



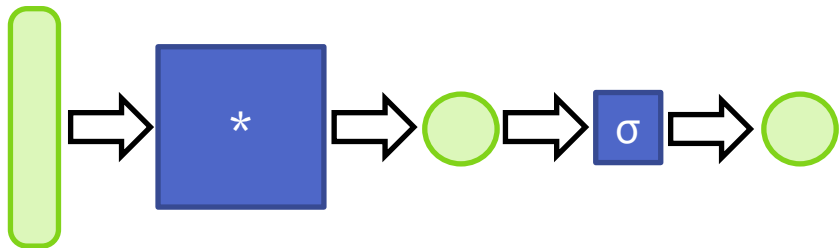
Deep learning models & how to train them

Alexey Zaytsev, Evgeny Burnaev



Logistic regression recap

Recap: logistic regression

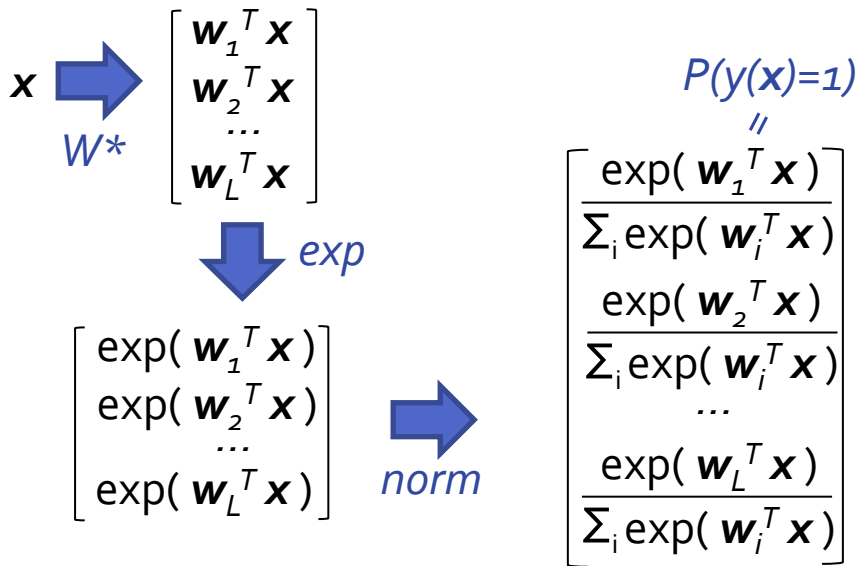


$$P(y(\mathbf{x}_i) = y_i | \mathbf{w}) = \frac{1}{1 + \exp(-y_i \mathbf{w}^T \mathbf{x}_i)} = \sigma(y_i \mathbf{w}^T \mathbf{x}_i)$$

Loss function for logistic regression

$$E(\mathbf{w}) = - \sum_{i=1} \log P(y(\mathbf{x}_i) = y_i | \mathbf{w})$$

Softmax: sigmoid generalization



Multinomial logistic loss

$$P(y(x) = i) = \frac{\exp w_i^T x}{\sum_j \exp w_j^T x}$$

Multinomial log loss (generalizes logistic loss):

$$\begin{aligned} E(w) &= - \sum_i \log P(y(x_i) = y_i) = \\ &= - \sum_i \left[w_{y_i}^T x_i - \log \sum_j \exp w_j^T x_i \right] \end{aligned}$$

(Part of the) gradient over \mathbf{w}_j :

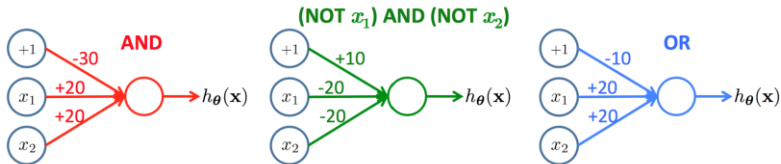
$$\frac{dE}{dw_j} = - \sum_i x_i ([y_i == j] - P(y(x_i) = j))$$

Few notes on logistic regression

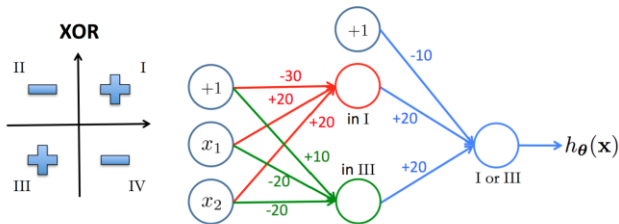
- Convex optimization problem.
Exercise: check that Hessian is positive definite
- Requires regularization for parameters: **on** by default in sklearn
- Admits multiclass classification
- Logistic regression is a generalized linear model & one-layer neural network

Capabilities are limited: need more layers

Building blocks:



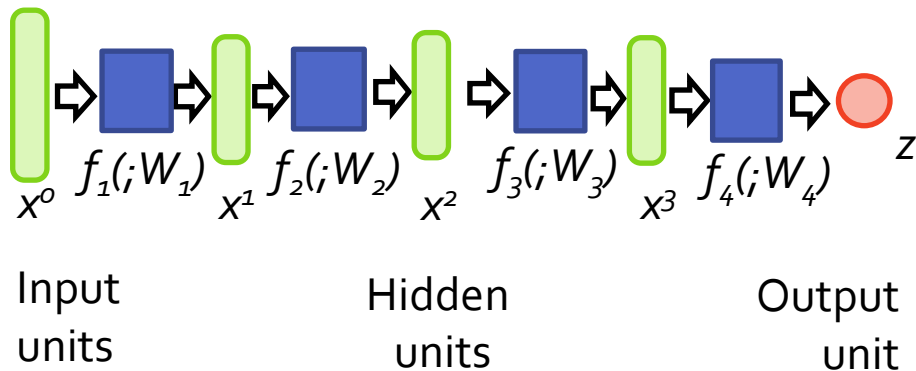
XOR function:



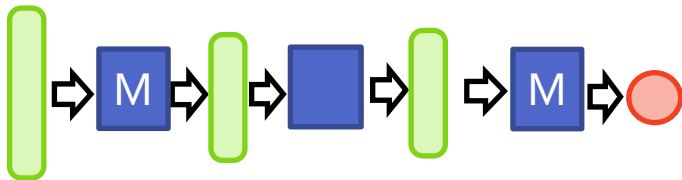


Fully connected neural networks

Multilayer fully-connected (FC) neural network



Universal approximation theorem



UAT: given non-polynomial non-linearity, a single hidden layer neural network can approximate any continuous function on any compact subset of \mathbb{R}^d up to an arbitrary precision [Tsybenko, 1989].

Caveat 1: the width of the network can be a very quickly growing function of space dimension and approximation accuracy. Deeper architectures are exponentially narrower for some classes of functions [Rollnick&Tegmark 2018]

Caveat 2: no guarantees on extrapolation beyond the compact set where the approximation is computed. Thus, designing a proper parameterization of your space is useful.

2006

CAPTCHA



Computer vision = 60%

$$0.6^{12} = 0.00217$$

2014



Completed • Swag • 215 teams

Dogs vs. Cats

Wed 25 Sep 2013 – Sat 1 Feb 2014 (8 months ago)

Dashboard ▼

Private Leaderboard - Dogs vs. Cats

This competition has completed. This leaderboard reflects the final standings.

See someone's profile

#	Δ1w	Team Name <small>* in the money</small>	Score <small>?</small>	Entries	Last Submission UTC (Best - Last)
1	—	Pierre Sermanet *	0.98914	5	Sat, 01 Feb 2014 21:43:19 (-)
2	↑26	orchid *	0.98309	17	Sat, 01 Feb 2014 23:52:30
3	—	Owen	0.98171	15	Sat, 01 Feb 2014 17:04:40 (-)
4	new	Paul Covington	0.98171	3	Sat, 01 Feb 2014 23:05:20
5	↓3	Maxim Milakov	0.98137	24	Sat, 01 Feb 2014 18:20:58

$$0.989^{12} = 0.875$$

2014

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ASIRRA



After 8 years of operation, Asirra is shutting down effective October 1, 2014. Thank you to all of our users!

Classic Machine learning, where representations are available

u – an object

A client

y – true label

Will leave in 3 months?

$x(u)$ – an object
representation

Salary, age

Problem: train a model that
can identify the true class for
 y

A gradient boosting
model

Object



Representation



Classifier



For structured data we need representation learning

u – an object

An image

y – true label

Cat breed? (1)

$x(u)$ – an object representation

NA (2)

Problems: (1) train a model that can identify the true class for y ; **(2) learn a representation**

A neural network:
Encoder +
Classifier

Object



(2) Encoder



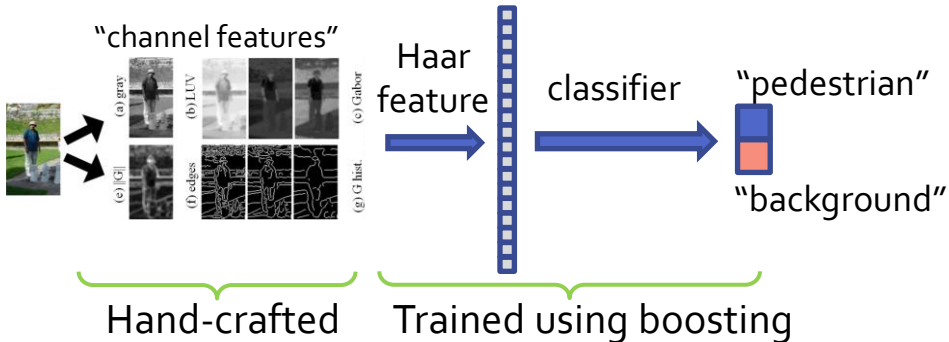
Representation



(1) Classifier



“Deep learning” is not only depth



- Previous CV systems were “deep”, they used multiple layers of representation with certain success
- But they were not called “deep learning”

Deep learning

End-to-end joint learning of all layers:

- multiple assemblable blocks
- each block is piecewise-differentiable
- gradients computed by backpropagation
- gradient-based optimization





Optimization for deep learning

Sequential computation: *backpropagation*

$\frac{dz}{dx^3}, \frac{dz}{dw_4}$ can be computed

$$\frac{dz}{dw_3} = \frac{dx^3}{dw_3}^T \cdot \frac{dz}{dx^3}$$

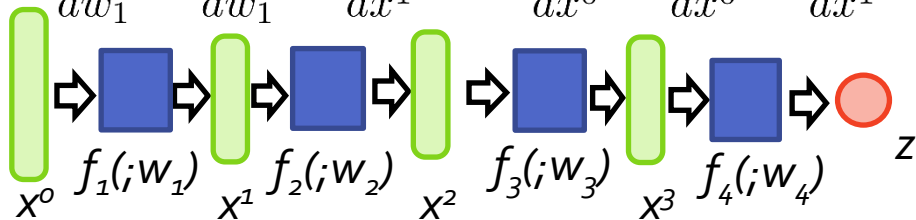
$$\frac{dz}{dw_2} = \frac{dx^2}{dw_2}^T \cdot \frac{dz}{dx^2}$$

$$\frac{dz}{dw_1} = \frac{dx^1}{dw_1}^T \cdot \frac{dz}{dx^1}$$

$$\frac{dz}{dx^2} = \frac{dx^3}{dx^2}^T \cdot \frac{dz}{dx^3}$$

$$\frac{dz}{dx^1} = \frac{dx^2}{dx^1}^T \cdot \frac{dz}{dx^2}$$

$$\frac{dz}{dx^0} = \frac{dx^1}{dx^0}^T \cdot \frac{dz}{dx^1}$$



Optimization for supervised ML

- $R(w)$ denotes regularization e.g. $\|w\|^2$
- $l(x_i, y_i, w)$ denotes loss for i -th example, e.g. $-\log P(y(x_i) = y_i \mid w)$
- The optimization objective is:

$$E(w) = \frac{1}{N} \sum_{i=1}^N l(x_i, y_i, w) + \lambda R(w)$$

Small scale setting: traditional optimization

$$E(w) = \frac{1}{N} \sum_{i=1}^N l(x_i, y_i, w) + \lambda R(w)$$

- Data are few, we can look through it at each optimization iteration
- Use adapted versions of standard optimization methods (gradient descent, quasi-Newton, quadratic programming,...)

Large-scale learning

$$E(w) = \frac{1}{N} \sum_{i=1}^N l(x_i, y_i, w) + \lambda R(w)$$

$$\frac{dE}{dw} = \frac{1}{N} \sum_{i=1}^N \frac{dl(x_i, y_i, w)}{dw} + \lambda \frac{dR}{dw}$$

- Evaluating gradient is very expensive
- It will only be good for one (small) step

Stochastic gradient descent (SGD) idea:

- Evaluate a coarse approximation to grad
- Make “quick” steps

Stochastic gradient descent (SGD)

Gradient:

$$\frac{dE}{dw} = \frac{1}{N} \sum_{i=1}^N \frac{dl(x_i, y_i, w)}{dw} + \lambda \frac{dR}{dw}$$

Stochastic gradient:

$$\frac{dE^i}{dw} = \frac{dl(x_i, y_i, w)}{dw} + \lambda \frac{dR}{dw}$$

Stochastic gradient is an unbiased estimate of the gradient:

$$\frac{dE}{dw} = \frac{1}{N} \sum_{i=1}^N \frac{dE^i}{dw}$$

Gradient descent (GD)

GD:

$$\begin{aligned}v[t] &= -\alpha[t] \nabla(E, w[t]) \\w[t+1] &= w[t] + v[t]\end{aligned}$$

where $\nabla(E, w[t]) = \frac{dE}{dw}(w[t])$

- $\alpha[t]$ is the learning rate, more on this later
- Convergence is guaranteed for good problems (deep learning optimization is not a good problem)

Stochastic gradient descent (SGD)

SGD:

$$\begin{aligned}v[t] &= -\alpha[t] \nabla(E, w[t]) \\w[t+1] &= w[t] + v[t]\end{aligned}$$

where $\nabla(E, w[t]) = \frac{dE^{i(t)}}{dw}(w[t])$

- $i(t)$ usually follow random permutations of training data
- One sweep over training data is called an **epoch**

Stochastic gradient descent (SGD)

SGD:

$$\begin{aligned}v[t] &= -\alpha[t] \nabla(E, w[t]) \\w[t+1] &= w[t] + v[t]\end{aligned}$$

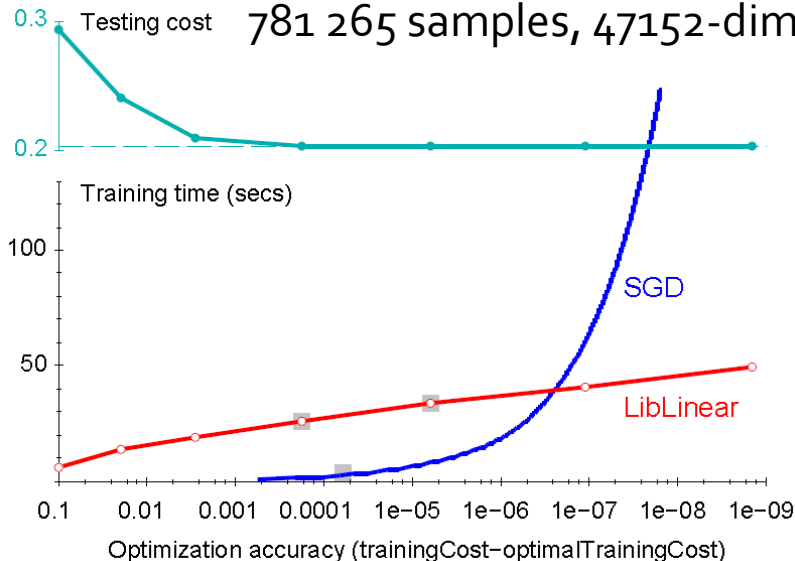
- One sweep over training data is called an **epoch**
- Popular choices for schedule $\alpha[t]$:
 - constant, e.g. $\alpha[t] = 0.0001$
 - piecewise constant, e.g. $\alpha[t]$ is decreased tenfold every N epochs
 - harmonic, e.g. $\alpha[t] = 0.001 / ([t/N] + 10)$

The efficiency of SGD ("shallow" learning)

[L.Bottou]

Document classification:

781 265 samples, 47152-dim BoW



Batch SGD

Gradient:

$$\frac{dE}{dw} = \frac{1}{N} \sum_{i=1}^N \frac{dl(x_i, y_i, w)}{dw} + \lambda \frac{dR}{dw}$$

Batch (aka mini-batch):

$$\{b_1, b_2, \dots, b_{N_b}\} \subset 1 \dots N$$

Batch stochastic gradient:

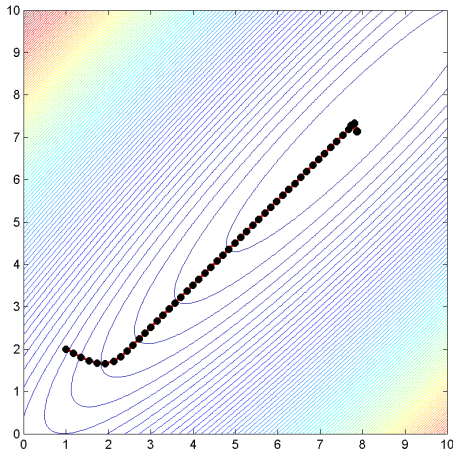
$$\frac{dE}{dw} = \frac{1}{N_b} \sum_{i=1}^{N_b} \frac{dl(x_{b(i)}, y_{b(i)}, w)}{dw} + \lambda \frac{dR}{dw}$$

Why do batching?

$$\frac{dE}{dw} = \frac{1}{N_b} \sum_{i=1}^{N_b} \frac{dl(x_{b(i)}, y_{b(i)}, w)}{dw} + \lambda \frac{dR}{dw}$$

- “Less stochastic” approximation, more stable convergence (questionable)
- **Main reason:** all modern architectures have parallelism, hence computing mini-batch grad is often as cheap as a single stochastic grad

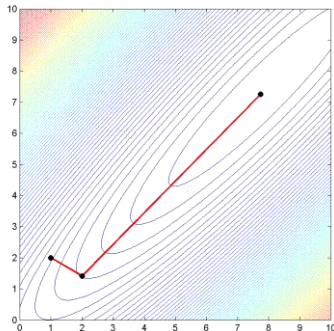
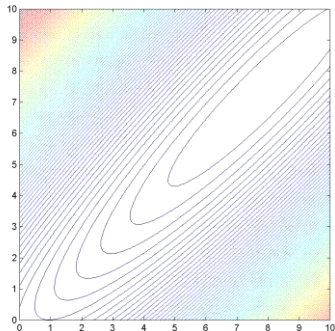
SGD inherits gradient descent problems



- Gradient descent is very poor “in ravines”
- SGD is no better

Better optimization methods

- Second order methods (Newton, Quasi-Newton)
- Krylov subspace methods, in particular *conjugate gradients*



Improving SGD using momentum

- Conjugate gradients use a combination of the current gradient and previous direction for the next step
- Similar idea for SGD (*momentum*):

$$\begin{aligned}v[t] &= -\alpha[t] \nabla(E, w[t]) \\w[t+1] &= w[t] + v[t]\end{aligned}$$



$$\begin{aligned}v[t] &= \mu v[t-1] - \alpha[t] \nabla(E, w[t]) \\w[t+1] &= w[t] + v[t]\end{aligned}$$

Typical $\mu = 0.9$

Exponentially decaying running average

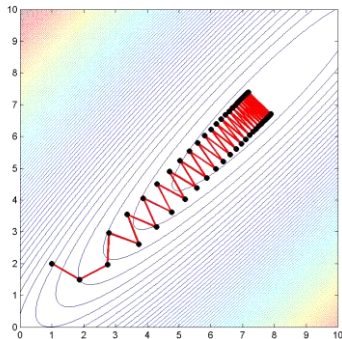
$$\begin{aligned}v[t] &= \mu v[t-1] - \alpha[t] \nabla (E, w[t]) \\w[t+1] &= w[t] + v[t]\end{aligned}$$

$$\begin{aligned}v[t] &= \mu v[t-1] - \alpha[t] \nabla (E, w[t]) = \\&= \mu^2 v[t-2] - \mu \alpha[t-1] \nabla (E, w[t-1]) \\&\quad - \alpha[t] \nabla (f, w[t]) = \\&= \mu^3 v[t-3] - \mu^2 \alpha[t-2] \nabla (E, w[t-2]) \\&\quad - \mu \alpha[t-1] \nabla (E, w[t-1]) - \alpha[t] \nabla (E, w[t]) = \\&= \mu^{k+1} v[t-k-1] + \sum_{i=0}^k \mu^i \alpha[t-i] \nabla (E, w[t-i])\end{aligned}$$

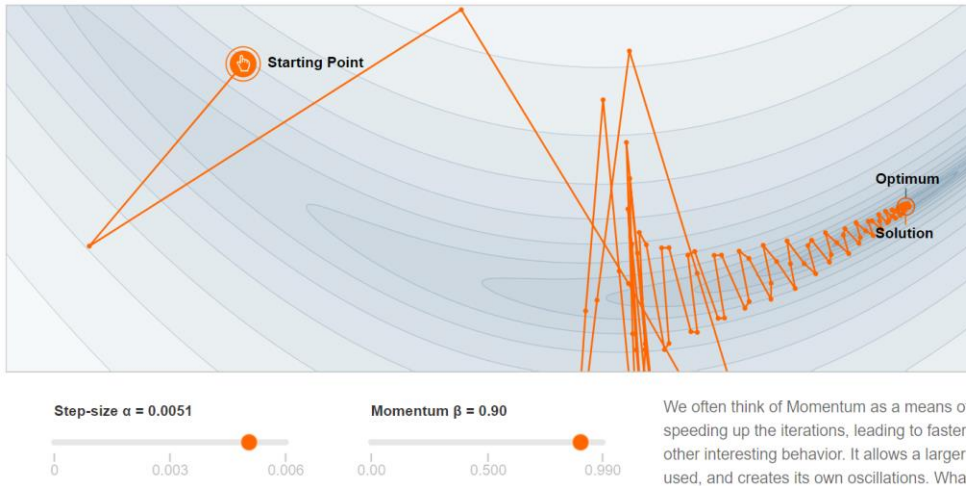
Momentum: why it works

$$v[t] \approx \sum_{i=0}^k \mu^i \alpha[t-i] \nabla(E, w[t-i])$$

- Smoothes out noise in SGD (~bigger batches)
- **Smoothes out oscillations inherent to gradient descent**
- Escapes local minima



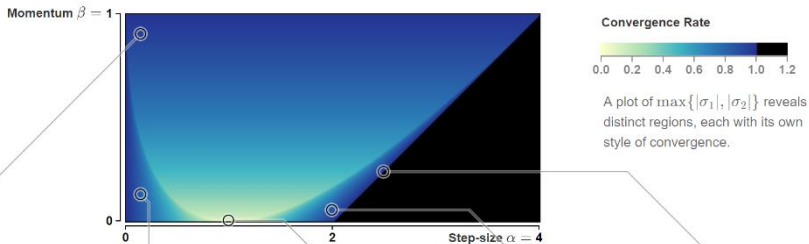
The effect of the momentum



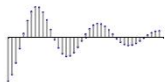
<https://distill.pub/2017/momentum/>

[Goh, Distill 2017]

Phase space along a single eigenvector



Ripples



R 's eigenvalues are complex, and the iterates display low frequency ripples. Surprisingly, the convergence rate $2\sqrt{\beta}$ is independent of α and λ_i .

Monotonic Decrease



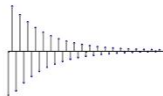
R 's eigenvalues are both real, are positive, and have norm less than one. The behavior here resembles gradient descent.

1-Step Convergence



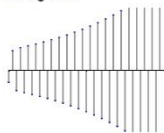
When $\alpha = 1/\lambda_i$, and $\beta = 0$, we converge in one step. This is a very special point, and kills the error in the eigenspace completely.

Monotonic Oscillations



When $\alpha > 1/\lambda_i$, the iterates flip between $+$ and $-$ at each iteration. These are often referred to as 'oscillations' in gradient descent.

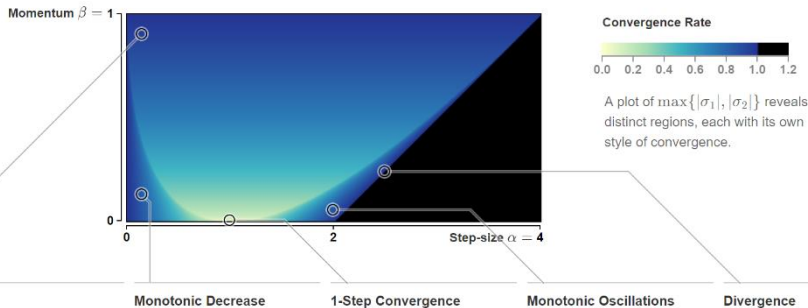
Divergence



When $\max\{|\sigma_1|, |\sigma_2|\} > 1$, the iterates diverge.

[Goh, Distill 2017]

Momentum: multiple eigenvalues



Optimal rate & momentum:

$$\alpha = \left(\frac{2}{\sqrt{\lambda_1} + \sqrt{\lambda_n}} \right)^2 \quad \beta = \left(\frac{\sqrt{\lambda_n} - \sqrt{\lambda_1}}{\sqrt{\lambda_n} + \sqrt{\lambda_1}} \right)^2$$

Optimal speed:

$$\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}$$

Convergence rate,
Momentum

$$\frac{\kappa - 1}{\kappa + 1}$$

Convergence rate,
Gradient Descent

[Goh, Distill 2017]

Momentum: multiple eigenvalues

Optimal rate &
momentum:

$$\alpha = \left(\frac{2}{\sqrt{\lambda_1} + \sqrt{\lambda_n}} \right)^2 \quad \beta = \left(\frac{\sqrt{\lambda_n} - \sqrt{\lambda_1}}{\sqrt{\lambda_n} + \sqrt{\lambda_1}} \right)^2$$

In real network we do not know eigenvalues, so:

- we set the momentum high (e.g. 0.9)
- then we tune the learning rate

Nesterov accelerated gradient

$$\begin{aligned}v[t] &= \mu v[t-1] - \alpha[t] \nabla(E, w[t]) \\w[t+1] &= w[t] + v[t]\end{aligned}$$

Before we even compute the gradient, we have a good approximation where we will end up: $w[t+1] \approx w[t] + \mu v[t-1]$

Let us use this knowledge:

$$\begin{aligned}v[t] &= \mu v[t-1] - \alpha[t] \nabla(E, w[t] + \mu v[t-1]) \\w[t+1] &= w[t] + v[t]\end{aligned}$$

(Computing the gradient at a more relevant spot)

Second-order methods

- Exponential smoothing helps, but still not optimal if large anisotropy exists
- Classic (Newton) solution: estimate the Hessian and make the update
$$v[t+1] = -H[t]^{-1} \nabla(E, w[t])$$
 (the lower the curvature the faster we go)
- Quasi-Newton methods: estimate some approximation to Hessian based on observed gradients

Adagrad method [Duchi et al. 2011]

Idea: scale updates along different dimensions according to accumulated gradient magnitude

$$g[t] = g[t-1] + \nabla(E, w[t]) \odot \nabla(E, w[t])$$

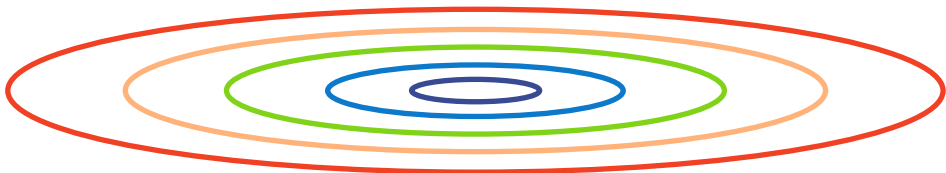
$$w[t+1] = w[t] - \frac{\alpha}{\sqrt{g[t] + \epsilon}} \odot \nabla(E, w[t])$$

Note: step lengths automatically decrease (perhaps too quickly).

Adagrad method [Duchi et al. 2011]

$$g[t] = g[t-1] + \nabla(E, w[t]) \odot \nabla(E, w[t])$$

$$w[t+1] = w[t] - \frac{\alpha}{\sqrt{g[t] + \epsilon}} \odot \nabla(E, w[t])$$



Adagrad in this case: find out that “vertical” derivatives are bigger, then make “vertical” steps smaller than “horizontal”

RMSPROP method [Hinton 2012]

Same as Adagrad, but replace accumulation of squared gradient with running averaging:

$$g[t] = \mu g[t-1] + (1-\mu) \nabla(E, w[t]) \odot \nabla(E, w[t])$$
$$w[t+1] = w[t] - \frac{\alpha[t]}{\sqrt{g[t]} + \epsilon} \odot \nabla(E, w[t])$$

Comparison: logistic regression

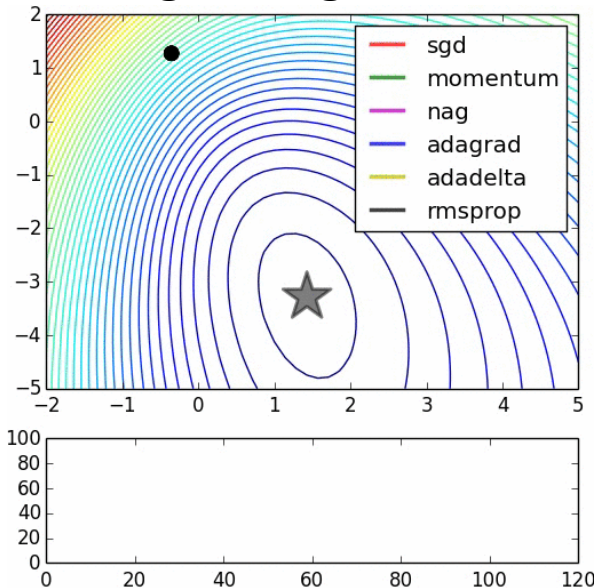


Image credit: Alec Redford

Further comparison

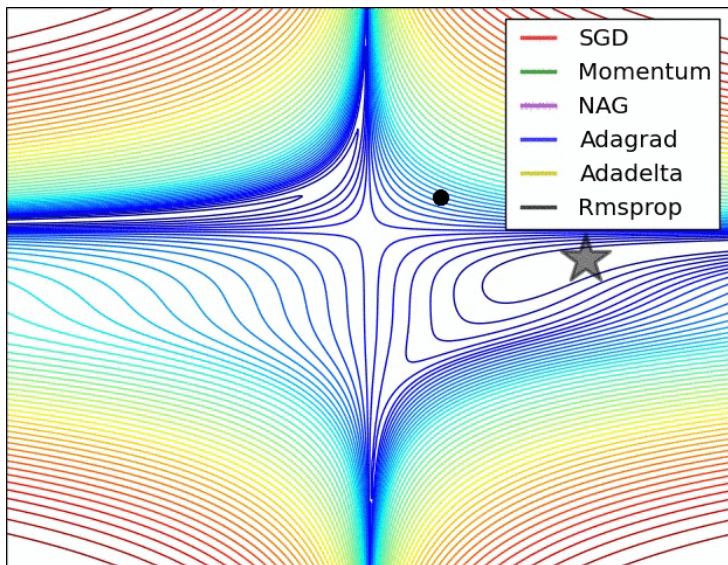


Image credit: Alec Redford

Further comparison: escaping from a saddle

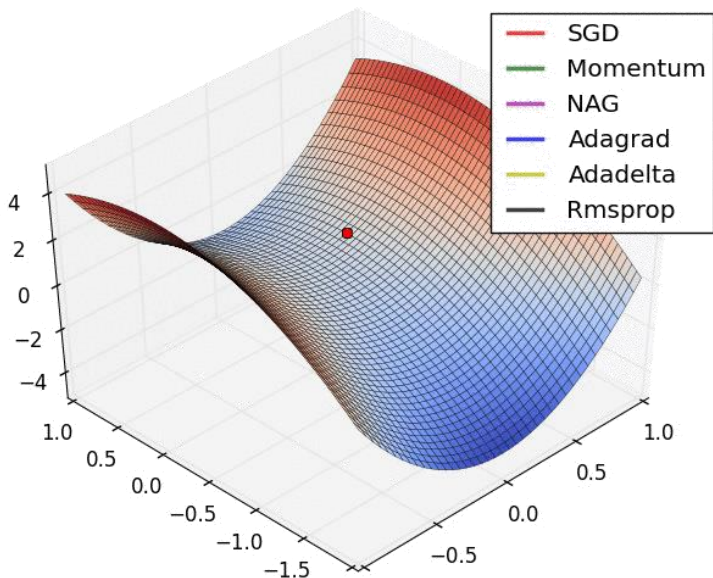


Image credit: Alec Redford

ADAM method [Kingma & Ba 2015]

ADAM = "ADaptive Moment Estimation"

$$v[t] = \beta v[t-1] + (1 - \beta) \nabla(E, w[t])$$

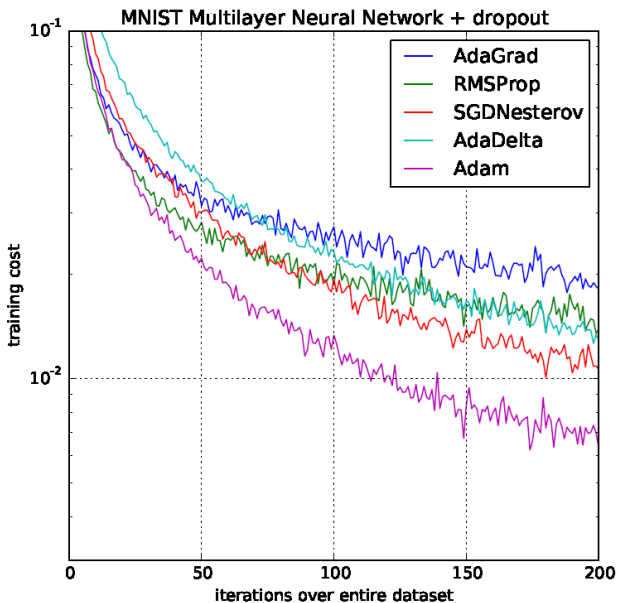
$$g[t] = \mu g[t-1] + (1 - \mu) \nabla(E, w[t]) \odot \nabla(E, w[t])$$

$$w[t+1] = w[t] - \alpha \frac{1}{\sqrt{g[t] + \epsilon}} \odot v[t]$$

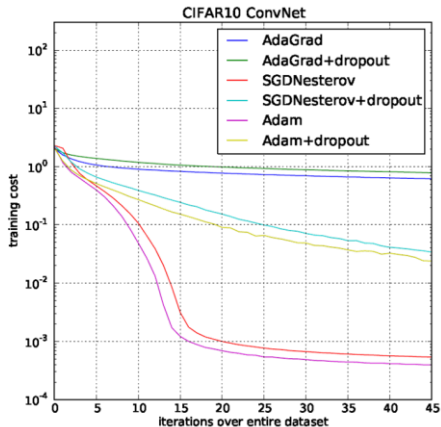
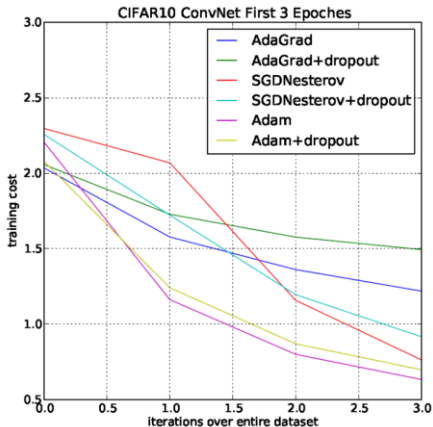
(Note: In the original image, blue annotations show the first term of the denominator is scaled by $1 - \mu^t$ and the second term by $1 - \beta^t$)

Recommended values: $\beta = 0.9$, $\mu = 0.999$, $\alpha = 0.001$, $\epsilon = 10^{-8}$

ADAM method [Kingma & Ba 2015]

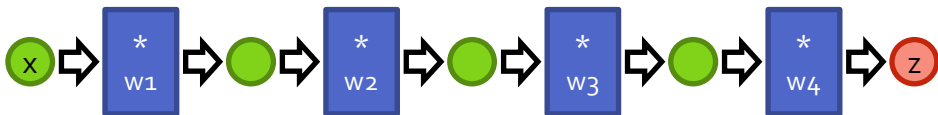


ADAM method [Kingma & Ba 2015]



Recap: optimization methods for DL

- Stochastic optimization is used always
- Optimization methods are not trying to estimate full Hessian (ignoring interaction between variables)



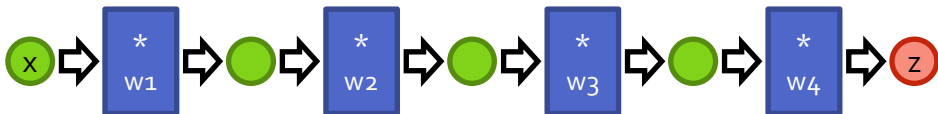
Toy example: $z = w_4 w_3 w_2 w_1 x$

$$\frac{dz}{dw_2} = w_4 w_3 w_1 x$$



Tricks for optimization of neural networks

Problems with DL optimization



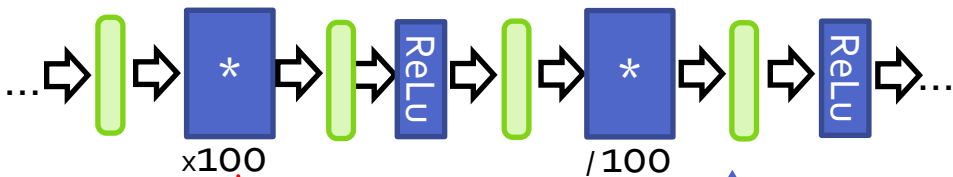
Toy example: $z = w_4 w_3 w_2 w_1 x$

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$$\frac{dz}{dw_3} = w_4 w_2 w_1 x$$

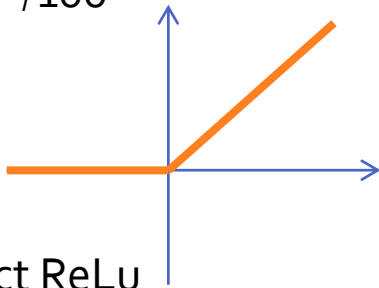
- $w = (1, 1, 1, 1)$ and $w = (1, 0.01, 100, 1)$ define the same function ("gauge freedom"), but very different derivatives
- In the first case, derivatives and values are of order 1.
- In the second case, derivatives and values are wildly different

Gauge freedom in ReLu Networks



$$\alpha > 0$$

$$1/\alpha \text{ ReLu}(\alpha x) = \text{ReLu}(x)$$



Thus: we can easily construct ReLu networks with **different** weights implementing the **same** function

Normalizing in the toy example



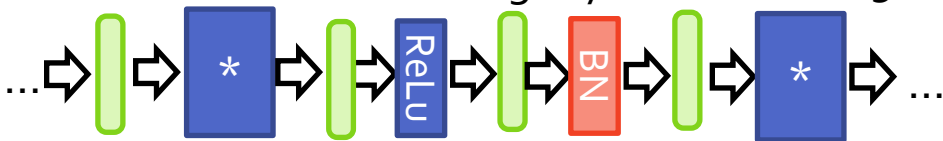
Toy example:
$$z_i = w_4 w_3 \frac{w_2 w_1 x_i}{\frac{1}{N} \sum_{j=1}^N w_2 w_1 x_j}$$

$$\left[\frac{dz}{dw_3} \right]^i = w_4 \frac{w_2 w_1 x_i}{\frac{1}{N} \sum_{j=1}^N w_2 w_1 x_j}$$

- Now, increasing w_2 or w_1 100x times will not change the partial derivative w.r.t. w_3 !
- The learning will become more stable

Batch normalization

[Szegedy and Ioffe 2015]



- Makes the training process invariant to some re-parameterizations
- Eliminates the bulk of cross-layer correlation between derivatives (off-diagonal Hessian vals)
- Use mini-batch statistics at training time to ensure that neuron activations are distributed “nicely” and the learning proceeds

Batch normalization layer

Input: Values of x over a mini-batch: $\mathcal{B} = \{x_{1...m}\}$;

Parameters to be learned: γ, β

Output: $\{y_i = \text{BN}_{\gamma, \beta}(x_i)\}$

covariant to reparameterization → $\mu_{\mathcal{B}} \leftarrow \frac{1}{m} \sum_{i=1}^m x_i$ // mini-batch mean

→ $\sigma_{\mathcal{B}}^2 \leftarrow \frac{1}{m} \sum_{i=1}^m (x_i - \mu_{\mathcal{B}})^2$ // mini-batch variance

$$\hat{x}_i \leftarrow \frac{x_i - \mu_{\mathcal{B}}}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}} \quad // \text{normalize}$$

$$y_i \leftarrow \gamma \hat{x}_i + \beta \equiv \text{BN}_{\gamma, \beta}(x_i) \quad // \text{scale and shift}$$

learnable by SGD

[Szegedy and Ioffe 2015]

Batch normalization layer

Input: Values of x over a mini-batch: $\mathcal{B} = \{x_1 \dots x_m\}$;

Parameters to be learned: γ, β

Output: $\{y_i = \text{BN}_{\gamma, \beta}(x_i)\}$

$$\mu_{\mathcal{B}} \leftarrow \frac{1}{m} \sum_{i=1}^m x_i \quad // \text{ mini-batch mean}$$

$$\sigma_{\mathcal{B}}^2 \leftarrow \frac{1}{m} \sum_{i=1}^m (x_i - \mu_{\mathcal{B}})^2 \quad // \text{ mini-batch variance}$$

$$\hat{x}_i \leftarrow \frac{x_i - \mu_{\mathcal{B}}}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}} \quad // \text{ normalize}$$

$$y_i \leftarrow \gamma \hat{x}_i + \beta \equiv \text{BN}_{\gamma, \beta}(x_i) \quad // \text{ scale and shift}$$

- At training time mean and variance are estimated per batch
- At test time, usually (running) averages over the dataset are used
- At test time, batch norm can be “merged in”
- For small batches, this is a big test \leftrightarrow train mismatch ☹

Solutions to train-test mismatch:

- Keep training time behavior
- Switch to test behavior and fine-tune

Alternatives to BatchNorm

- Layer Norm [Ba et al. NIPS'16], Instance Norm [Ulyanov et al. Arxiv16], Group renorm [Wu and He, ECCV18] – normalize over statistics of certain specific groups of variables **within** the same sample
- Batch Renorm [Ioffe NIPS'17]: gradually switch between train and test time behavior during training
- Weight norm [Salimans and Kingma NIPS'16]: decouple direction and magnitude of weight matrices

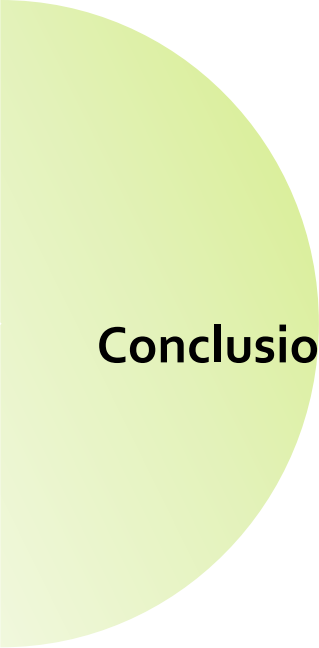
Initialization schemes

- **Basic idea 1:** units should be initialized to have comparable total input weights
- **Basic idea 2:** use layers which keep magnitude (otherwise both forwardprop and backprop will suffer from explosion/attenuation to zero; normalization layers solve this issue)
- E.g. [Glorot&Bengio 2010] aka “Xavier-initialization”:

$$W \sim U\left[-\frac{\sqrt{6}}{\sqrt{n_j + n_{j+1}}}, \frac{\sqrt{6}}{\sqrt{n_j + n_{j+1}}}\right]$$

- E.g. [He et al, Arxiv15] for ReLu networks:

$$W \sim \mathcal{N}(0, \sqrt{2/n_i})$$



Conclusions

Recap

- Batch SGD optimization is used in large-scale setting
- Advanced SGD methods use running averages to smooth and rescale SGD steps
- Normalization layers are important and used in most modern deep architectures

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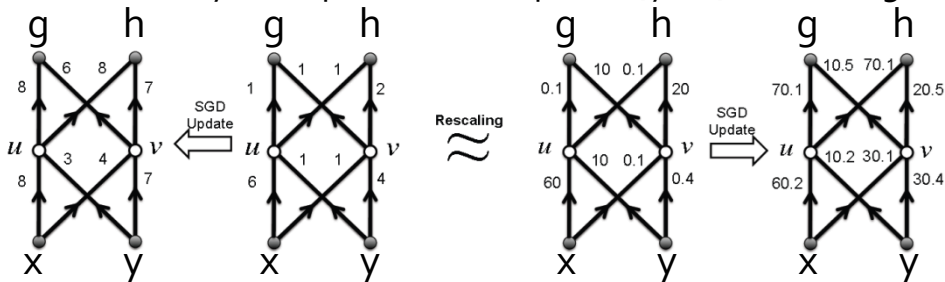
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Initialization schemes

One more toy example: 1 SGD step for $(x,y = 1,1)$ and $L = g+h$



[Neyshabur, Salakhutdinov, Srebro, Path-SGD: Path-Normalized Optimization in Deep Neural Networks, NIPS2015]

Units of measurements

- Let our coordinates be measured in meters. What is the unit of measurement for gradients?
Assume unitless function...
- (Stochastic) gradient descent is inconsistent.
- Newton method is consistent.



Adadelta method [Zeiler 2012]

$$g[t] = \mu g[t-1] + (1 - \mu) \nabla(E, w[t]) \odot \nabla(E, w[t])$$

$$w[t+1] = w[t] - \frac{\sqrt{d[t]} + \epsilon}{\sqrt{g[t]} + \epsilon} \odot \nabla(E, w[t])$$

$$d[t+1] = \mu d[t] + (1 - \mu) (w[t+1] - w[t]) \odot (w[t+1] - w[t])$$

- No step length parameter (good!)
- Correct units within the updates