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ADAM: A Method for Stochastic Optimization

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What is optimization?

The process of finding the best solution from all possible solutions

What is optimization in machine learning?

The process of adjusting model parameters to <u>minimize the objective function</u> (loss function) and improve model performance.

Line-up

1. Optimization algorithms
2. Related work
3. Adam
4. Convergence analysis
5. Codes
6. Experiments
7. Limitations

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Big picture!

- Optimization algorithms
  - Descent direction methods
    - Fibonacci search
    - Bisection method
    - Line search
    - Approximate line search
    - Trust region methods
  - First order methods
    - Gradient descent (GD)
      - Batch GD
      - Mini-batch GD
      - Stochastic GD
      - GD with momentum
      - Conjugate GD
    - Adaptive learning rate methods
      - RMSProp
      - Adam
      - Adagrad
      - Adadelta
  - Second order methods
    - Newton’s method
    - Quasi-Newton methods
      - BFGS
      - L-BFGS

Big picture!

Optimization algorithms

Descent direction methods

- Fibonacci search
- Bisection method
- Line search
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First order methods

Gradient descent (GD)

- Batch GD
- Mini-batch GD
- Stochastic GD
- GD with momentum
- Conjugate GD

Adaptive learning rate methods

- RMSProp
- Adam
- Adagrad
- Adadelta

Second order methods

- Newton's method
- Quasi-Newton methods
  - BFGS
  - L-BFGS

Line-up

1	2	3	4	5	6	7
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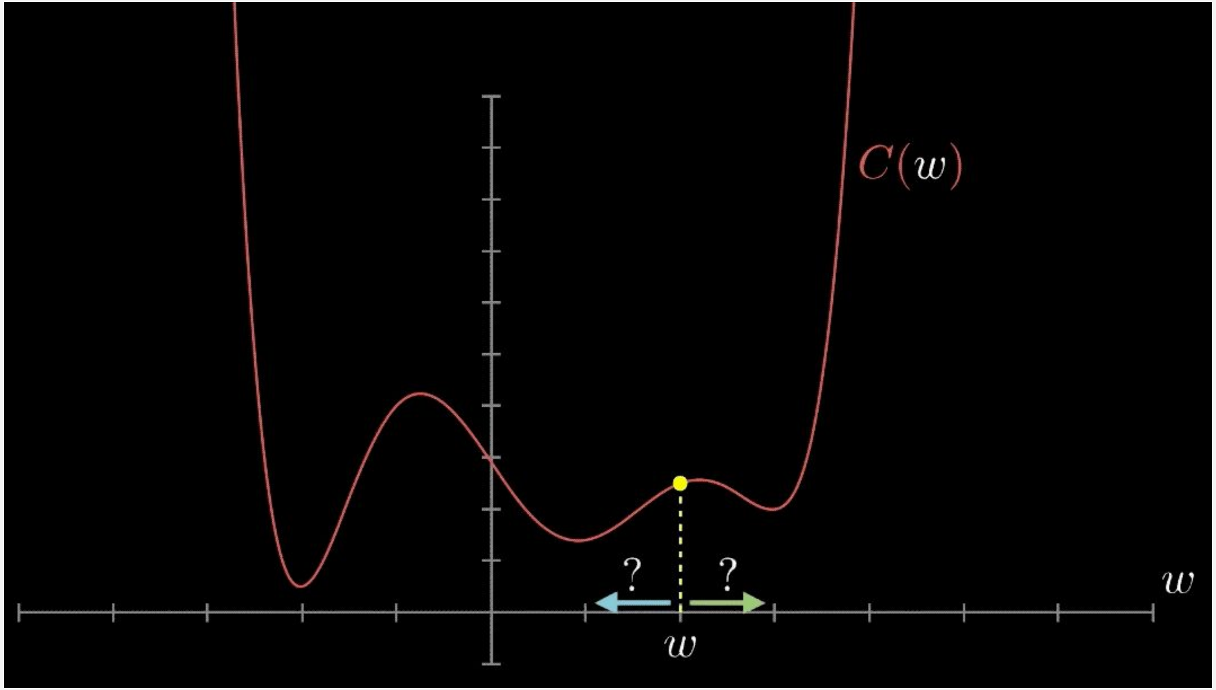
Recap: Gradient descent

$$\mathrm{w} = \mathrm{w} - \alpha \frac{\partial}{\partial w}[C(w)]$$

w: model parameter

$C(w)$: objective function



Credits: https://mlfromscratch.com/optimizers-explained

Gradient descent variants
Batch gradient descent

$$X_{(n\times m)} = \left[x^{(1)}\ x^{(2)}\ \dots\ x^{(m)}\right]$$

$$Y_{(1\times m)} = \left[y^{(1)}\ y^{(2)}\ \dots\ y^{(m)}\right]$$

w: weight parameter

b : bias parameter

$J(w,b)$: loss function

$$J(w,b) = \frac{1}{m}\sum_{i=1}^{m} L(\hat{y}^{(i)}, y^{(i)})$$

$$\mathrm{w} = \mathrm{w} - \alpha \frac{\partial}{\partial w}[J(w,b)]$$

$$b = b - \alpha \frac{\partial}{\partial b}[J(w,b)]$$

- All training examples are processed at once
- High computational cost (utilizes vectorization w/o for loops)
- Slow convergence (1 parameters per epoch)

Mini-batch gradient descent

$$X_{(n\times m)} = [\underbrace{x^{(1)}\, x^{(2)} \dots x^{(b)}}_{X^{\{1\}}_{(n\times b)}} \mid \underbrace{x^{(b+1)}\, x^{(b+2)} \dots x^{(2b)}}_{X^{\{2\}}_{(n\times b)}} \mid \dots]$$

$$Y_{(1\times m)} = [\underbrace{y^{(1)}\, y^{(2)} \dots y^{(b)}}_{Y^{\{1\}}_{(1\times b)}} \mid \underbrace{y^{(b+1)}\, y^{(b+2)} \dots y^{(2b)}}_{Y^{\{2\}}_{(1\times b)}} \mid \dots]$$

$X^{\{t\}}$: t[th] mini-batch of training examples
$Y^{\{t\}}$: t[th] mini-batch of targets

$$J^{\{t\}}(w,b) = \frac{1}{b}\sum_{i=1}^{b} L(\hat{y}^{(i)}, y^{(i)})$$

$$\mathrm{w} = \mathrm{w} - \alpha \frac{\partial}{\partial w}[J^{\{t\}}(w,b)]$$

$$b = b - \alpha \frac{\partial}{\partial b}[J^{\{t\}}(w,b)]$$

- All training examples are processed in mini-batches
- Medium computational cost (reduced vectorization w/ for loops)
- Fastest learning (parameters get updated ceil(m/b) number of steps per epoch)

Stochastic gradient descent

$$X_{(n\times m)} = [\underbrace{x^{(1)}}_{X^{\{1\}}_{(n\times 1)}}\ x^{(2)} \ldots \underbrace{x^{(m)}}_{X^{\{m\}}_{(n\times 1)}}]$$

$$Y_{(1\times m)} = [\underbrace{y^{(1)}}_{Y^{\{1\}}_{(1\times 1)}}\ y^{(2)} \ldots \underbrace{y^{(m)}}_{Y^{\{m\}}_{(1\times 1)}}]$$

$b = 1$: here mini-batch size is one

$X^{\{t\}}$: t^th mini-batch of training examples

$Y^{\{t\}}$: t^th mini-batch of targets

$$J^{\{t\}}(w,b) = \frac{1}{b}\sum_{i=1}^{b} L(\hat{y}^{(i)}, y^{(i)})$$

$$\mathrm{w} = \mathrm{w} - \alpha \frac{\partial}{\partial w}[J^{\{t\}}(w,b)]$$

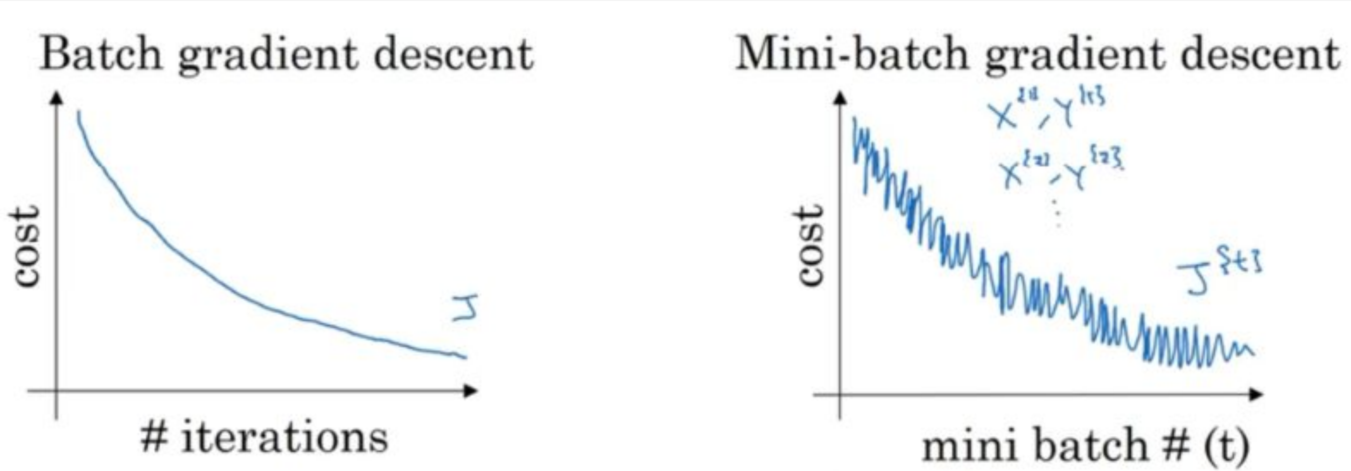
$$b = b - \alpha \frac{\partial}{\partial b}[J^{\{t\}}(w,b)]$$

- All training examples are processed one sample at a time
- Low computational cost per update
- Fast but oscillates, loses speedup from vectorization (parameters get updated per sample per epoch)

Training

Low noise in updates

More noise in updates
(less noise than SGD)



Credits: Deep learning specialization by Prof. Andrew Ng, Coursera

Stochasticity

Randomness or unpredictability in a system or process

E.g.,

- Mini-batch gradient descent
- SGD

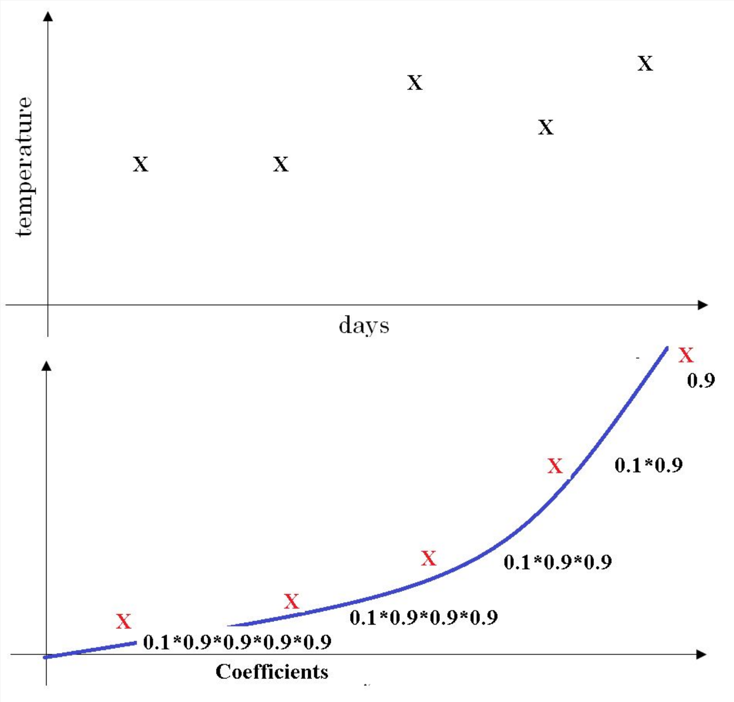
Stochastic objective functions

EWA (Exponentially Weighted Average)

$v_t = \beta v_{t-1} + (1 - \beta)\theta_t$ β is usually a decimal close to 1 (e.g. 0.9, 0.99, etc.)

$$v_0 = 0$$
$$v_1 = (1 - \beta)\theta_1$$
$$v_2 = \beta v_1 + (1 - \beta)\theta_2 \Leftrightarrow v_2 = \beta((1 - \beta)\theta_1) + (1 - \beta)\theta_2$$
$$v_3 = \beta v_2 + (1 - \beta)\theta_3 \Leftrightarrow v_3 = \beta(\beta((1 - \beta)\theta_1) + (1 - \beta)\theta_2) + (1 - \beta)\theta_3$$
$$\Updownarrow$$
$$v_3 = \beta^2(1 - \beta)\theta_1 + \beta(1 - \beta)\theta_2 + (1 - \beta)\theta_3$$

Why ‘exponential’?

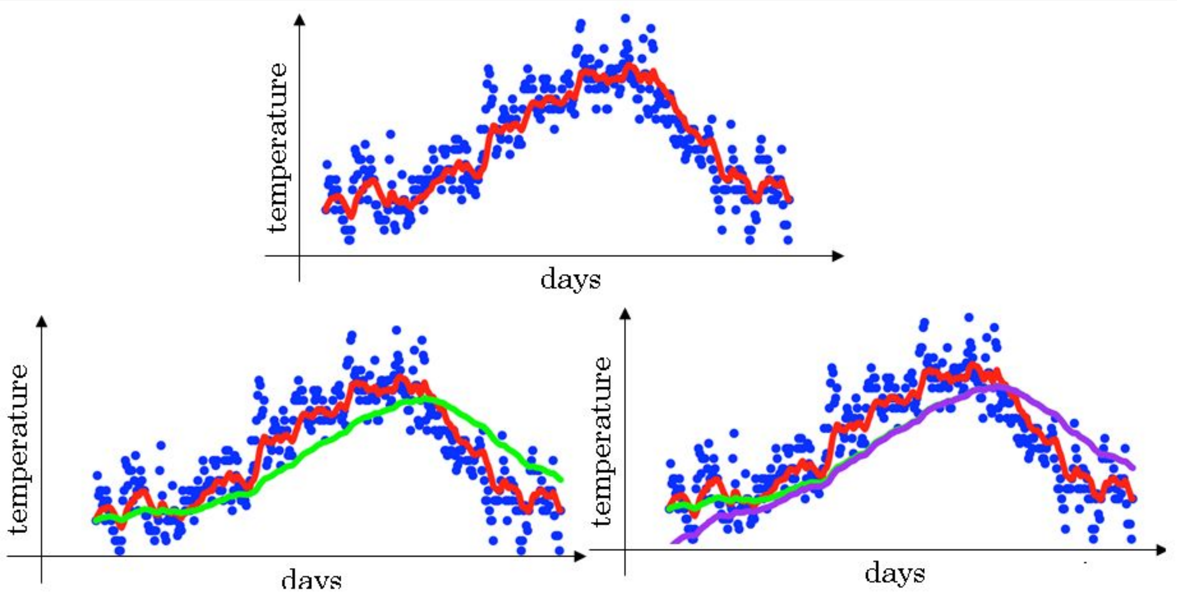


Credits: upscfever.com

$\beta = 0.9$
$(1-\beta) = 0.1$

- Places greater weights on the most recent data
- The weighting for older data points decrease exponentially
- Computationally efficient
- Saves storage (overrides)

Bias correction



Credits: Deep learning specialization by Prof. Andrew Ng, Coursera

$$v_t = \beta v_{t-1} + (1-\beta)\theta_t$$

- Initially biased towards initialization
- Bias corrected term:

$$\hat{v}_t = \frac{v_t}{1-\beta^t}$$

- Green plot: bias not corrected
- Purple plot: bias corrected

Gradient descent with momentum

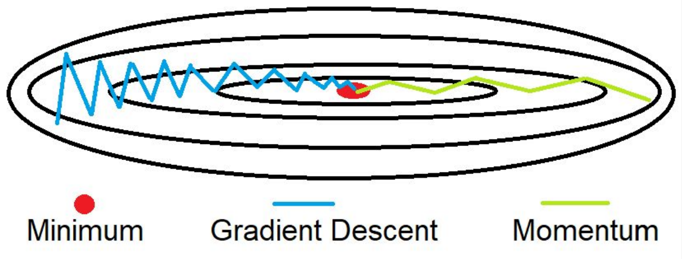
First moment estimate/estimate for mean of gradients

$$m_{t,w} = \beta_1 m_{t-1,w} + (1-\beta_1) g_{t,w}$$

$$m_{t,b} = \beta_1 m_{t-1,b} + (1-\beta_1) g_{t,b}$$

Bias correction: $\hat{m}_{t,w} = \frac{m_{t,w}}{1-\beta_1^t}$ $\hat{m}_{t,b} = \frac{m_{t,b}}{1-\beta_1^t}$

Parameter updates: $W = W - \alpha \hat{m}_{t,w}$ $b = b - \alpha \hat{m}_{t,b}$



Credits: andreaperlato.com

Gradient w.r.t. Stochastic objective at timestep t:

$$g_{t,w} = \frac{\partial}{\partial w}[J^{\{t\}}(w,b)]$$

$$g_{t,b} = \frac{\partial}{\partial b}[J^{\{t\}}(w,b)]$$

- Minimizes the vertical direction gradient component

Adagrad (Adaptive gradient)

$$g_t = \nabla_\theta J(\theta_t)$$

Accumulates the squares of past gradients:

$$G_t = G_{t-1} + g_t^2$$

Update rule for parameters:

$$\theta_{t+1} = \theta_t - \frac{\eta}{\sqrt{G_t + \epsilon}} \odot g_t$$

Adaptive learning rate methods

RMSProp

Second moment estimate/estimate for variance of gradients

$$v_{t,w} = \beta_2 v_{t-1,w} + (1-\beta_2) g_{t,w}^2$$

$$v_{t,b} = \beta_2 v_{t-1,b} + (1-\beta_2) g_{t,b}^2$$

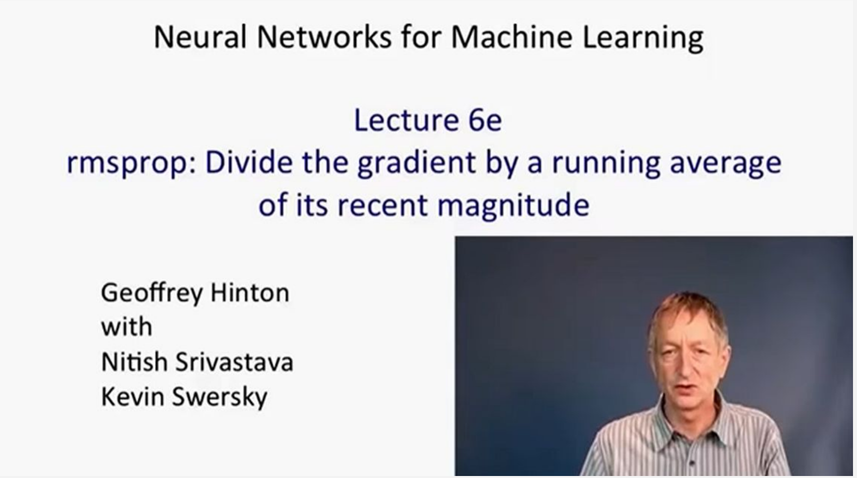
Bias correction:

$$\hat{v}_{t,w} = \frac{v_{t,w}}{1-\beta_2^t} \qquad \hat{v}_{t,b} = \frac{v_{t,b}}{1-\beta_2^t}$$

Parameter updates:

$$W = W - \alpha \frac{g_{t,w}}{\sqrt{\hat{v}_{t,w} + \varepsilon}}$$

$$b = b - \alpha \frac{g_{t,b}}{\sqrt{\hat{v}_{t,b} + \varepsilon}}$$



Root
Mean
Square
Propagation

RMSProp

- Minimizes variance in gradients

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Adam (Adaptive moment estimation)

1st moment estimate (momentum term):

$$m_{t,w} = \beta_1 m_{t-1,w} + (1-\beta_1) g_{t,w} \qquad m_{t,b} = \beta_1 m_{t-1,b} + (1-\beta_1) g_{t,b}$$

$$\hat{m}_{t,w} = \frac{m_{t,w}}{1-\beta_1^t} \qquad \hat{m}_{t,b} = \frac{m_{t,b}}{1-\beta_1^t}$$

2nd moment estimate (RMSProp term):

$$v_{t,w} = \beta_2 v_{t-1,w} + (1-\beta_2) g_{t,w}^2 \qquad v_{t,b} = \beta_2 v_{t-1,b} + (1-\beta_2) g_{t,b}^2$$

$$\hat{v}_{t,w} = \frac{v_{t,w}}{1-\beta_2^t} \qquad \hat{v}_{t,b} = \frac{v_{t,b}}{1-\beta_2^t}$$

Parameter updates:

$$W = W - \alpha \frac{\hat{m}_{t,w}}{\sqrt{\hat{v}_{t,w}} + \varepsilon} \qquad b = b - \alpha \frac{\hat{m}_{t,b}}{\sqrt{\hat{v}_{t,b}} + \varepsilon}$$

Algorithm

β1: Exponential decay rate parameter for past gradient estimates

β2: Exponential decay rate parameter for past squared gradient estimates

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Algorithm 1: *Adam*, our proposed algorithm for stochastic optimization. See section 2 for details, and for a slightly more efficient (but less clear) order of computation. g_t^2 indicates the elementwise square $g_t \odot g_t$. Good default settings for the tested machine learning problems are $\alpha = 0.001$, $\beta_1 = 0.9$, $\beta_2 = 0.999$ and $\epsilon = 10^{-8}$. All operations on vectors are element-wise. With β_1^t and β_2^t we denote β_1 and β_2 to the power t.

Require: α: Stepsize
Require: $\beta_1, \beta_2 \in [0, 1)$: Exponential decay rates for the moment estimates
Require: $f(\theta)$: Stochastic objective function with parameters θ
Require: θ_0: Initial parameter vector
  $m_0 \leftarrow 0$ (Initialize 1st moment vector)
  $v_0 \leftarrow 0$ (Initialize 2nd moment vector)
  $t \leftarrow 0$ (Initialize timestep)
  while θ_t not converged **do**
    $t \leftarrow t + 1$
    $g_t \leftarrow \nabla_\theta f_t(\theta_{t-1})$ (Get gradients w.r.t. stochastic objective at timestep t)
    $m_t \leftarrow \beta_1 \cdot m_{t-1} + (1 - \beta_1) \cdot g_t$ (Update biased first moment estimate)
    $v_t \leftarrow \beta_2 \cdot v_{t-1} + (1 - \beta_2) \cdot g_t^2$ (Update biased second raw moment estimate)
    $\widehat{m}_t \leftarrow m_t / (1 - \beta_1^t)$ (Compute bias-corrected first moment estimate)
    $\widehat{v}_t \leftarrow v_t / (1 - \beta_2^t)$ (Compute bias-corrected second raw moment estimate)
    $\theta_t \leftarrow \theta_{t-1} - \alpha \cdot \widehat{m}_t / (\sqrt{\widehat{v}_t} + \epsilon)$ (Update parameters)
  end while
  return θ_t (Resulting parameters)

Adam's update rule

$$\Delta_t = \alpha \cdot \widehat{m}_t / \sqrt{\widehat{v}_t}$$

case $(1-\beta_1) > \sqrt{1-\beta_2}$ $\quad |\Delta_t| \le \alpha \cdot (1-\beta_1)/\sqrt{1-\beta_2}$

If $\underbrace{\text{gradient}}_{g_t}$ has been zero at all time steps except current step,

$$m_t \approx (1-\beta_1) g_t \Longrightarrow \hat{m}_t \approx \frac{(1-\beta_1) g_t}{(1-\beta_1^t)}$$

$$V_t \approx (1-\beta_2) g_t^2 \Longrightarrow \hat{V}_t \simeq \frac{(1-\beta_2) g_t^2}{(1-\beta_2^t)}$$

when $t \uparrow$ $\beta_1^t, \beta_2^t \simeq 0$

$\hat{m}_t \simeq m_t$

$\hat{V}_t \simeq V_t$

$$\Longrightarrow \left| \frac{\hat{m}_t}{\sqrt{\hat{V}_t}} \right| = \left| \frac{(1-\beta_1) g_t}{\sqrt{(1-\beta_2) g_t^2}} \right| = \frac{1-\beta_1}{\sqrt{1-\beta_2}}$$

$(1-\beta_1) > \sqrt{1-\beta_2}$

$$|\Delta_t| \le \alpha \cdot \frac{(1-\beta_1)}{\sqrt{1-\beta_2}} \lesssim \alpha \cdot 1$$

Tighter upper bound (for sparsity)

Adam's update rule

$$\Delta_t = \alpha \cdot \widehat{m}_t / \sqrt{\widehat{v}_t}$$

Common case: $|\Delta_t| \leq \alpha$

SNR (signal to noise ratio)

Jensen's inequality

For any stochastic gradient, g_t:

1st moment estimate $\hat{m}_t$

2nd moment est. v_t

$$\frac{E[g_t]}{\sqrt{E[g_t^2]}} \leq 1$$

$\therefore$ General case $|\Delta_t| \leq \alpha \cdot 1$

- Adam is bounded
- Does not grow exponentially

Line-up

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PyTorch

Adam

CLASS torch.optim.Adam(*params*, *lr=0.001*, *betas=(0.9, 0.999)*, *eps=1e-08*, *weight_decay=0*, *amsgrad=False*, ***, *foreach=None*, *maximize=False*, *capturable=False*, *differentiable=False*, *fused=None*) [SOURCE]

Parameters

- **params** (*iterable*) – iterable of parameters or named_parameters to optimize or iterable of dicts defining parameter groups. When using named_parameters, all parameters in all groups should be named
- **lr** (*float*, *Tensor*, *optional*) – learning rate (default: 1e-3). A tensor LR is not yet supported for all our implementations. Please use a float LR if you are not also specifying fused=True or capturable=True.
- **betas** (*Tuple*[*float*, *float*], *optional*) – coefficients used for computing running averages of gradient and its square (default: (0.9, 0.999))
- **eps** (*float*, *optional*) – term added to the denominator to improve numerical stability (default: 1e-8)
- **weight_decay** (*float*, *optional*) – weight decay (L2 penalty) (default: 0)

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Experiments

Logistic regression (convex)

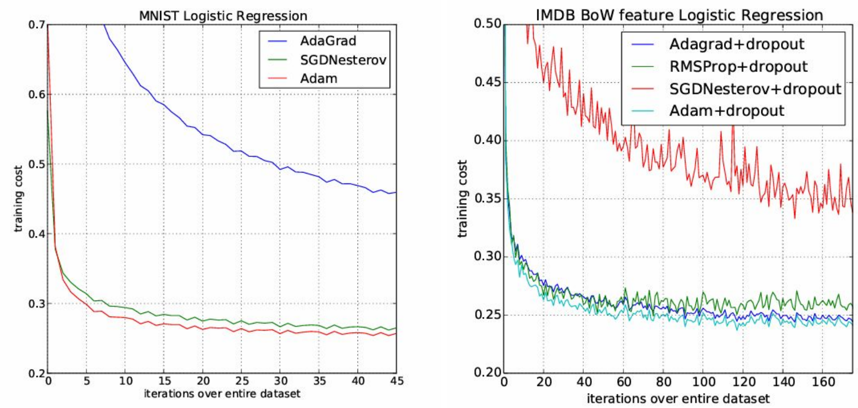


Figure 1: Logistic regression training negative log likelihood on MNIST images and IMDB movie reviews with 10,000 bag-of-words (BoW) feature vectors.

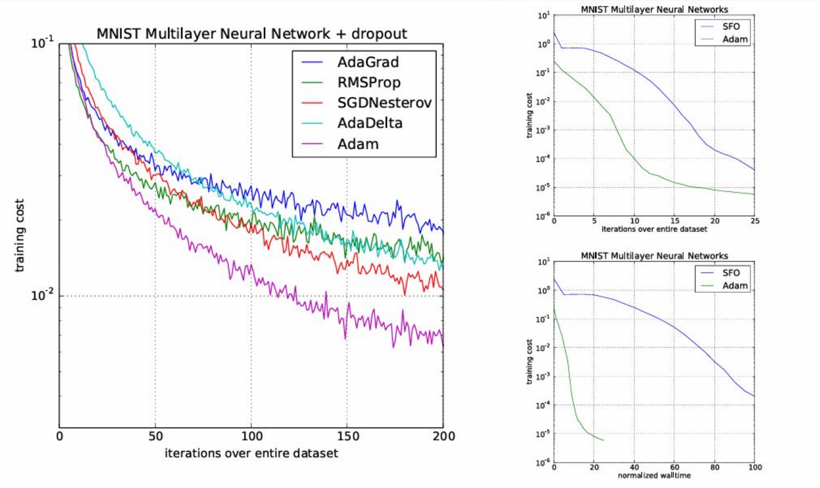
Adam's learning rate decay:

$$\alpha_t = \frac{\alpha}{\sqrt{t}}$$

- The 10,000 dimension BoW feature vector for each review is highly sparse
- Adam can take advantage of sparse features and obtain faster convergence

Experiments

Multi-layer neural network (non-convex)



(a) (b)

Figure 2: Training of multilayer neural networks on MNIST images. (a) Neural networks using dropout stochastic regularization. (b) Neural networks with deterministic cost function. We compare with the sum-of-functions (SFO) optimizer (Sohl-Dickstein et al., 2014)

- A neural network model with:
  - 2 fully connected
  - Hidden layers with 1000 hidden units each
  - ReLU activation
- Mini-batch size of 128
- L2 weight decay on the parameters to prevent over-fitting
- Normalized walltime: actual elapsed time (walltime) adjusted or normalized relative to a reference standard

Experiments

CNN (non-convex)

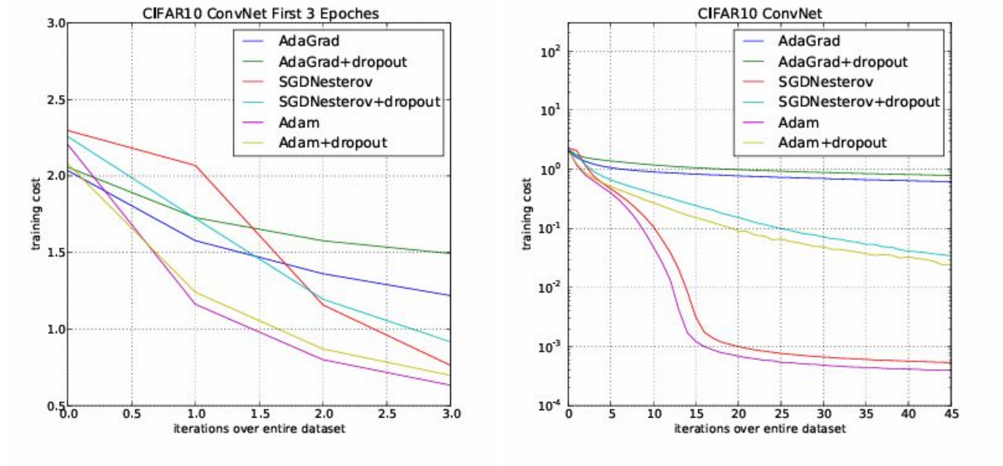


Figure 3: Convolutional neural networks training cost. (left) Training cost for the first three epochs. (right) Training cost over 45 epochs. CIFAR-10 with c64-c64-c128-1000 architecture.

- CNN architecture
  - three alternating stages of 5x5 convolution filters
  - 3x3 max pooling with stride of 2
  - fully connected layer of 1000 rectified linear hidden units (ReLU's)

Experiments (Ablation)

Bias correction term

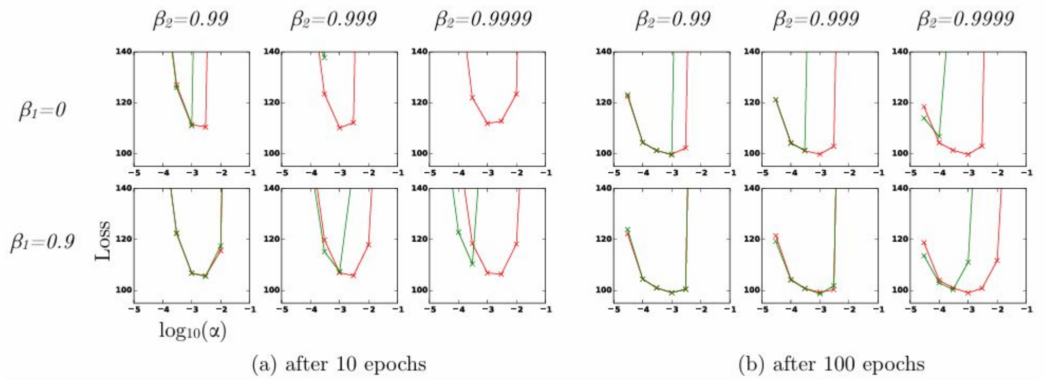


Figure 4: Effect of bias-correction terms (red line) versus no bias correction terms (green line) after 10 epochs (left) and 100 epochs (right) on the loss (y-axes) when learning a Variational Auto-Encoder (VAE) (Kingma & Welling, 2013), for different settings of stepsize α (x-axes) and hyper-parameters β_1 and β_2.

- Values of **β**2 close to 1, required for robustness to sparse gradients, results in larger initialization bias
- values **β**2 close to 1 indeed lead to instabilities in training when no bias correction term was present, especially at first few epochs of the training

Extensions

AdaMax

Algorithm 2: *AdaMax*, a variant of Adam based on the infinity norm. See section 7.1 for details. Good default settings for the tested machine learning problems are $\alpha = 0.002$, $\beta_1 = 0.9$ and $\beta_2 = 0.999$. With β_1^t we denote β_1 to the power t. Here, $(\alpha/(1-\beta_1^t))$ is the learning rate with the bias-correction term for the first moment. All operations on vectors are element-wise.

Require: α: Stepsize
Require: $\beta_1, \beta_2 \in [0, 1)$: Exponential decay rates
Require: $f(\theta)$: Stochastic objective function with parameters θ
Require: θ_0: Initial parameter vector
  $m_0 \leftarrow 0$ (Initialize 1st moment vector)
  $u_0 \leftarrow 0$ (Initialize the exponentially weighted infinity norm)
  $t \leftarrow 0$ (Initialize timestep)
  while θ_t not converged **do**
    $t \leftarrow t + 1$
    $g_t \leftarrow \nabla_\theta f_t(\theta_{t-1})$ (Get gradients w.r.t. stochastic objective at timestep t)
    $m_t \leftarrow \beta_1 \cdot m_{t-1} + (1 - \beta_1) \cdot g_t$ (Update biased first moment estimate)
    $u_t \leftarrow \max(\beta_2 \cdot u_{t-1}, |g_t|)$ (Update the exponentially weighted infinity norm)
    $\theta_t \leftarrow \theta_{t-1} - (\alpha/(1 - \beta_1^t)) \cdot m_t/u_t$ (Update parameters)
  end while
  return θ_t (Resulting parameters)

- We don't need to correct for initialization bias in this case
- Also note that the magnitude of parameter updates has a simpler bound with AdaMax than Adam

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Limitations

- **Non-Convergence Issues:** fail to converge to global minima in certain scenarios, particularly when the learning rates do not diminish over time

  [Dereich et al. 2024. Non-convergence of Adam and other adaptive stochastic gradient descent optimization methods for non-vanishing learning rates]

- **Limit Cycles and Oscillations:** Adam can exhibit limit cycles, leading to oscillations around suboptimal points rather than converging smoothly to an optimal solution

  [Bock et al. 2019. Non-convergence and Limit Cycles in the Adam Optimizer]

Thank you!

Credits: meme-arsenal