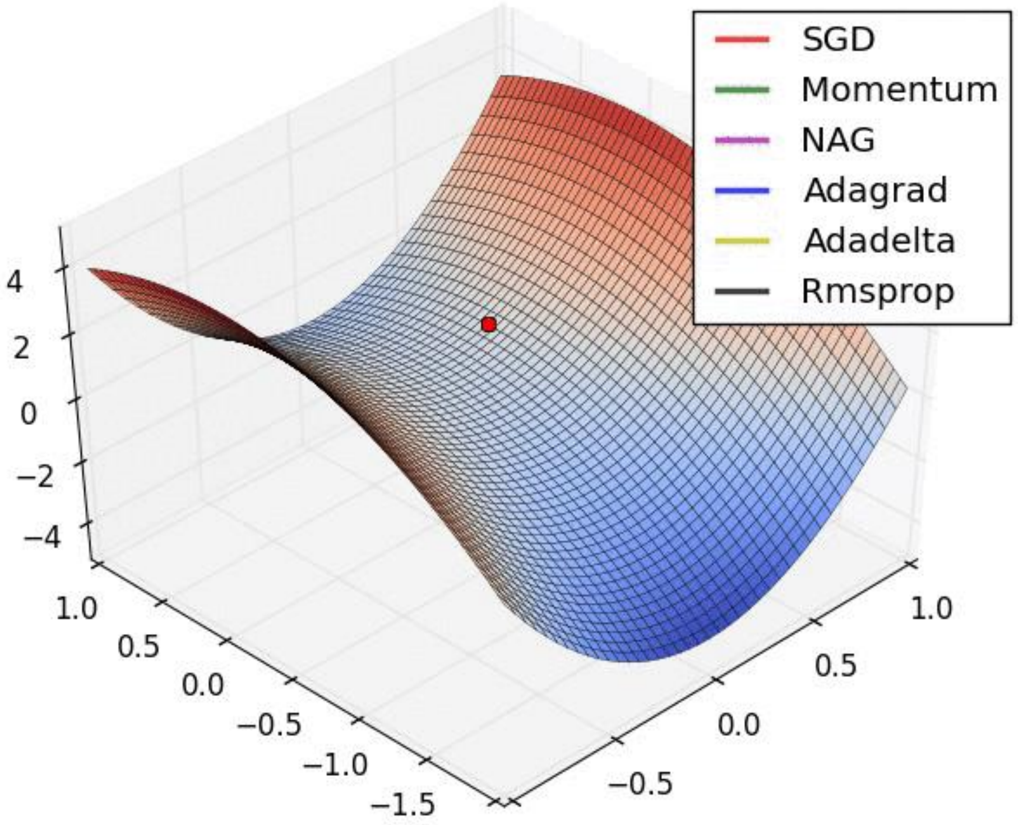

Image Credit: [1]

BP + Momentum

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[3]: Gradient descent is a man walking down a hill. He follows the steepest path downwards; his progress is slow, but steady. Momentum is a heavy ball rolling down the same hill. The added inertia acts both as a smoother and an accelerator, dampening oscillations and causing us to barrel through narrow valleys, small humps and local minima.

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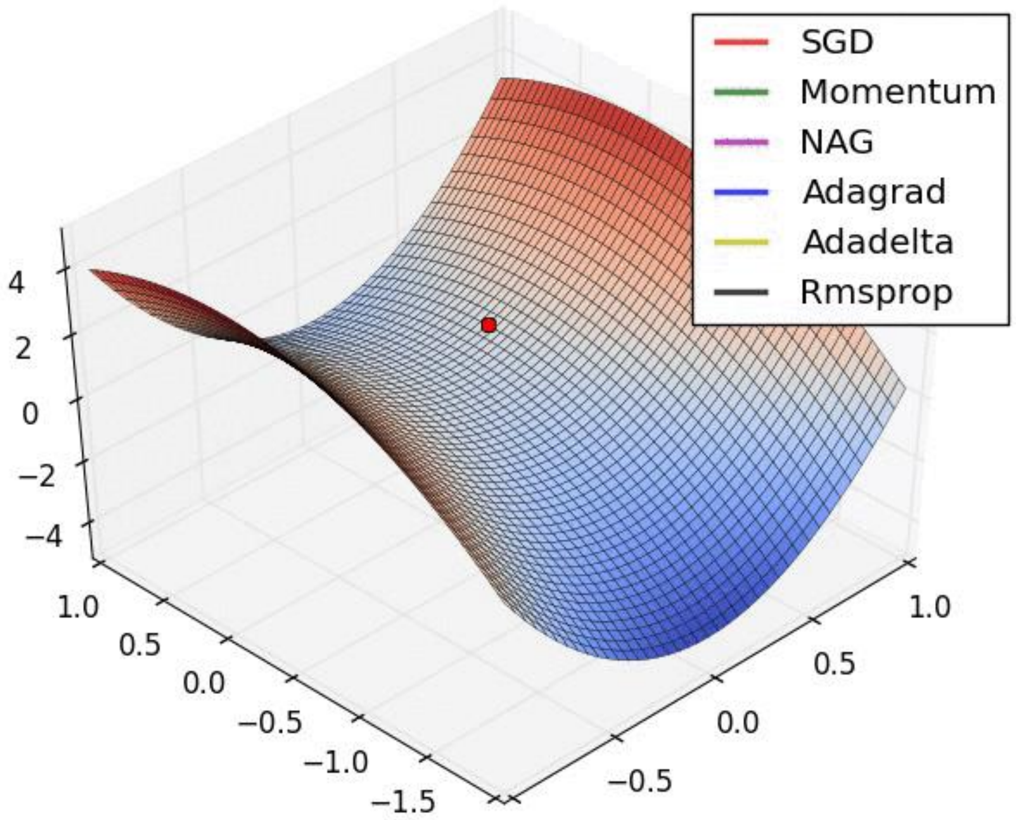
Alternative form (so-called Nesterov momentum) in the literature, see, e.g., [4]

BP + Momentum



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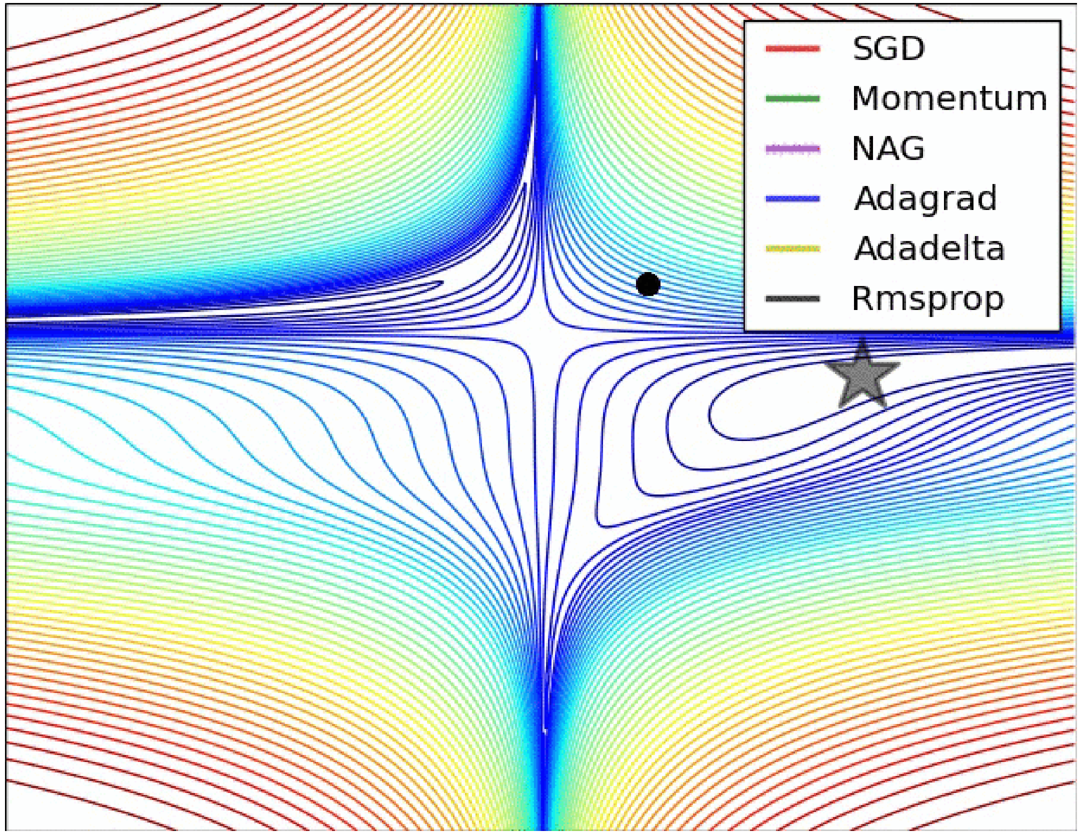

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Demo: https://distill.pub/2017/momentum/

BP + Adaptive Learning Rate

Denoting $g^t = \frac{\partial L(W^{t-1}, X^t, Y^t)}{\partial W}$, recall in GD/SGD, we have the following update rule:

$$W^t = W^{t-1} - \eta g^t$$

How can we tune the learning rate?

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How can we tune the learning rate?

AdaGrad (Adaptive Gradient) [5] proposes to assign larger learning rates to infrequently updated weights and smaller ones to frequently updated weights:

$$G^t = \sum_{\tau=1}^{t} g^\tau {g^\tau}^\top$$

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Let us look at the element-wise update rule of AdaGrad:

$$W^t[i] = W^{t-1}[i] - \frac{\eta}{\sqrt{\epsilon + G^t[i,i]}} g^t[i]$$

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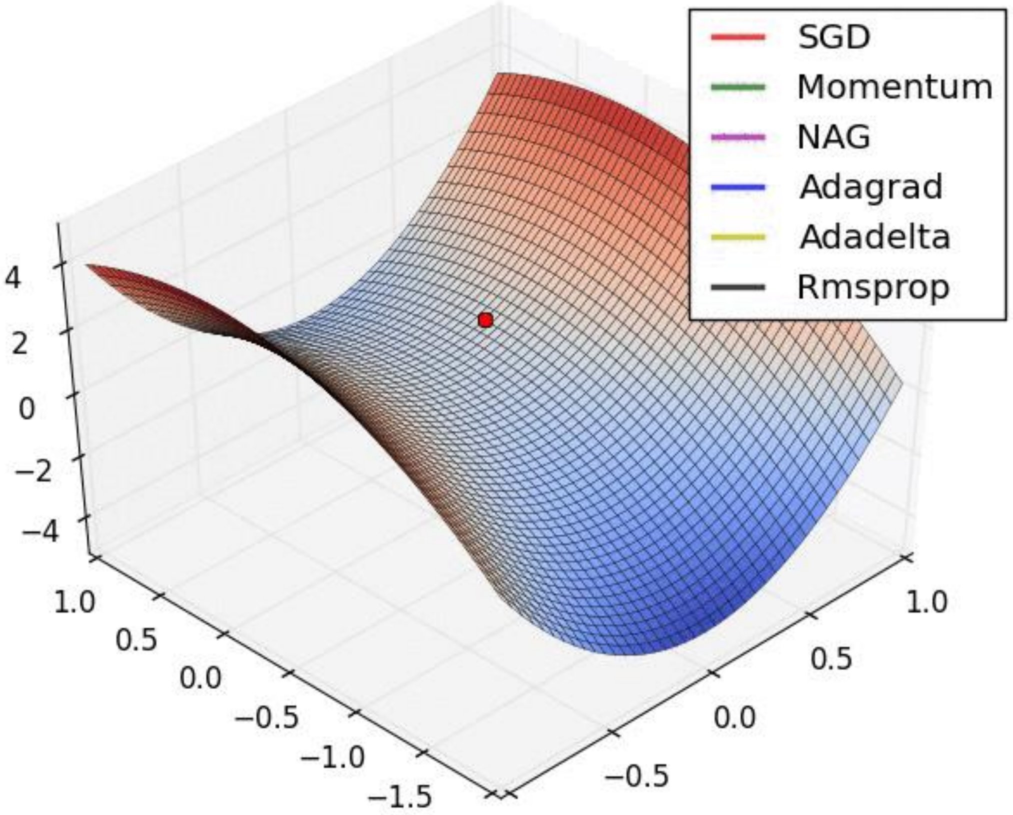
Adadelta [7] leverages the same EMA trick (denominator) and additional weighting (numerator) based on parameter updates.

Comparison Again



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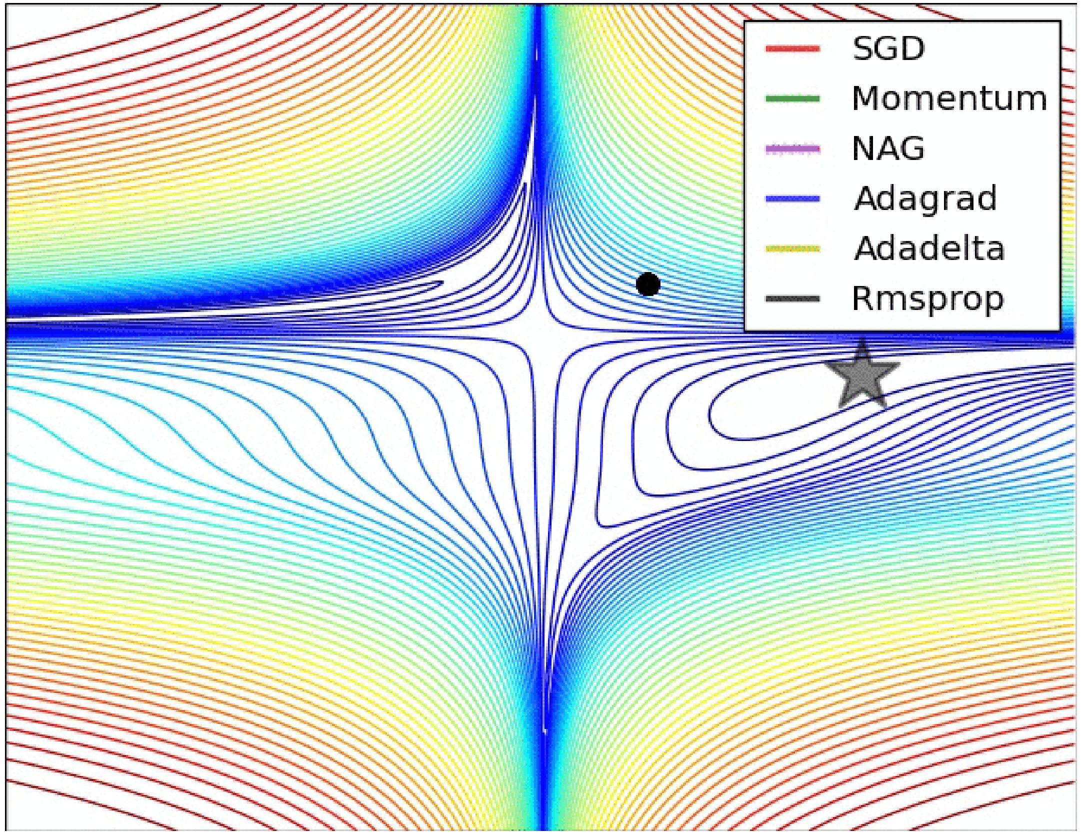

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These are powers of scalars (abuse of superscript)

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$$\begin{aligned}\mathbb{E}\left[\tilde{g}^t\right] &= \mathbb{E}\left[\beta_1 \tilde{g}^{t-1} + (1-\beta_1) g^t\right] = \mathbb{E}\left[\beta_1\left(\beta_1 \tilde{g}^{t-2} + (1-\beta_1) g^{t-1}\right) + (1-\beta_1) g^t\right] \\ &= \mathbb{E}\left[\beta_1^2 \tilde{g}^{t-2} + \beta_1 (1-\beta_1) g^{t-1} + (1-\beta_1) g^t\right] \\ &= \mathbb{E}\left[\sum_{i=1}^{t} \beta_1^{t-i} (1-\beta_1) g^i + \beta_1^t \tilde{g}^0\right]\end{aligned}$$

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W^t &= W^{t-1} - \eta_t \mathrm{diag}\left(\epsilon I + G^t\right)^{-1/2} \tilde{g}^t \\
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\end{aligned}
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&= \mathbb{E}\left[\beta_1^2 \tilde{g}^{t-2} + \beta_1 (1-\beta_1) g^{t-1} + (1-\beta_1) g^t\right] \\
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We ignore this term due to the zero initialization and assume gradients at each time step are stationary!

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&= \mathbb{E}\left[\sum_{i=1}^{t} \beta_1^{t-i} (1-\beta_1) g^i + \boxed{\beta_1^t \tilde{g}^0}\right] \\
&\approx \sum_{i=1}^{t} \beta_1^{t-i} (1-\beta_1) \mathbb{E}\left[g^i\right] \\
&= \left(\sum_{i=0}^{t-1} \beta_1^i\right) (1-\beta_1) \mathbb{E}\left[g^i\right] = (1-\beta_1^t) \mathbb{E}\left[g^i\right]
\end{aligned}$$

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Where does this bias-correction term (red box) come from?

Similar reasoning applies to G^t. We have $\mathbb{E}\left[G^t\right] \approx (1 - \beta_2^t) \mathbb{E}\left[g^i {g^i}^\top\right]$ $\mathbb{E}\left[g^t\right] \approx (1 - \beta_1^t) \mathbb{E}\left[g^i\right]$

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Check the update (blue box) element-wise:

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Where does this bias-correction term (red box) come from?

Similar reasoning applies to G^t. We have $\mathbb{E}\left[G^t[j,j]\right] \approx (1-\beta_2^t)\mathbb{E}\left[\left(g^i[j]\right)^2\right]$ $\qquad \mathbb{E}\left[\tilde{g}^t\right] \approx (1-\beta_1^t)\mathbb{E}\left[g^i\right]$

Check the update (blue box) element-wise:

$$\mathbb{E}\left[\Delta W^t[j]\right] = \mathbb{E}\left[\eta_t \frac{1}{\sqrt{\epsilon + G^t[j,j]}} \tilde{g}^t[j]\right] \boxed{\approx \eta_t \mathbb{E}\left[\frac{1}{\sqrt{G^t[j,j]}} \tilde{g}^t[j]\right]}$$

ignore epsilon

BP + Adaptive Learning Rate + Momentum (Adam)

Now that we can tune the learning rate adaptively, how can we incorporate momentum?

Based on RMSProp, Adam (Adaptive Momentum) [8] proposes to keep another EMA of past gradients:

$$\tilde{g}^t = \beta_1 \tilde{g}^{t-1} + (1-\beta_1) g^t$$

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Independent assumption of G^t and $\tilde{g}^t$

$$= \boxed{\eta_t \frac{\mathbb{E}\left[\tilde{g}^t[j]\right]}{\mathbb{E}\left[\sqrt{G^t[j,j]}\right]}}$$

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A crude assumption (Jensen's inequality is tight) on G^t

$$= \eta_t \frac{\mathbb{E}\left[\tilde{g}^t[j]\right]}{\mathbb{E}\left[\sqrt{G^t[j,j]}\right]} \approx \boxed{\eta_t \frac{\mathbb{E}\left[\tilde{g}^t[j]\right]}{\sqrt{\mathbb{E}\left[G^t[j,j]\right]}}}$$

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Substitute with above results

$$= \eta_t \frac{\mathbb{E}\left[\tilde{g}^t[j]\right]}{\mathbb{E}\left[\sqrt{G^t[j,j]}\right]} \approx \eta_t \frac{\mathbb{E}\left[\tilde{g}^t[j]\right]}{\sqrt{\mathbb{E}\left[G^t[j,j]\right]}}$$

$$\approx \eta_t \frac{(1-\beta_1^t)\mathbb{E}\left[g^i[j]\right]}{\sqrt{1-\beta_2^t}\sqrt{\mathbb{E}\left[\left(g^i[j]\right)^2\right]}}$$

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$$\approx \eta_t \frac{(1-\beta_1^t)\mathbb{E}\left[g^i[j]\right]}{\sqrt{1-\beta_2^t}\sqrt{\mathbb{E}\left[\left(g^i[j]\right)^2\right]}} \leq \boxed{\eta_t \frac{(1-\beta_1^t)}{\sqrt{1-\beta_2^t}}} = \eta$$

Jensen's Inequality

$$\mathbb{E}\left[g^i[j]\right] \leq \sqrt{\mathbb{E}\left[\left(g^i[j]\right)^2\right]}$$

BP + Adaptive Learning Rate + Momentum (Adam)

In summary, Adam is shown in below

Algorithm 1 Adam

Input: step T, initial learning Rate η, initial W^0, batch size B, $\beta_1 = 0.9$, $\beta_2 = 0.999$, $\epsilon = 10^{-8}$, $m^0 = 0$, $v^0 = 0$

For $t = 1, \cdots, T$

  Get mini-batch data (X^t, Y^t)

  $L(W^{t-1}, X^t, Y^t) = \frac{1}{B}\sum_{i=1}^{B} \ell(f(W^{t-1}, X^t[i]), Y^t[i])$

  $g^t = \frac{\partial L(W^{t-1}, X^t, Y^t)}{\partial W}$

  $m^t = \beta_1 m^{t-1} + (1 - \beta_1) g^t$

  $v^t = \beta_2 v^{t-1} + (1 - \beta_2)(g^t \odot g^t)$

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Return W^T

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9: **Return** W^T

Adam [8] has been cited by 165,000+ times since its publication in 2015! It is by far the most popular optimizer in deep learning!

Outline

- Learning Algorithm for Feedforward Neural Networks:
  - Backpropagation
  - Weight Initialization
  - Learning Rate & Momentum & Adam
  - **Weight Decay & Early Stopping**

Weight Decay

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We can control the lambda to trade-off model complexity and overfitting.

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It only adds a term to the existing gradient:

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But for Adam, we have two possibilities: 1) add it to the gradient and then perform gradient update; 2) add it to the gradient update

This ordering change makes a difference in practice and 2) is called AdamW [9]!

AdamW

Let us look at Adam again:

Algorithm 1 Adam

1: **Input**: step T, initial learning Rate η, initial W^0, batch size B, $\beta_1 = 0.9$, $\beta_2 = 0.999$, $\epsilon = 10^{-8}$, $m^0 = 0$, $v^0 = 0$
2: **For** $t = 1, \cdots, T$
3: Get mini-batch data (X^t, Y^t)
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9: **Return** W^T

We can it here by replacing the rex box with:

$$g^t = \frac{\partial L(W^{t-1}, X^t, Y^t)}{\partial W} + \lambda W^{t-1}$$

But then weight decay also goes through EMA!

AdamW

We can add it in the final gradient update:

Algorithm 1 AdamW

1: **Input**: step T, initial learning Rate η, initial W^0, batch size B, $\beta_1 = 0.9$, $\beta_2 = 0.999$, $\epsilon = 10^{-8}$, $m^0 = 0$, $v^0 = 0$, weight decay λ

2: **For** $t = 1, \cdots, T$

3: Get mini-batch data (X^t, Y^t)

4: $L(W^{t-1}, X^t, Y^t) = \frac{1}{B}\sum_{i=1}^{B} \ell(f(W^{t-1}, X^t[i]), Y^t[i])$

5: $g^t = \frac{\partial L(W^{t-1}, X^t, Y^t)}{\partial W}$

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7: $v^t = \beta_2 v^{t-1} + (1-\beta_2)(g^t \odot g^t)$

8: $W^t = W^{t-1} - \eta \left(\frac{\sqrt{1-\beta_2^t}}{1-\beta_1^t} \frac{m^t}{\sqrt{v^t}+\epsilon} + \lambda W^{t-1} \right)$

9: **Return** W^T

This change works significantly better in some cases [9]!

Early Stopping

We do not necessarily need to run the optimization until the maximum number of iterations or until its convergence.

Algorithm 1 AdamW

Input: step T, initial learning Rate η, initial W^0, batch size B, $\beta_1 = 0.9$, $\beta_2 = 0.999$, $\epsilon = 10^{-8}$, $m^0 = 0$, $v^0 = 0$, weight decay λ

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  $L(W^{t-1}, X^t, Y^t) = \frac{1}{B}\sum_{i=1}^{B} \ell(f(W^{t-1}, X^t[i]), Y^t[i])$

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Return W^T

Image Credit: [10]

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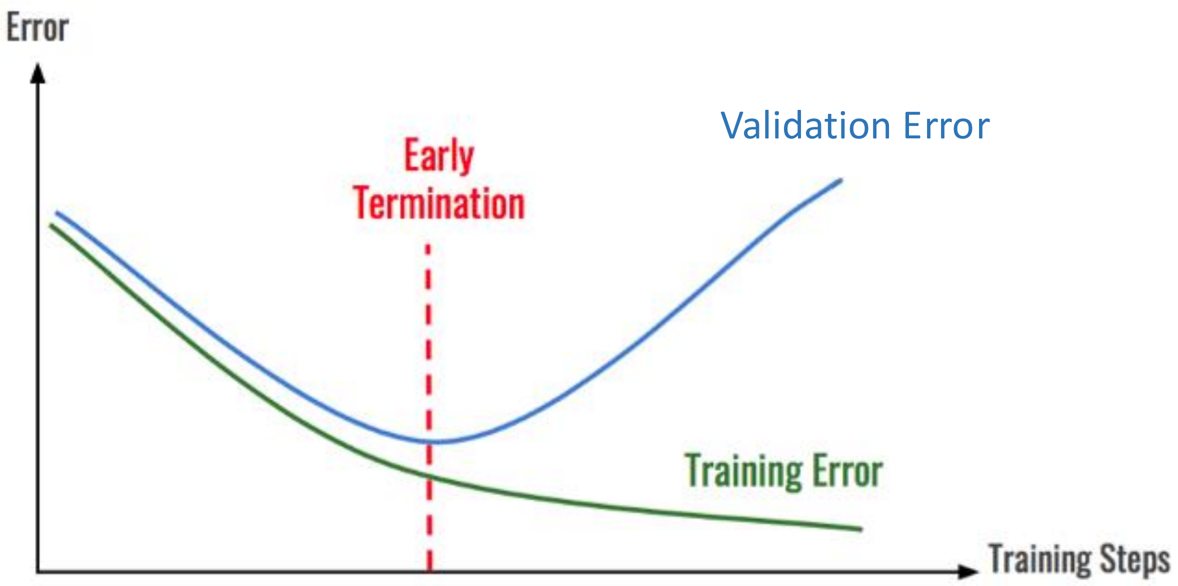

We can check the validation error and if it is keep increasing within a time window, then we stop the training!

If you worry that it will go down again, run until the maximum number of iterations and pick the model with the least validation error.

Image Credit: [10]

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Questions?