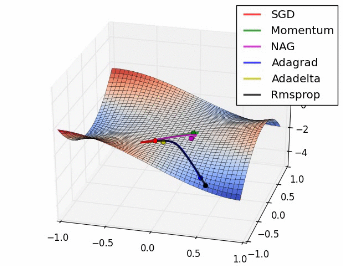
Optimization in Machine Learning

First order methods
Adam and friends

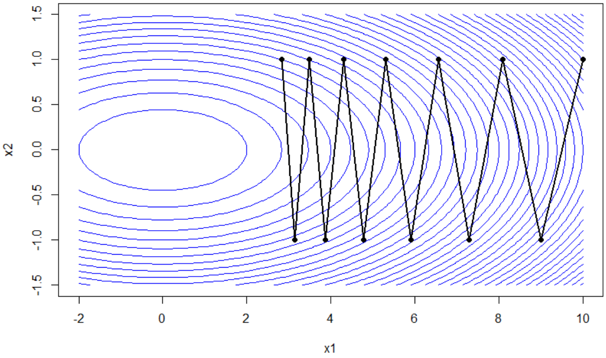


Learning goals

- Adaptive step sizes
- AdaGrad
- RMSProp
- Adam

ADAPTIVE STEP SIZES

- Step size is probably the most important control parameter
- Has strong influence on performance
- Natural to use different step size for each input individually and automatically adapt them



ADAGRAD

- AdaGrad adapts step sizes by scaling them inversely proportional to square root of the sum of the past squared derivatives
  - Inputs with large derivatives get smaller step sizes
  - Inputs with small derivatives get larger step sizes
- Accumulation of squared gradients can result in premature small step sizes (Goodfellow et al., 2016)

ADAGRAD / 2

Algorithm AdaGrad

```
require Global step size α
require Initial parameter θ
require Small constant β, perhaps 10^{-7}, for numerical stability
Initialize gradient accumulation variable r = 0
while stopping criterion not met do
    Sample minibatch of m examples from the training set {x̃^(1), ..., x̃^(m)}
    Compute gradient estimate: ĝ ← (1/m) ∇_θ Σ_i L(y^(i), f(x̃^(i) | θ))
    Accumulate squared gradient r ← r + ĝ ⊙ ĝ
    Compute update: ∇θ = −α/(β+√r) ⊙ ĝ (operations element-wise)
    Apply update: θ ← θ + ∇θ
end while
```

- **require** Global step size α
- **require** Initial parameter $\boldsymbol{\theta}$
- **require** Small constant β, perhaps 10^{-7}, for numerical stability
- **Initialize** gradient accumulation variable $\mathbf{r} = \mathbf{0}$
- **while** stopping criterion not met **do**
  - Sample minibatch of m examples from the training set $\{\tilde{\mathbf{x}}^{(1)}, \dots, \tilde{\mathbf{x}}^{(m)}\}$
  - Compute gradient estimate: $\hat{\mathbf{g}} \leftarrow \frac{1}{m} \nabla_{\boldsymbol{\theta}} \sum_i L\left(y^{(i)}, f\left(\tilde{\mathbf{x}}^{(i)} \mid \boldsymbol{\theta}\right)\right)$
  - Accumulate squared gradient $\mathbf{r} \leftarrow \mathbf{r} + \hat{\mathbf{g}} \odot \hat{\mathbf{g}}$
  - Compute update: $\nabla \boldsymbol{\theta} = -\frac{\alpha}{\beta + \sqrt{\mathbf{r}}} \odot \hat{\mathbf{g}}$ (operations element-wise)
  - Apply update: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \nabla \boldsymbol{\theta}$
- **end while**

$\odot$: element-wise product (Hadamard)

RMSPROP

- Modification of AdaGrad
- Resolves AdaGrad's radically diminishing step sizes.
- Gradient accumulation is replaced by exponentially weighted moving average
- Theoretically, leads to performance gains in non-convex scenarios
- Empirically, RMSProp is a very effective optimization algorithm. Particularly, it is employed routinely by DL practitioners.

RMSPROP / 2

Algorithm RMSProp

require Global step size α and decay rate $\rho \in [0, 1)$
require Initial parameter $\boldsymbol{\theta}$
require Small constant β, perhaps 10^{-6}, for numerical stability
Initialize gradient accumulation variable $\mathbf{r} = \mathbf{0}$
while stopping criterion not met **do**
    Sample minibatch of m examples from the training set $\{\tilde{\mathbf{x}}^{(1)}, \ldots, \tilde{\mathbf{x}}^{(m)}\}$
    Compute gradient estimate: $\hat{\mathbf{g}} \leftarrow \frac{1}{m} \nabla_\theta \sum_i L\left(y^{(i)}, f\left(\tilde{\mathbf{x}}^{(i)} \mid \boldsymbol{\theta}\right)\right)$
    Accumulate squared gradient $\mathbf{r} \leftarrow \rho \mathbf{r} + (1 - \rho) \hat{\mathbf{g}} \odot \hat{\mathbf{g}}$
    Compute update: $\nabla \boldsymbol{\theta} = -\frac{\alpha}{\beta + \sqrt{\mathbf{r}}} \odot \hat{\mathbf{g}}$
    Apply update: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \nabla \boldsymbol{\theta}$
end while

ADAM

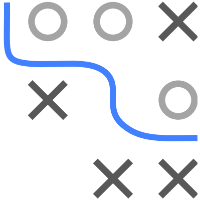
- Adaptive Moment Estimation also has adaptive step sizes
- Uses the 1st and 2nd moments of gradients
  - Keeps an exponentially decaying average of past gradients (1st moment)
  - Like RMSProp, stores an exp-decaying avg of past squared gradients (2nd moment)
  - Can be seen as combo of RMSProp + momentum.

ADAM / 2

Algorithm Adam

require Global step size α (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 β (suggested default 10^{-8})
require Initial parameters $\boldsymbol{\theta}$
Initialize time step $t = 0$
Initialize 1st and 2nd moment variables $\mathbf{s}^{[0]} = 0, \mathbf{r}^{[0]} = 0$
while stopping criterion not met **do**
    $t \leftarrow t + 1$
    Sample a minibatch of m examples from the training set $\{\tilde{x}^{(1)}, \ldots, \tilde{x}^{(m)}\}$
    Compute gradient estimate: $\hat{\mathbf{g}}^{[t]} \leftarrow \frac{1}{m} \nabla_{\boldsymbol{\theta}} \sum_i L\left(y^{(i)}, f\left(\tilde{\mathbf{x}}^{(i)} \mid \boldsymbol{\theta}\right)\right)$
    Update biased first moment estimate: $\mathbf{s}^{[t]} \leftarrow \rho_1 \mathbf{s}^{[t-1]} + (1 - \rho_1)\hat{\mathbf{g}}^{[t]}$
    Update biased second moment estimate: $\mathbf{r}^{[t]} \leftarrow \rho_2 \mathbf{r}^{[t-1]} + (1 - \rho_2)\hat{\mathbf{g}}^{[t]} \odot \hat{\mathbf{g}}^{[t]}$
    Correct bias in first moment: $\hat{\mathbf{s}} \leftarrow \frac{\mathbf{s}^{[t]}}{1-\rho_1^t}$
    Correct bias in second moment: $\hat{\mathbf{r}} \leftarrow \frac{\mathbf{r}^{[t]}}{1-\rho_2^t}$
    Compute update: $\nabla\boldsymbol{\theta} = -\alpha \frac{\hat{\mathbf{s}}}{\sqrt{\hat{\mathbf{r}}}+\beta}$
    Apply update: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \nabla\boldsymbol{\theta}$
end while

ADAM / 3



- Initializes moment variables **s** and **r** with zero $\Rightarrow$ Bias towards zero

$$\mathbb{E}[\mathbf{s}^{[t]}] \neq \mathbb{E}[\hat{\mathbf{g}}^{[t]}] \quad \text{and} \quad \mathbb{E}[\mathbf{r}^{[t]}] \neq \mathbb{E}[\hat{\mathbf{g}}^{[t]} \odot \hat{\mathbf{g}}^{[t]}]$$

($\mathbb{E}$ calculated over minibatches)

- Indeed: Unrolling $\mathbf{s}^{[t]}$ yields

$$\begin{aligned}
\mathbf{s}^{[0]} &= 0 \\
\mathbf{s}^{[1]} &= \rho_1 \mathbf{s}^{[0]} + (1-\rho_1)\hat{\mathbf{g}}^{[1]} = (1-\rho_1)\hat{\mathbf{g}}^{[1]} \\
\mathbf{s}^{[2]} &= \rho_1 \mathbf{s}^{[1]} + (1-\rho_1)\hat{\mathbf{g}}^{[2]} = \rho_1(1-\rho_1)\hat{\mathbf{g}}^{[1]} + (1-\rho_1)\hat{\mathbf{g}}^{[2]} \\
\mathbf{s}^{[3]} &= \rho_1 \mathbf{s}^{[2]} + (1-\rho_1)\hat{\mathbf{g}}^{[3]} = \rho_1^2(1-\rho_1)\hat{\mathbf{g}}^{[1]} + \rho_1(1-\rho_1)\hat{\mathbf{g}}^{[2]} + (1-\rho_1)\hat{\mathbf{g}}^{[3]}
\end{aligned}$$

- Therefore: $\mathbf{s}^{[t]} = (1-\rho_1)\sum_{i=1}^{t} \rho_1^{t-i}\hat{\mathbf{g}}^{[i]}$.
- **Note:** Contributions of past $\hat{\mathbf{g}}^{[i]}$ decreases rapidly

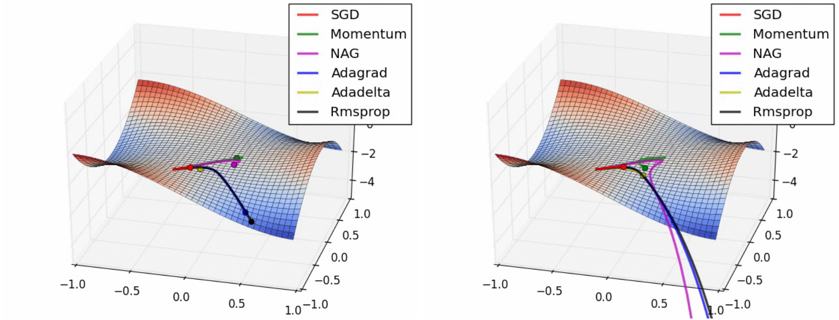
ADAM / 4

- We continue with

$$\begin{aligned}\mathbb{E}[\mathbf{s}^{[t]}] &= \mathbb{E}[(1-\rho_1)\sum_{i=1}^{t}\rho_1^{t-i}\hat{\mathbf{g}}^{[i]}] \\ &= \mathbb{E}[\hat{\mathbf{g}}^{[t]}](1-\rho_1)\sum_{i=1}^{t}\rho_1^{t-i} + \zeta \\ &= \mathbb{E}[\hat{\mathbf{g}}^{[t]}](1-\rho_1^t) + \zeta,\end{aligned}$$

  where we approximated $\hat{\mathbf{g}}^{[i]}$ by $\hat{\mathbf{g}}^{[t]}$. The resulting error is put in ζ and be kept small due to the exponential weights of past gradients.
- Therefore: $\mathbf{s}^{[t]}$ is a biased estimator of $\hat{\mathbf{g}}^{[t]}$
- But bias vanishes for $t \to \infty$ ($\rho_1^t \to 0$)
- Ignoring ζ, we correct for the bias by $\hat{\mathbf{s}}^{[t]} = \frac{\mathbf{s}^{[t]}}{(1-\rho_1^t)}$
- Analogously: $\hat{\mathbf{r}}^{[t]} = \frac{\mathbf{r}^{[t]}}{(1-\rho_2^t)}$

COMPARISON OF OPTIMIZERS: ANIMATION



Credits: Dettmers (2015) and Radford

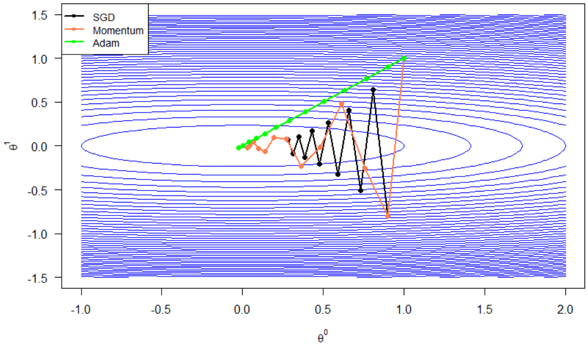
Comparison of SGD optimizers near saddle point.

Left: After start. **Right:** Later.

All methods accelerate compared to vanilla SGD.

Best is RMSProp, then AdaGrad. (Adam is missing here.)

COMPARISON ON QUADRATIC FORM



SGD vs. SGD with Momentum vs. Adam on a quadratic form.