Deep learning models & how to train them

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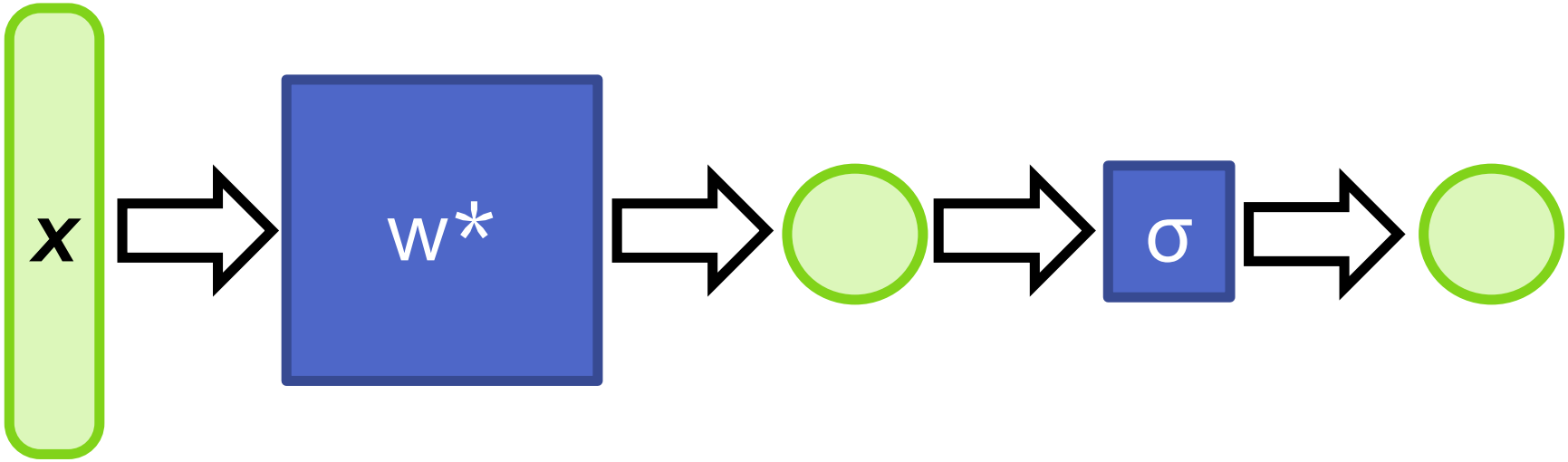
Slides mostly by Viktor Lempitsky

Logistic regression recap

Recap: Logistic regression

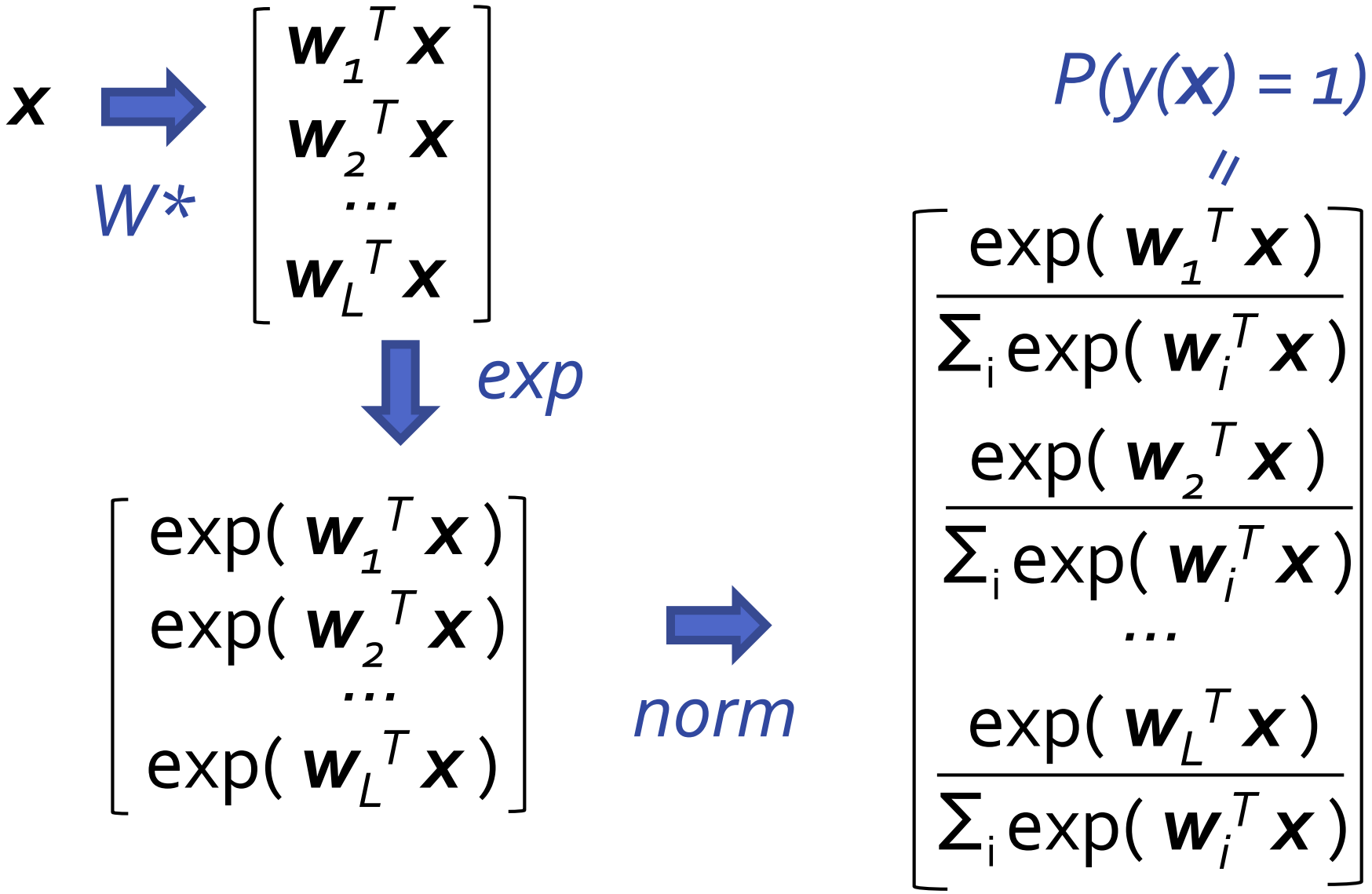


$$P(y(\boldsymbol{x}_i) = y_i|\boldsymbol{w}) = \frac{1}{1+\exp(-y_i\boldsymbol{w}^T\boldsymbol{x}_i)} = \sigma(y_i\boldsymbol{w}^T\boldsymbol{x}_i)$$

The loss function for the logistic regression

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

Softmax: a sigmoid generalization for L-class classification



Multinomial logistic loss

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

Multinomial log loss is a generalizes logistic loss:

$$E(w) = -\sum_i \log P(y(x_i) = y_i) =$$

$$= -\sum_i \left[w_{y_i}^T x_i - \log \sum_j \exp w_j^T x_i \right]$$

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

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

Few notes on logistic regression

- Convex optimization problem.
  Exercise: check that Hessian is positive definite

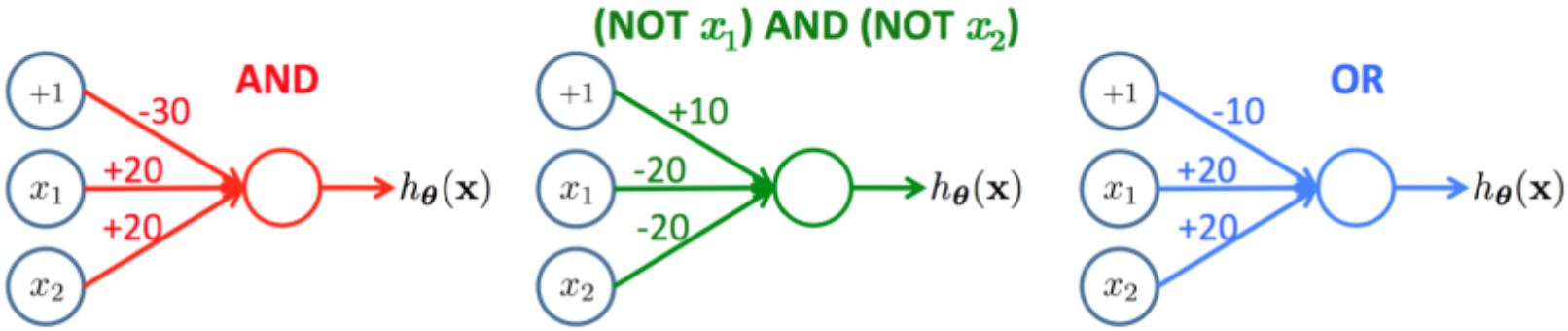
- Requires regularization for parameters: **on** by default in sklearn

- Admits multiclass classification

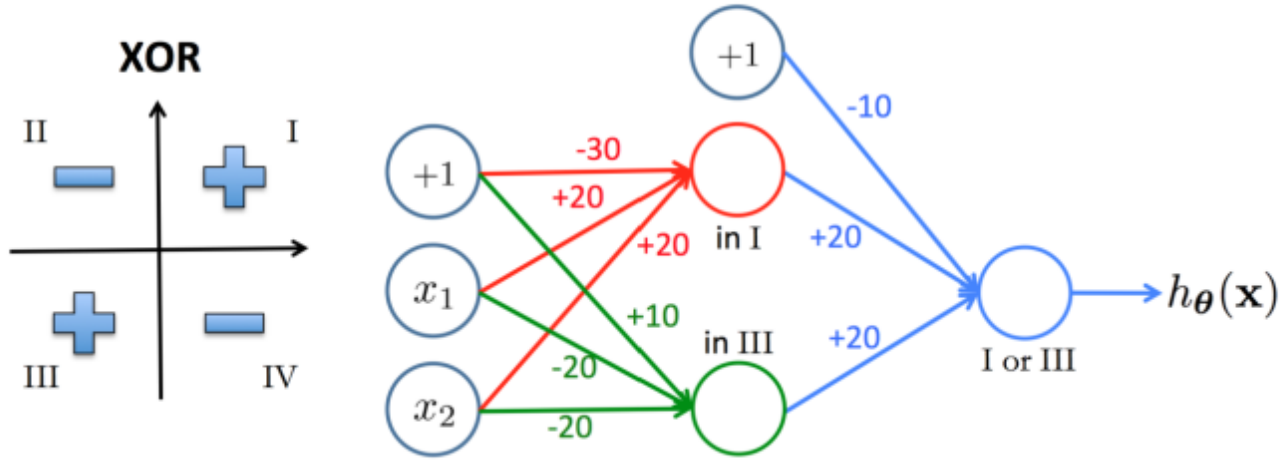
- Logistic regression is a generalized linear model (GLM) & a one-layer neural network

Capabilities are limited: need more layers

Building blocks:

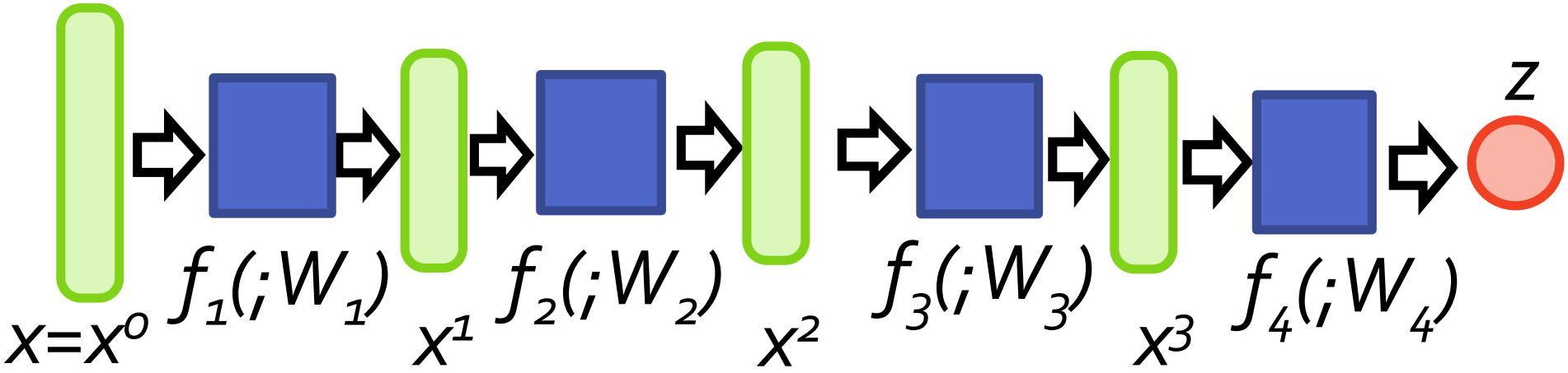


XOR function:



Fully connected neural networks

Multilayer fully-connected (FC) neural network

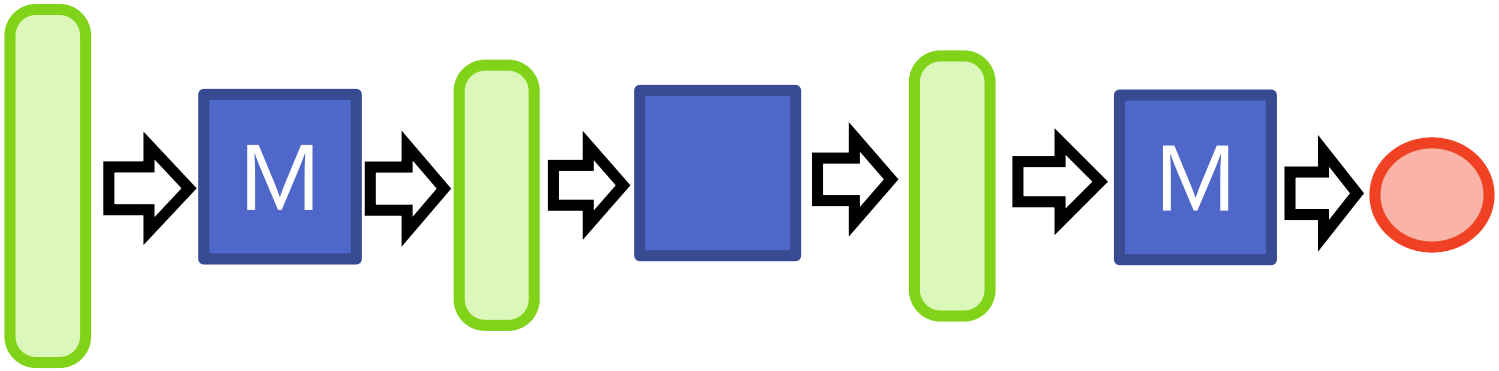


Input units

Hidden units

Output unit

Universal approximation theorem



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

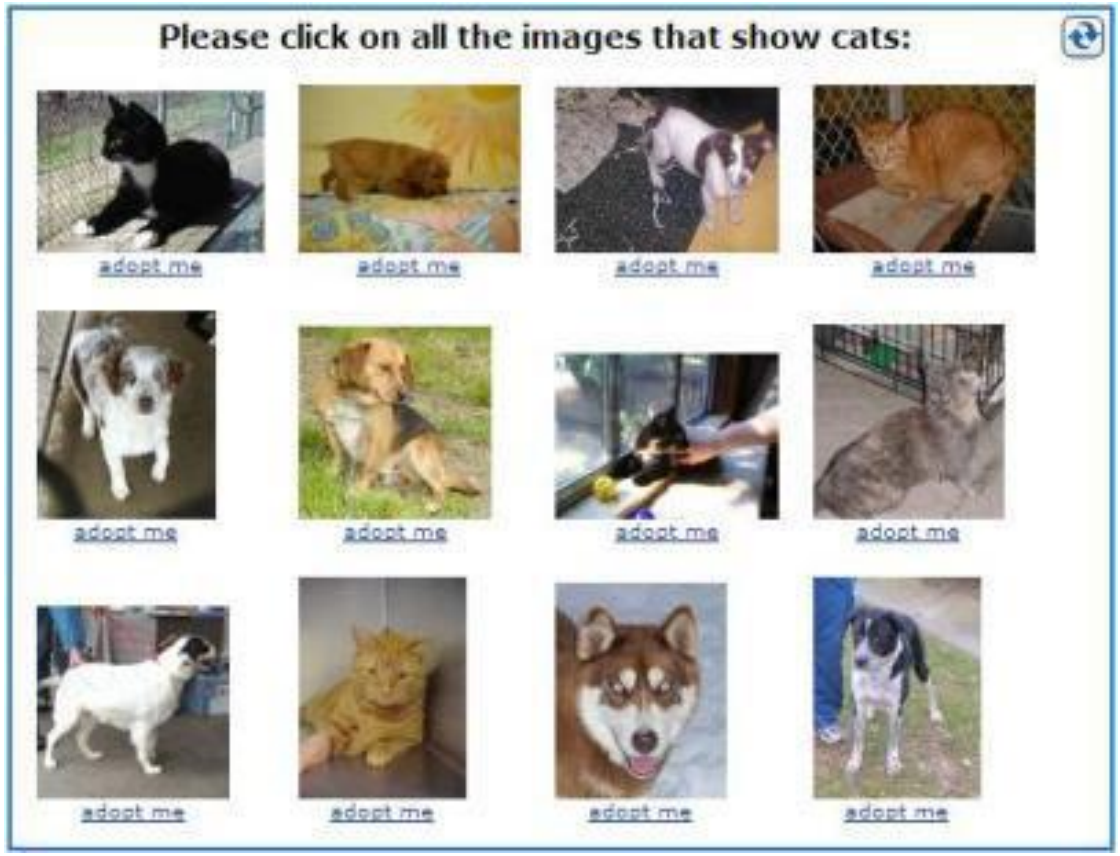
Caveat 1: the width of the network can be a very quickly growing function of space dimension and approximation accuracy. Deeper architectures are exponentially narrower for some classes of functions [Rollnick&Tegmark 2018]

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

asirra



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

#	Δ1w	Team Name * in the money	Score	Entries	Last Submission UTC (Best – Las
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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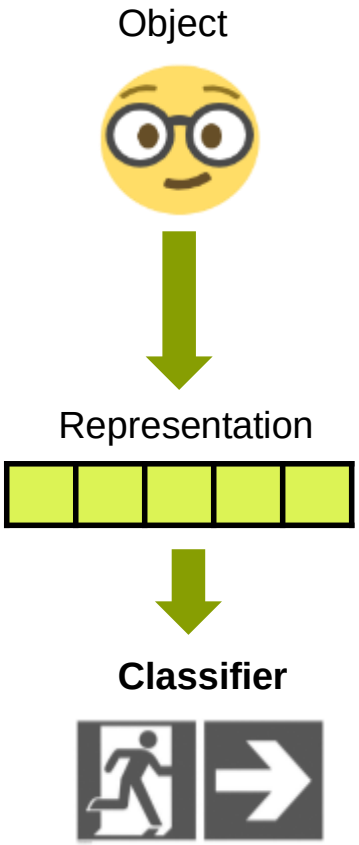
ASIRRA

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

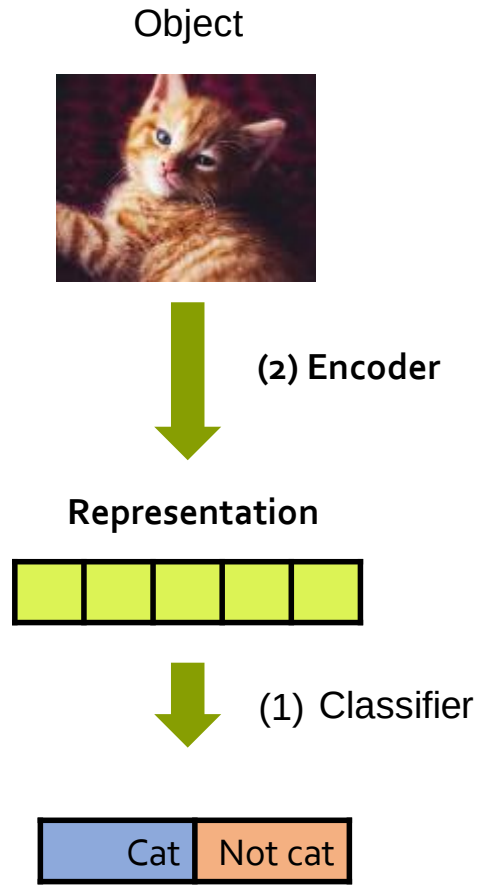
Classic Machine learning, where representations are available

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

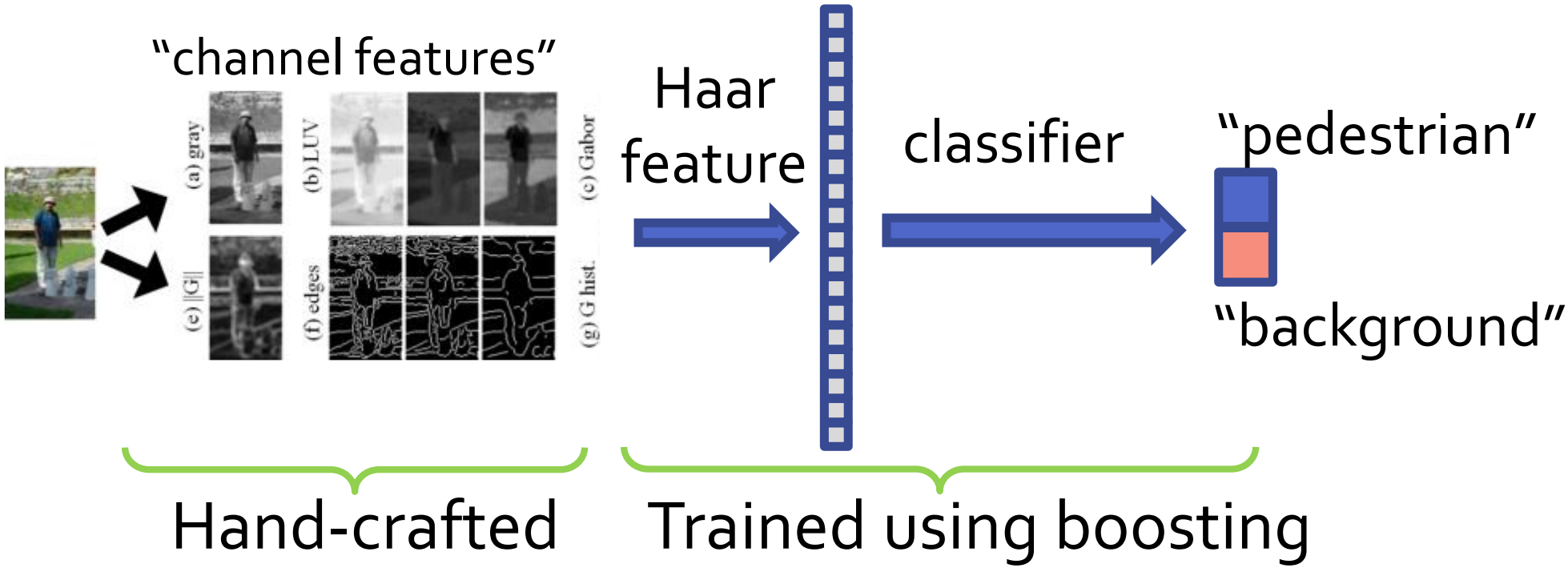


For structured data we need representation learning

u – an object	An image
y – true label	Cat breed? (1)
x(u) – an object representation	NA (2)
Problem**s**: (1) train a model that can identify the true class for *y;* **(2) learn a representation**	A neural network: Encoder + 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 machine learning recap

Optimization for supervised ML

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

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

Small scale setting: traditional optimization

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

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

Gradient descent

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

$$\frac{dE(\boldsymbol{w})}{d\boldsymbol{w}} = \frac{1}{N}\sum_{i=1}^{N} \frac{dl(\boldsymbol{x}_i, y_i, \boldsymbol{w})}{d\boldsymbol{w}} + \lambda \frac{dR(\boldsymbol{w})}{d\boldsymbol{w}},$$

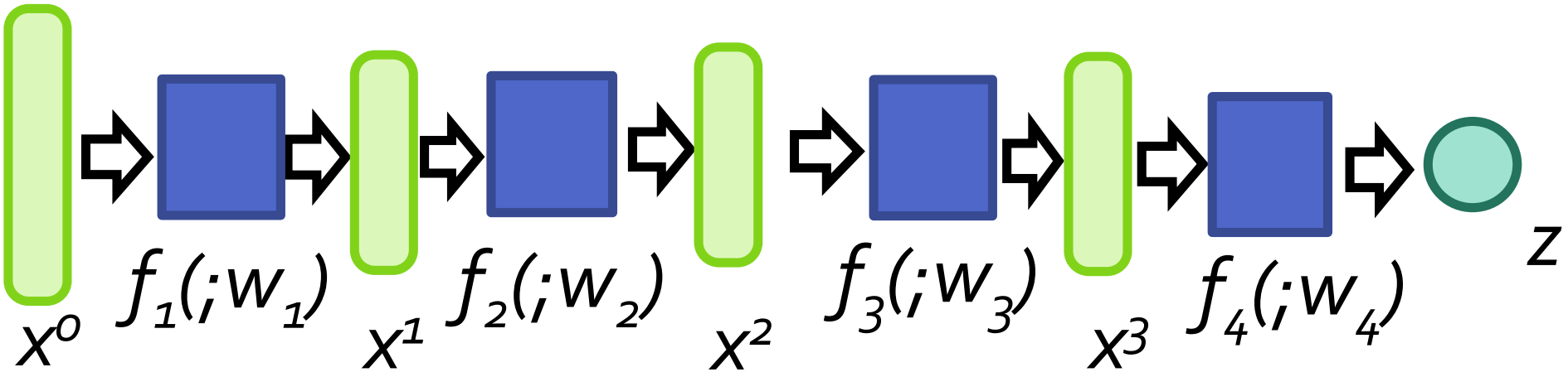
$$\boldsymbol{w}^{t+1} = \boldsymbol{w}^{t} - \alpha \frac{dE(\boldsymbol{w})}{d\boldsymbol{w}}\Big|_{w=w^t}$$

Sequential computation: *backpropagation*

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

$$\frac{dz}{dw_3} = \frac{dx^3}{dw_3}^T \cdot \frac{dz}{dx^3} \qquad \frac{dz}{dx^2} = \frac{dx^3}{dx^2}^T \cdot \frac{dz}{dx^3}$$

$$\frac{dz}{dw_1} = \frac{dx^1}{dw_1}^T \cdot \frac{dz}{dx^1} \qquad \frac{dz}{dx^0} = \frac{dx^1}{dx^0}^T \cdot \frac{dz}{dx^1}$$



Optimization for deep learning

Large-scale learning

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

$$\frac{dE(\boldsymbol{w})}{d\boldsymbol{w}} = \frac{1}{N}\sum_{i=1}^{N} \frac{dl(\boldsymbol{x}_i, y_i, \boldsymbol{w})}{d\boldsymbol{w}} + \lambda \frac{dR(\boldsymbol{w})}{d\boldsymbol{w}}$$

- 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:

$$\frac{dE(\boldsymbol{w})}{d\boldsymbol{w}} = \frac{1}{N}\sum_{i=1}^{N}\frac{dl(\boldsymbol{x}_i, y_i, \boldsymbol{w})}{d\boldsymbol{w}} + \lambda\frac{dR(\boldsymbol{w})}{d\boldsymbol{w}}$$

Stochastic gradient:

$$\frac{dE^i}{d\boldsymbol{w}} = \frac{dl(\boldsymbol{x}_i, y_i, \boldsymbol{w})}{d\boldsymbol{w}} + \lambda\frac{dR(\boldsymbol{w})}{d\boldsymbol{w}}$$

Stochastic gradient is an unbiased estimate of the gradient:

$$\frac{dE}{d\boldsymbol{w}} = \frac{1}{N}\sum_{i=1}^{N}\frac{dE^i}{d\boldsymbol{w}}$$

Gradient descent (GD)

GD:

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

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

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

Stochastic gradient descent (SGD)

SGD:

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

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:

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

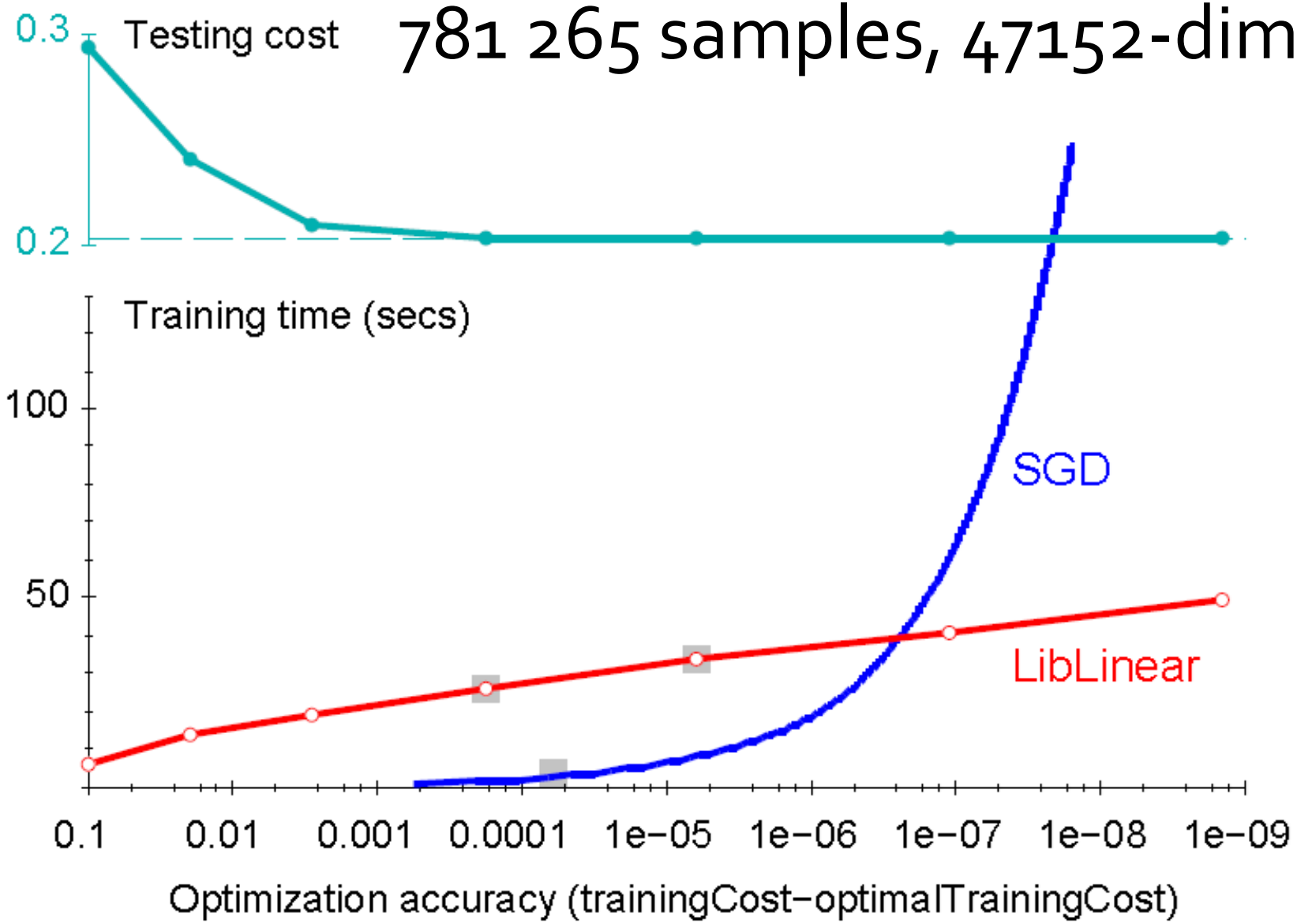
- One sweep over training data is called an **epoch**
- Popular choices for schedule $\alpha[t]$:
  - constant, e.g. $\alpha[t] = 0.0001$
  - piecewise constant, e.g. $\alpha[t]$ is decreased tenfold every N epochs
  - harmonic, e.g. $\alpha[t] = 0.001 / ([t/N] + 10)$

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 is a subset of indexes:

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

Batch stochastic gradient:

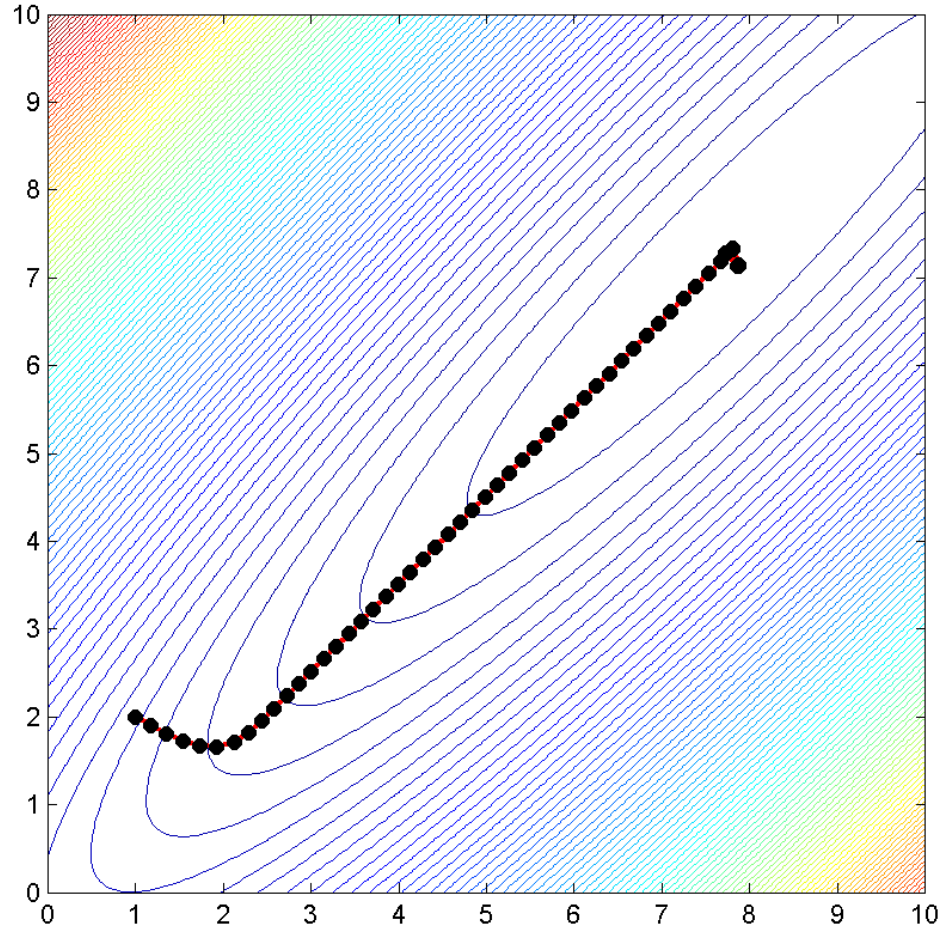
$$\frac{dE}{dw} = \frac{1}{N_b}\sum_{i=1}^{N_b}\frac{dl(x_{b(i)}, y_{b(i)}, w)}{dw} + \lambda\frac{dR}{dw}$$

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

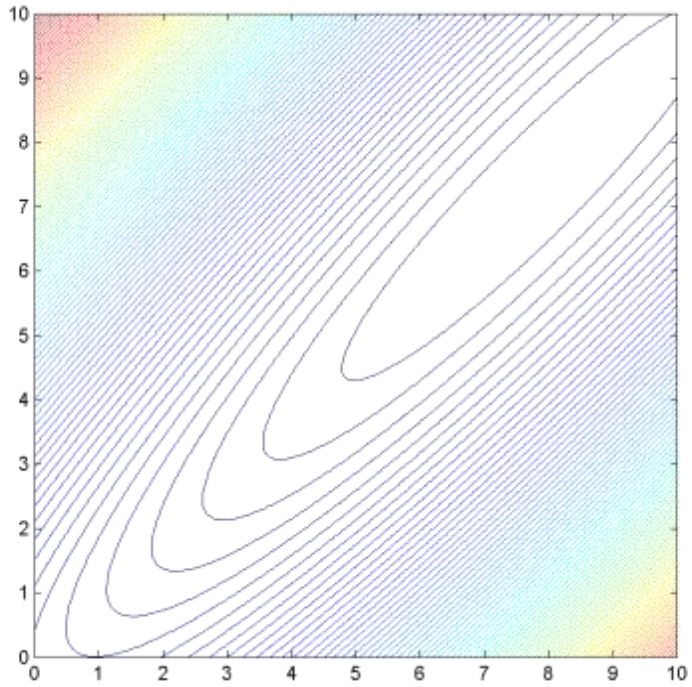
SGD inherits gradient descent problems

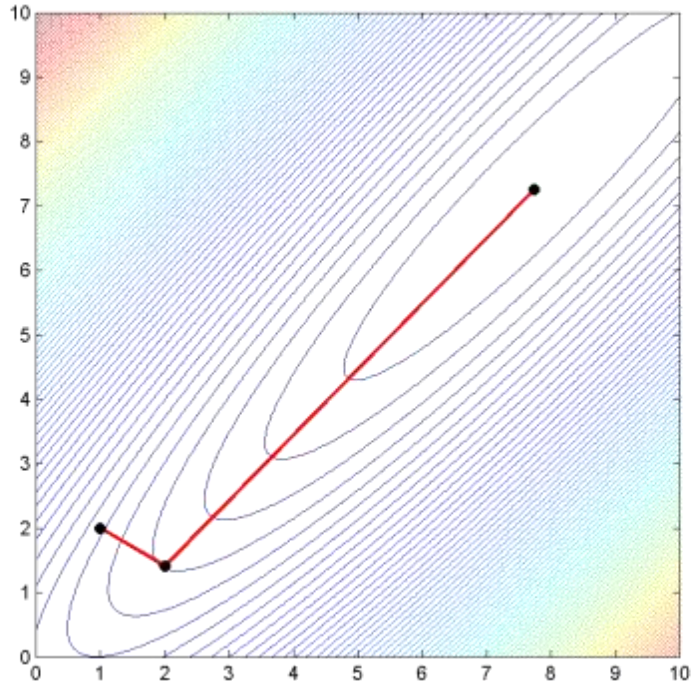


- Gradient descent is very poor “in ravines”
- SGD is no better

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*):

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

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

Typical $\mu = 0.9$

Exponentially decaying running average

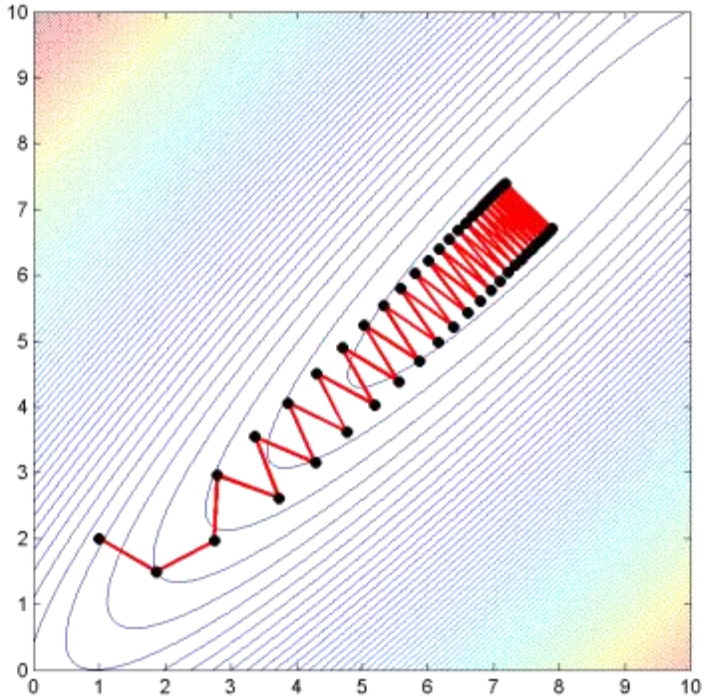
$$v[t] = \mu\, v[t-1] - \alpha[t]\, \nabla(E, w[t])$$
$$w[t+1] = w[t] + v[t]$$

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

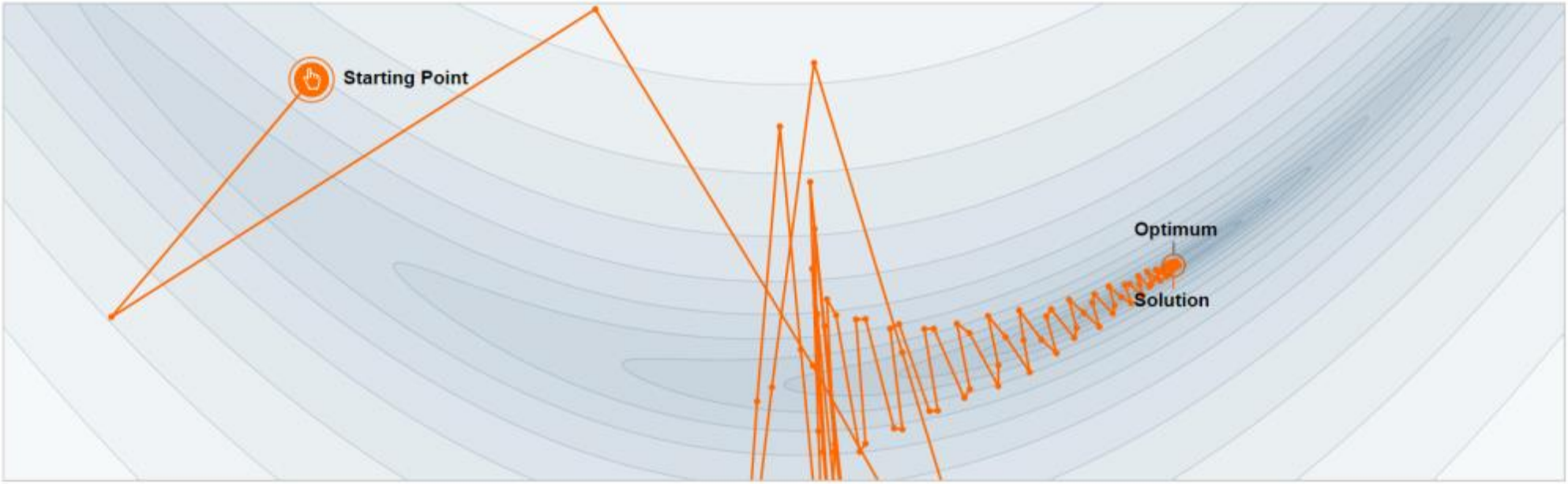
Momentum: why it works

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

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



The effect of the momentum



Step-size α = 0.0051

0 0.003 0.006

Momentum β = 0.90

0.00 0.500 0.990

We often think of Momentum as a means of dampening oscillations and speeding up the iterations, leading to faster convergence. But it has other interesting behavior. It allows a larger range of step-sizes to be used, and creates its own oscillations. What is going on?

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

[Goh, Distill 2017]

Simplified case: quadratic problem, no momentum

$$E(\boldsymbol{w}) = \frac{1}{2}\boldsymbol{w}^T A\boldsymbol{w} - \boldsymbol{b}^T\boldsymbol{w},$$

A is a positive-definite matrix with eigenvalues $\{\lambda_1, \dots, \lambda_d\}$

$$E\left(\boldsymbol{w}^k\right) - E(\boldsymbol{w}^*) = \sum(1 - \alpha\lambda_i)^{2k}\lambda_i\left[w_i^0\right]^2,$$

$$\text{rate}(\alpha) = \max\{|1 - \alpha\lambda_1|, |1 - \alpha\lambda_d|\},$$

$$\text{rate}(\alpha^*) = \frac{2}{\lambda_1 + \lambda_n}, \alpha^* = \frac{\lambda_n/\lambda_1 - 1}{\lambda_n/\lambda_1 + 1}$$

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

[Goh, Distill 2017]

Simplified case: quadratic problem with momentum

$$\text{rate}(\alpha, \beta) = \max\{|\sigma_1|, |\sigma_2|\},$$

σ_1, σ_2 are eigenvalues of the matrix R:

$$\text{R} = (\beta, \lambda_i; -\alpha\beta, 1 - \alpha\lambda_i)$$

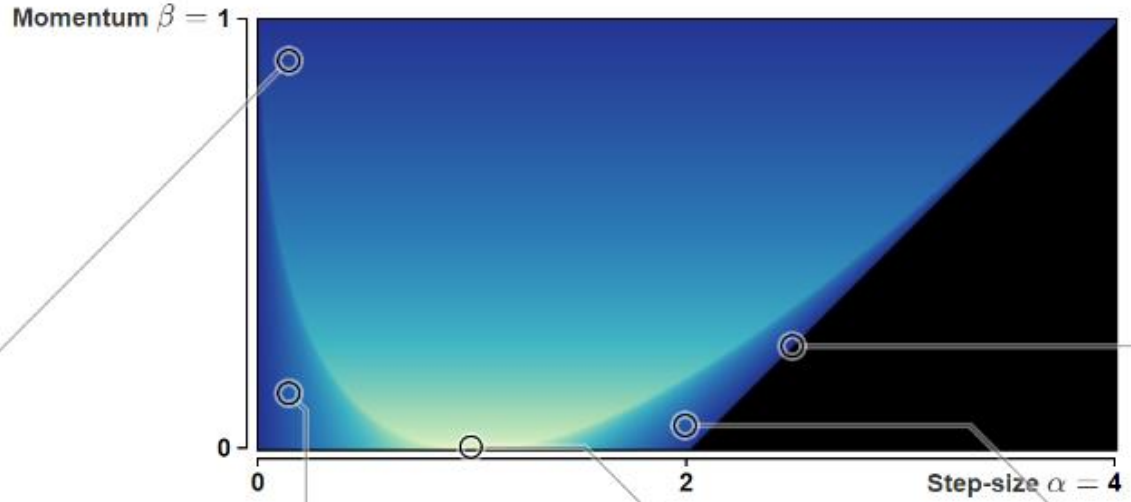
A bit more complex, but e.g. converges is observed for

$$0 < \alpha\lambda_i < 2 + 2\beta, \beta \in [0, 1)$$

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

[Goh, Distill 2017]

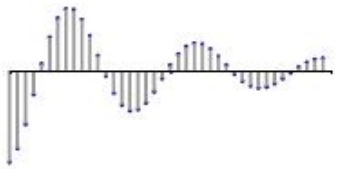
Phase space along a single eigenvector



Convergence Rate

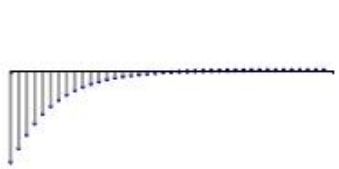
A plot of $\max\{|\sigma_1|, |\sigma_2|\}$ reveals distinct regions, each with its own style of convergence.

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

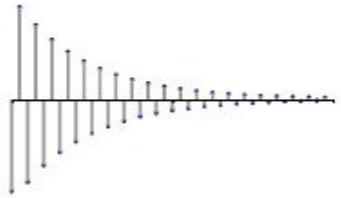


R's eigenvalues are both real, are positive, and have norm less than one. The behavior here resembles gradient descent.

1-Step Convergence

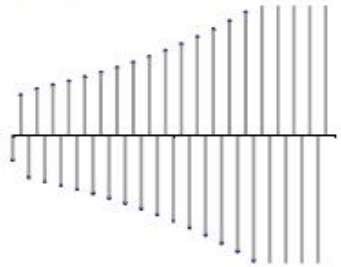
When $\alpha = 1/\lambda_i$, and $\beta = 0$, we converge in one step. This is a very special point, and kills the error in the eigenspace completely.

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.

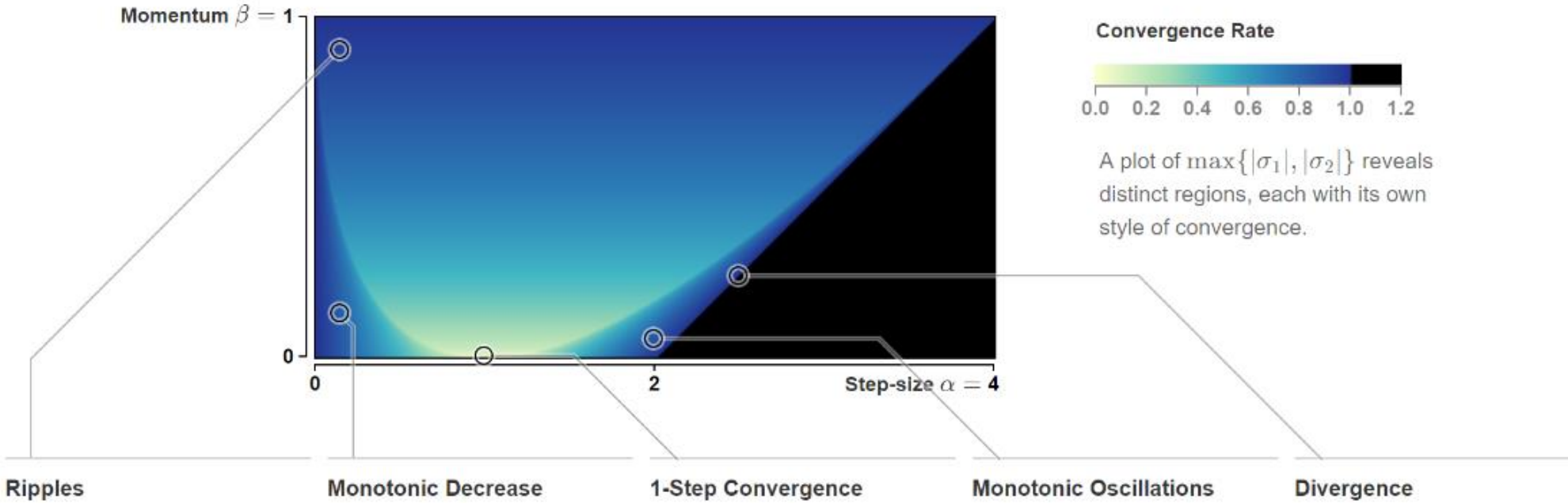
Divergence



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

[Goh, Distill 2017]

Momentum: multiple eigenvalues



Optimal rate & momentum:

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

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:

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

In real network we do not know eigenvalues and their change with iterations, so:

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

[Goh, Distill 2017]

Nesterov accelerated gradient

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

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:

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

(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

Recap from statistics

Let us define the Fisher information matrix

$$I(\boldsymbol{w}) = -\mathrm{E}\left[\frac{\partial^2}{\partial \boldsymbol{w}^2} \log f(\boldsymbol{x}, y|\boldsymbol{w}) \,\middle|\, \boldsymbol{w}\right],$$

where $\mathrm{E}(\mathbf{w}) = f(\boldsymbol{x}, y|\boldsymbol{w})$ is the likelihood for a given data point (e.g. scaled squared error)

Under regularity conditions, it holds that

$$I_{ij}(\boldsymbol{w}) = \mathrm{E}\left[\frac{\partial}{\partial w_i} \log f(\boldsymbol{x}, y|\boldsymbol{w}) \frac{\partial}{\partial w_j} \log f(\boldsymbol{x}, y|\boldsymbol{w}) \,\middle|\, \boldsymbol{w}\right].$$

- The first form is the Hessian for our problem
- We can use sample-based estimates instead
- We can look only at the first derivatives

Adagrad method [Duchi et al. 2011]

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

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

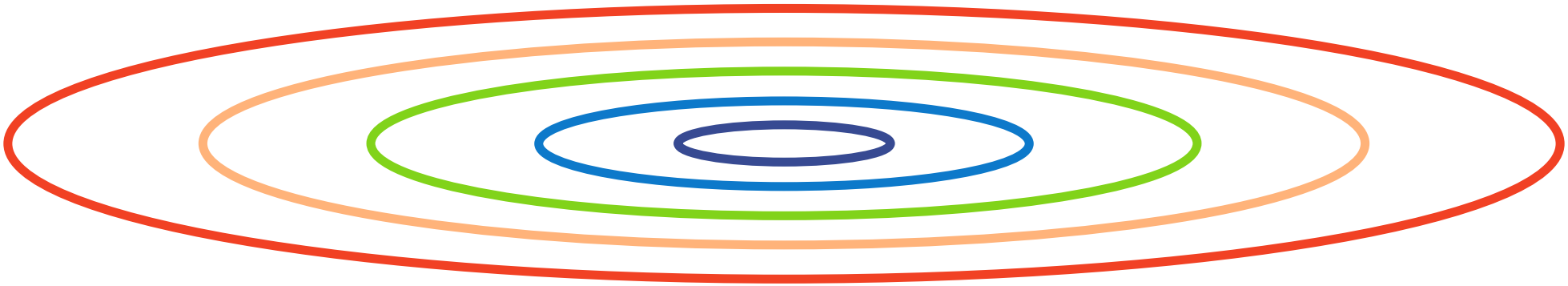
$$w[t+1] = w[t] - \frac{\alpha}{\sqrt{g[t] + \epsilon}} \odot \nabla(E, w[t])$$

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

Adagrad method [Duchi et al. 2011]

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

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



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 the running average:

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

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

Comparison: logistic regression

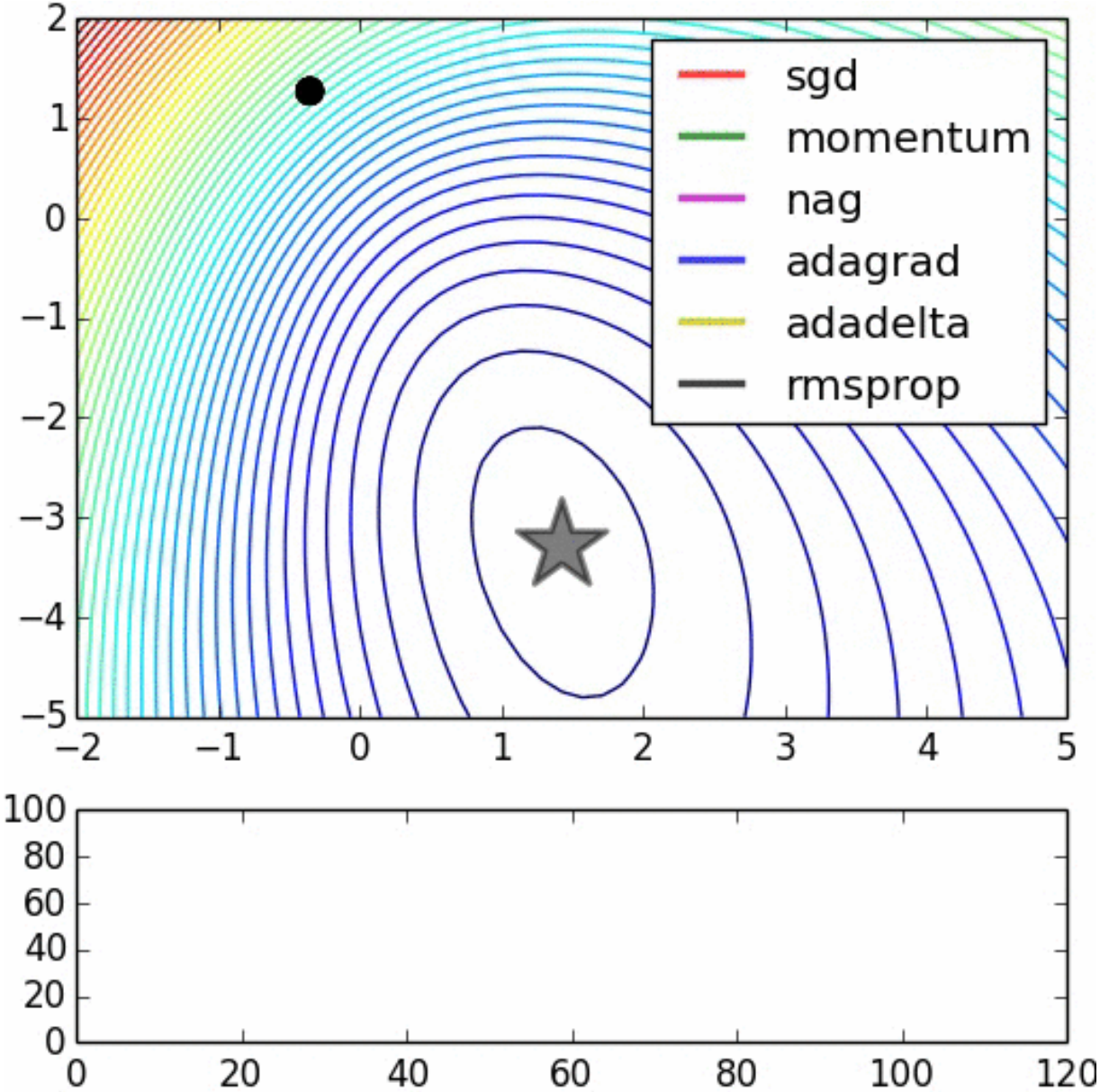


Image credit: Alec Redford

Further comparison

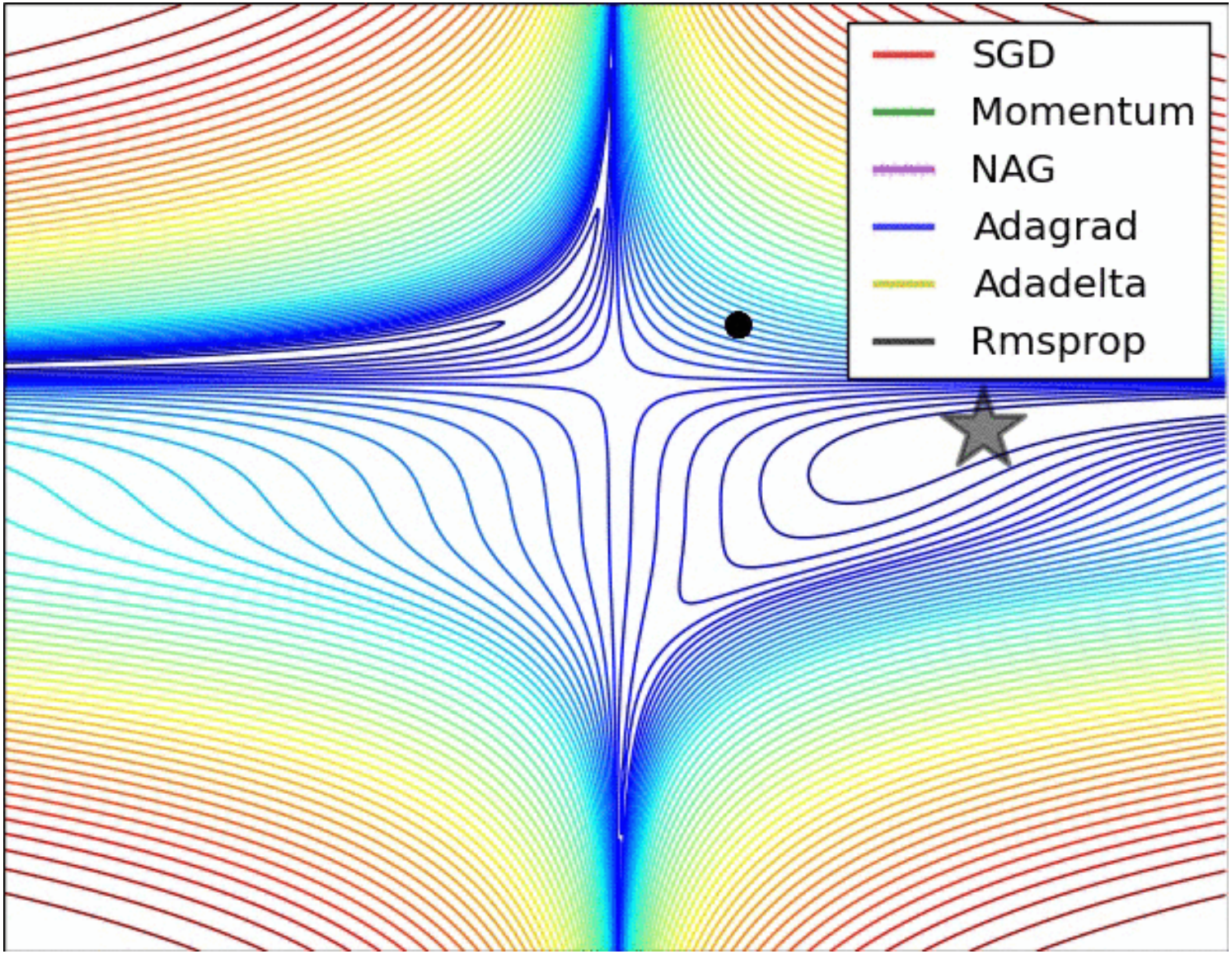


Image credit: Alec Redford

Further comparison: escaping from a saddle

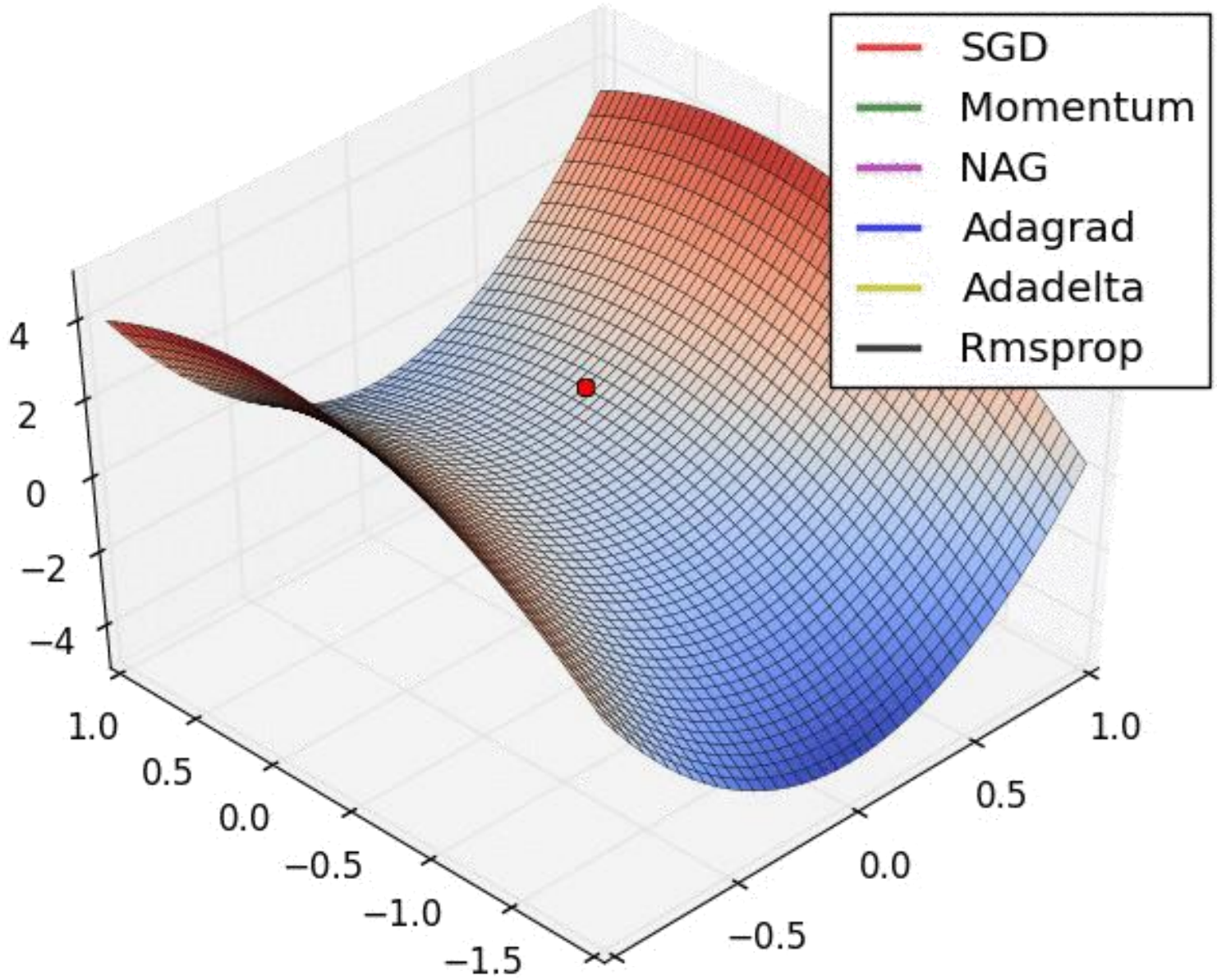


Image credit: Alec Redford

ADAM method [Kingma & Ba 2015]

ADAM = "ADAptive Moment Estimation"

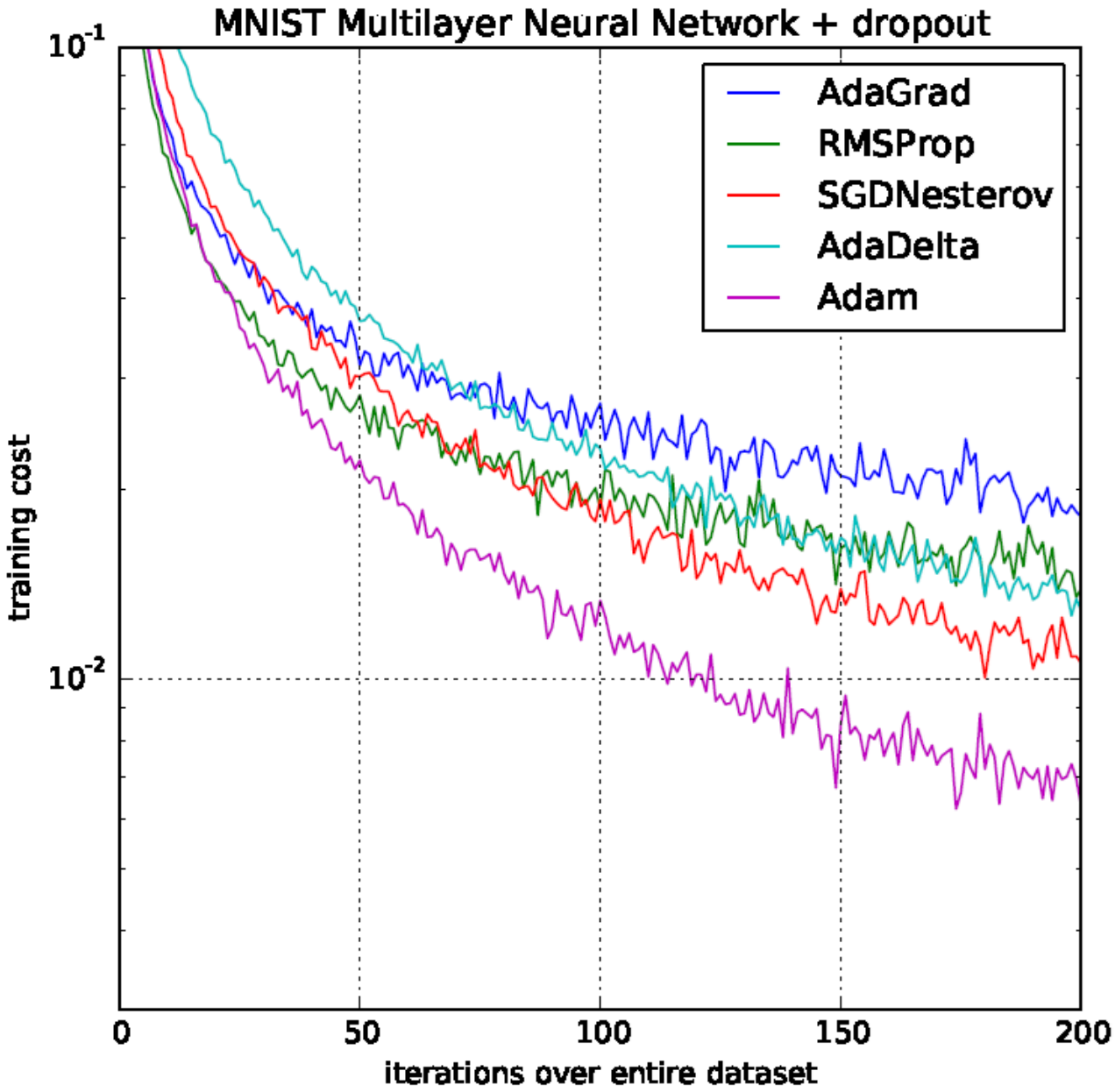
$$v[t] = \beta\, v[t\text{-}1] + (1-\beta)\,\nabla(E, w[t])$$

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

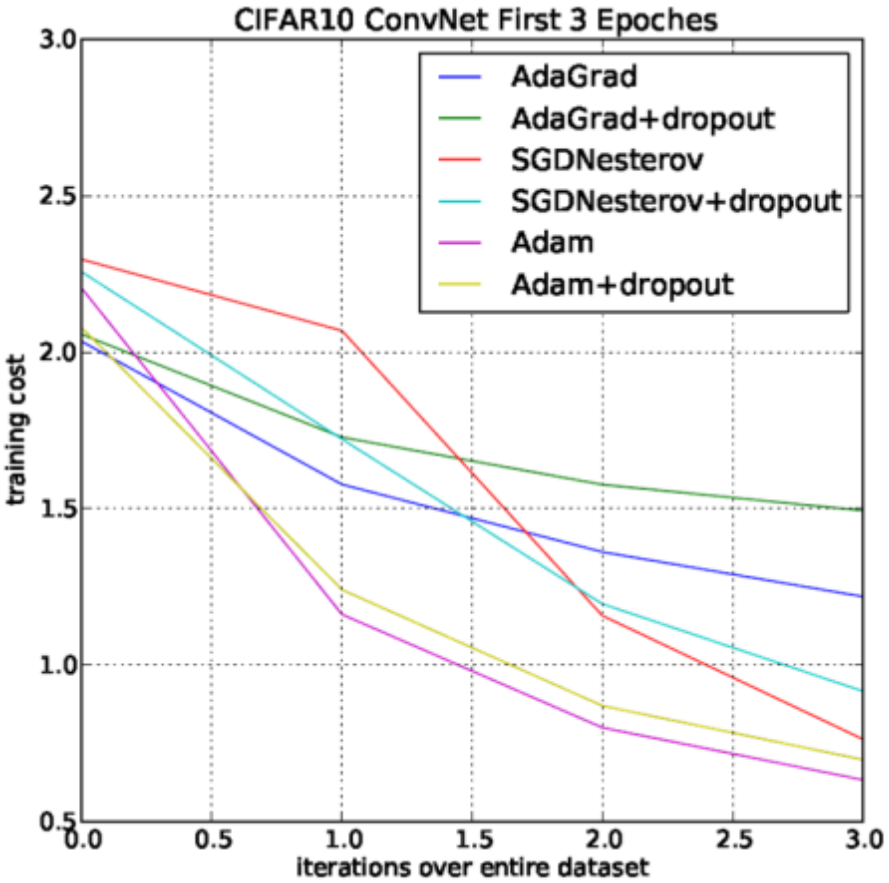
$$w[t+1] = w[t] - \alpha \frac{1}{\sqrt{g[t] + \epsilon}} \odot v[t] \Big/ \frac{1-\beta^t}{1-\mu^t}$$

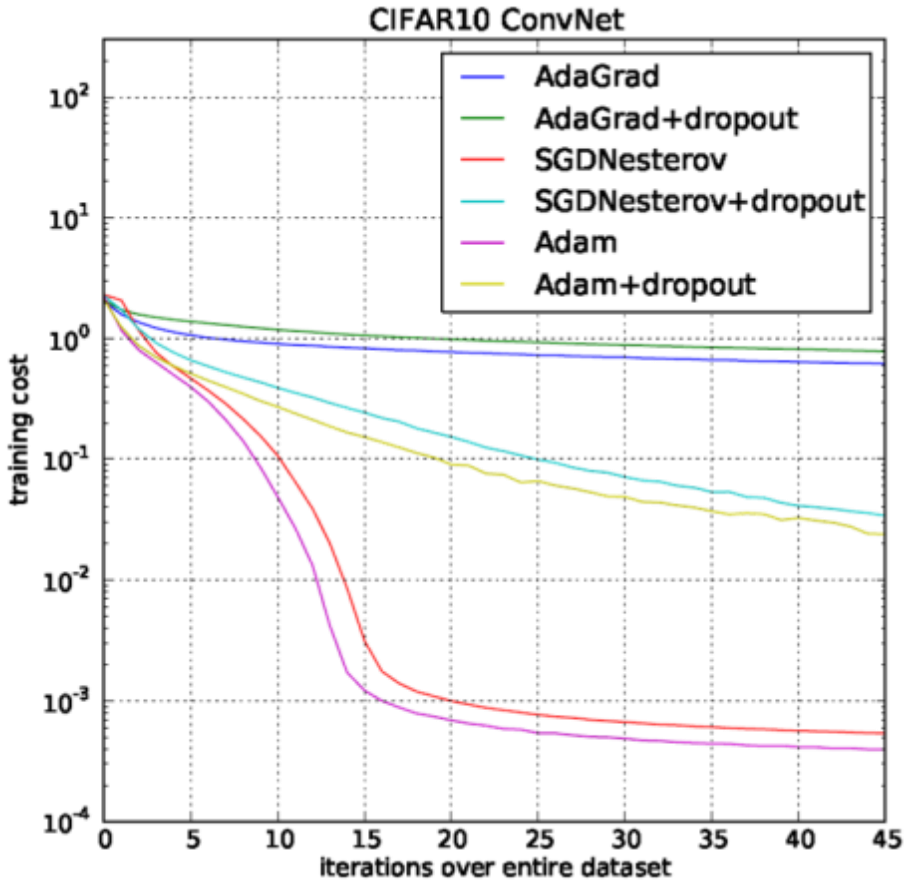
Recommended values: $\beta = 0.9$, $\mu = 0.999$, $\alpha = 0.001$, $\varepsilon = 10^{-8}$

ADAM method [Kingma & Ba 2015]



ADAM method [Kingma & Ba 2015]



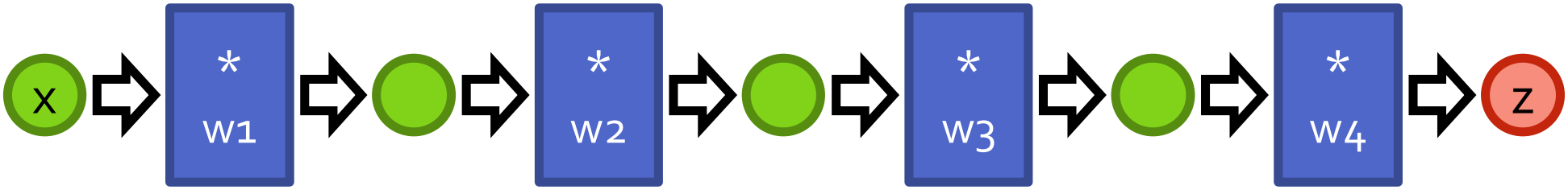


Recap: optimization methods for DL

- Stochastic optimization is used always
- Optimization methods are not trying to estimate full Hessian, ignoring interaction between variables
- ADAM is the most common option
- Also see Nesterov accelerated gradient

Tricks for optimization of neural networks

Problems with DL optimization

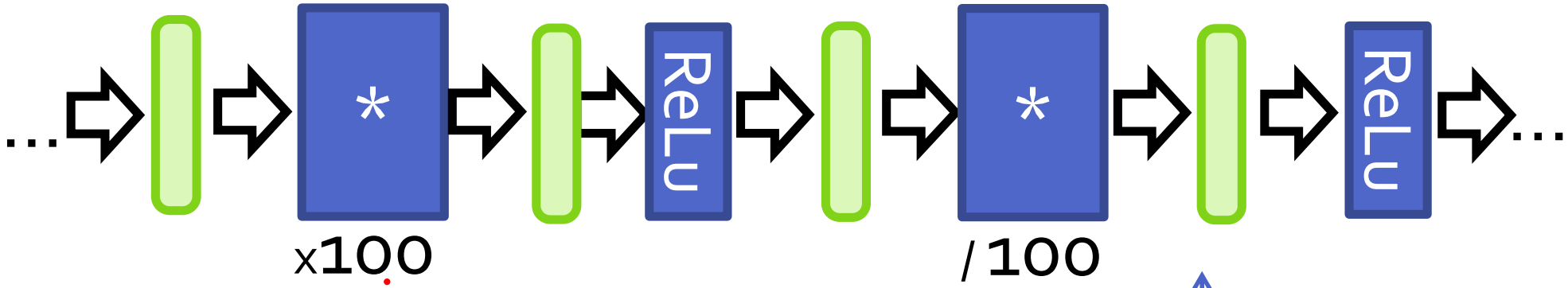


Toy example: $z = w_4\, w_3\, w_2\, w_1\, x$

$$\frac{dz}{dw_2} = w_4\, w_3\, w_1\, x \qquad \frac{dz}{dw_3} = w_4\, w_2\, w_1\, x$$

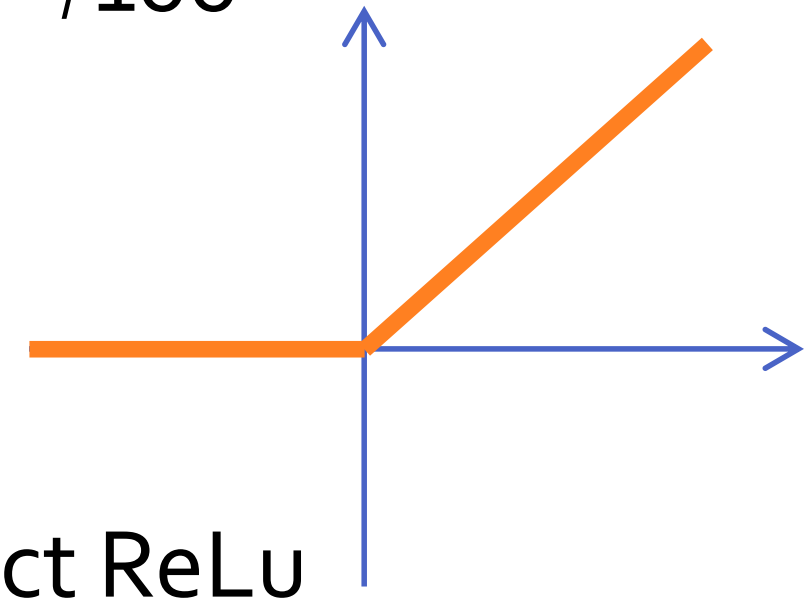
- *w = (1, 1, 1, 1)* and *w = (1,0.01,100,1)* define the same function ("gauge freedom"), but very different derivatives
- In the first case, derivatives and values are of order 1.
- In the second case, derivatives and values are wildly different

Gauge freedom in ReLu Networks



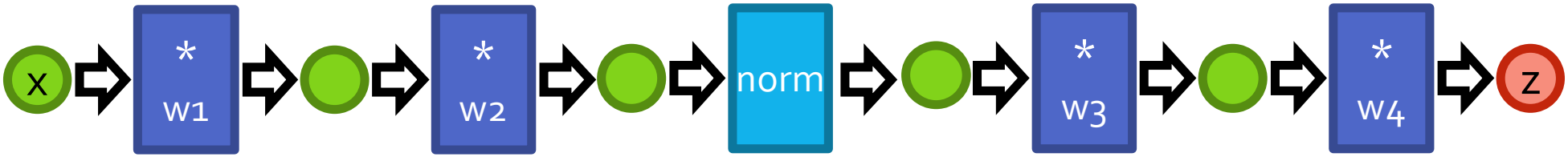
$\alpha > 0$

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



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

Normalizing in the toy example



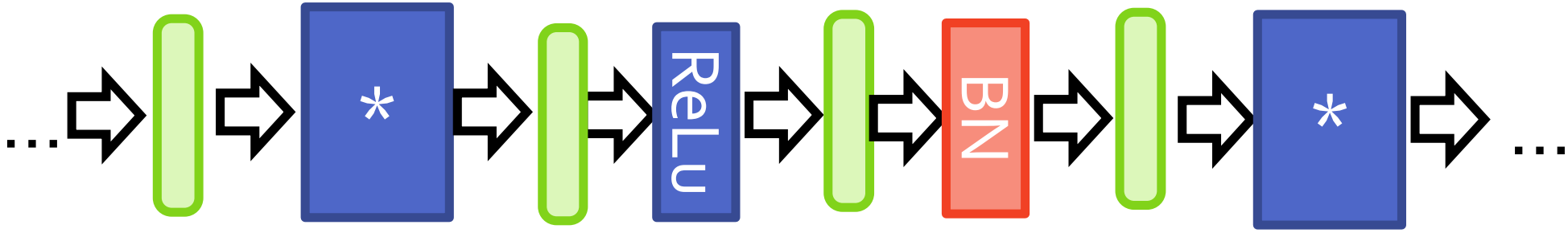
Toy example: $$z_i = w_4\, w_3\, \frac{w_2\, w_1\, x_i}{\frac{1}{N}\sum_{j=1}^{N} w_2\, w_1\, x_j}$$

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

- Now, increasing w2 or w1 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: $\{y_i = \mathrm{BN}_{\gamma,\beta}(x_i)\}$

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

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

$$\widehat{x}_i \leftarrow \frac{x_i - \mu_{\mathcal{B}}}{\sqrt{\sigma^2_{\mathcal{B}} + \epsilon}} \qquad \text{// normalize}$$

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

covariant to reparameterization

learnable by SGD

[Szegedy and Ioffe 2015]

Batch normalization layer

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

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

- 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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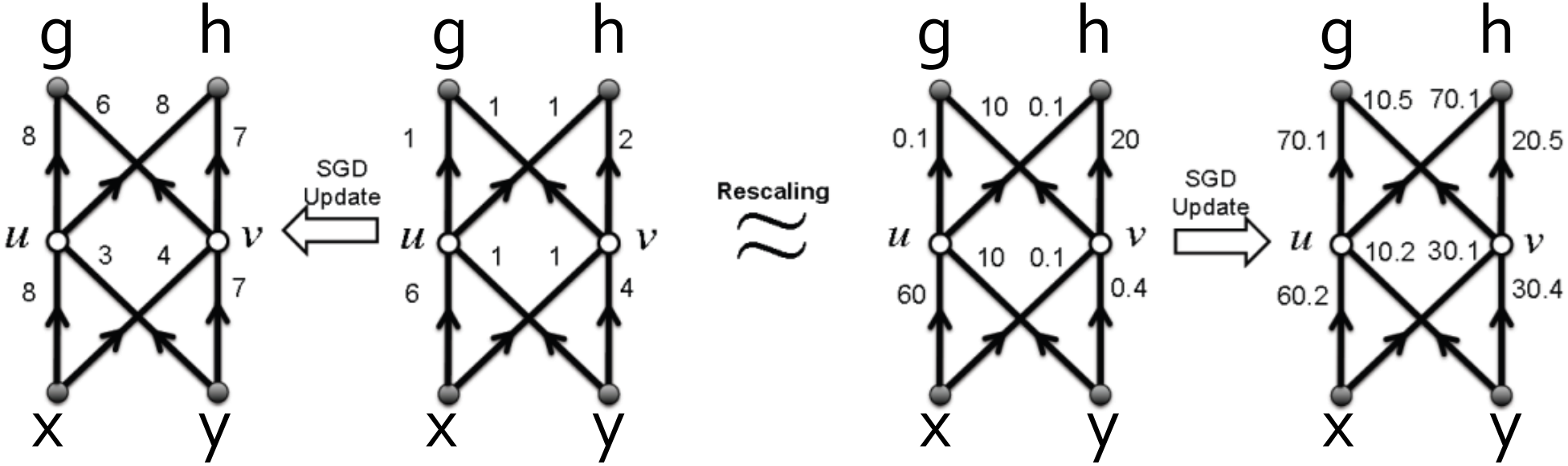
Initialization schemes

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