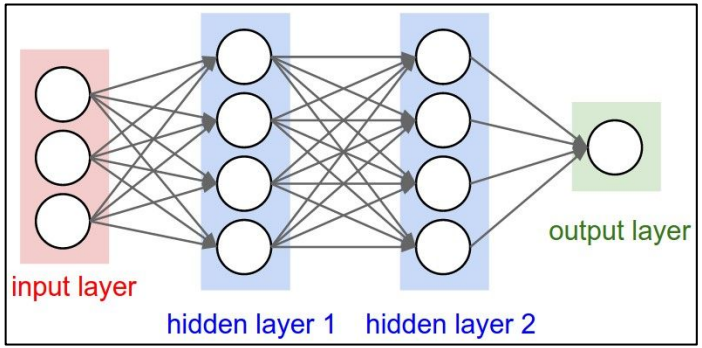
Lecture 6:

Training Neural Networks, Part 2

Mini-batch SGD

Loop:

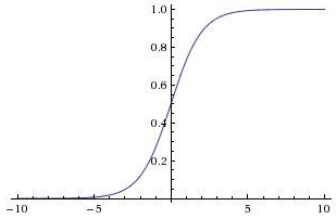
1. **Sample** a batch of data
2. **Forward** prop it through the graph, get loss
3. **Backprop** to calculate the gradients
4. **Update** the parameters using the gradient



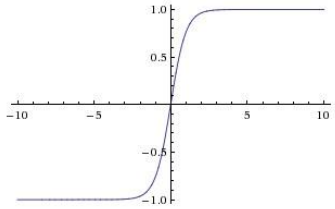
Activation Functions

Sigmoid

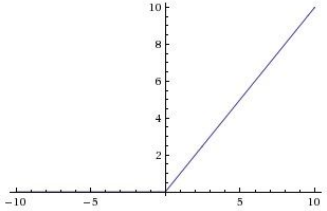
$$\sigma(x) = 1/(1+e^{-x})$$



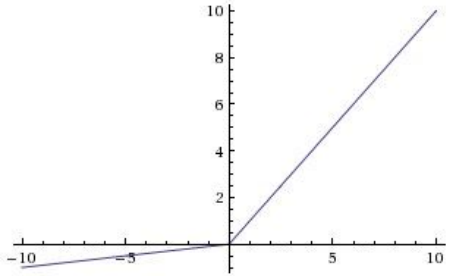
tanh tanh(x)



ReLU max(0,x)



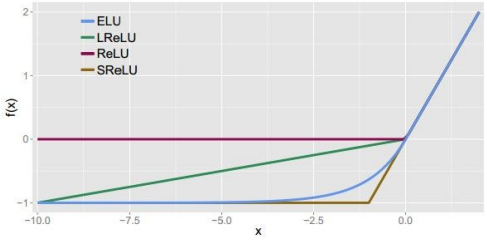
Leaky ReLU
max(0.1x, x)



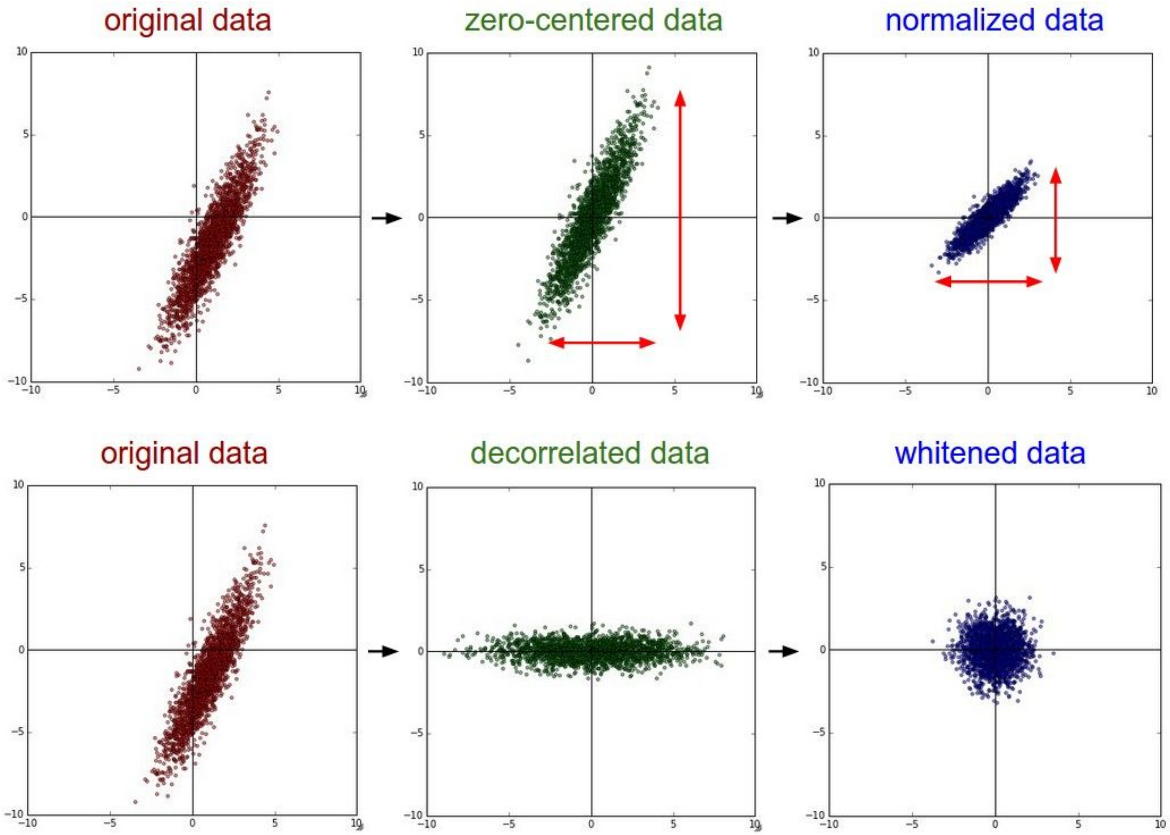
Maxout $\max(w_1^T x + b_1, w_2^T x + b_2)$

ELU

$$f(x) = \begin{cases} x & \text{if } x > 0 \\ \alpha\,(\exp(x) - 1) & \text{if } x \leq 0 \end{cases}$$



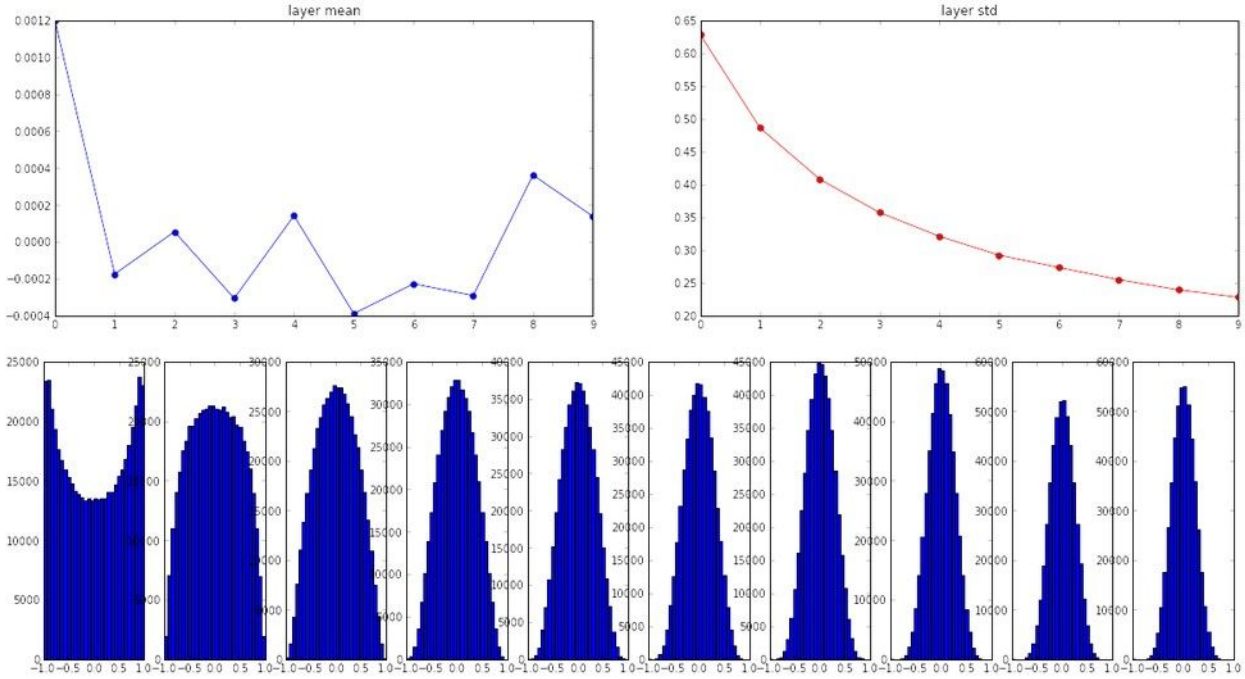
Data Preprocessing



```
input layer had mean 0.001800 and std 1.001311
hidden layer 1 had mean 0.001198 and std 0.627953
hidden layer 2 had mean -0.000175 and std 0.486051
hidden layer 3 had mean 0.000055 and std 0.407723
hidden layer 4 had mean -0.000306 and std 0.357108
hidden layer 5 had mean 0.000142 and std 0.320917
hidden layer 6 had mean -0.000389 and std 0.292116
hidden layer 7 had mean -0.000228 and std 0.273387
hidden layer 8 had mean -0.000291 and std 0.254935
hidden layer 9 had mean 0.000361 and std 0.239266
hidden layer 10 had mean 0.000139 and std 0.228008
```

```
W = np.random.randn(fan_in, fan_out) / np.sqrt(fan_in) # layer initialization
```

"Xavier initialization"
[Glorot et al., 2010]



Reasonable initialization.
(Mathematical derivation assumes linear activations)

Weight Initialization

Batch Normalization

[Ioffe and Szegedy, 2015]

Normalize:

$$\widehat{x}^{(k)} = \frac{x^{(k)} - \mathrm{E}[x^{(k)}]}{\sqrt{\mathrm{Var}[x^{(k)}]}}$$

And then allow the network to squash the range if it wants to:

$$y^{(k)} = \gamma^{(k)}\widehat{x}^{(k)} + \beta^{(k)}$$

- Improves gradient flow through the network
- Allows higher learning rates
- Reduces the strong dependence on initialization
- Acts as a form of regularization in a funny way, and slightly reduces the need for dropout, maybe

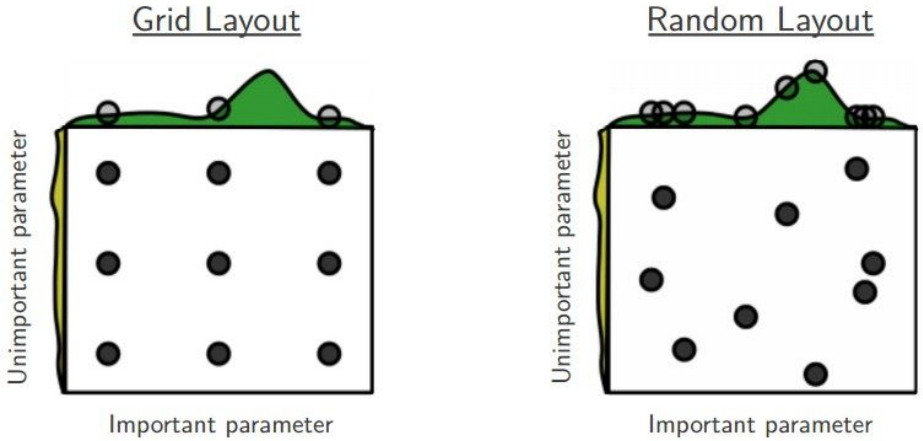
Babysitting the learning process

```
model = init_two_layer_model(32*32*3, 50, 10) # input size, hidden size, number of classes
trainer = ClassifierTrainer()
best_model, stats = trainer.train(X_train, y_train, X_val, y_val,
                                  model, two_layer_net,
                                  num_epochs=10, reg=0.000001,
                                  update='sgd', learning_rate_decay=1,
                                  sample_batches = True,
                                  learning_rate=1e-6, verbose=True)
```

```
Finished epoch 1 / 10: cost 2.302576, train: 0.080000, val 0.103000, lr 1.000000e-06
Finished epoch 2 / 10: cost 2.302582, train: 0.121000, val 0.124000, lr 1.000000e-06
Finished epoch 3 / 10: cost 2.302558, train: 0.119000, val 0.138000, lr 1.000000e-06
Finished epoch 4 / 10: cost 2.302519, train: 0.127000, val 0.151000, lr 1.000000e-06
Finished epoch 5 / 10: cost 2.302517, train: 0.158000, val 0.171000, lr 1.000000e-06
Finished epoch 6 / 10: cost 2.302518, train: 0.179000, val 0.172000, lr 1.000000e-06
Finished epoch 7 / 10: cost 2.302466, train: 0.180000, val 0.176000, lr 1.000000e-06
Finished epoch 8 / 10: cost 2.302452, train: 0.175000, val 0.185000, lr 1.000000e-06
Finished epoch 9 / 10: cost 2.302459, train: 0.206000, val 0.192000, lr 1.000000e-06
Finished epoch 10 / 10: cost 2.302420, train: 0.190000, val 0.192000, lr 1.000000e-06
finished optimization. best validation accuracy: 0.192000
```

Loss barely changing:
Learning rate is probably too low

Cross-validation



TODO

- Parameter update schemes
- Learning rate schedules
- Dropout
- Gradient checking
- Model ensembles

Parameter Updates

Training a neural network, main loop:

```
while True:
  data_batch = dataset.sample_data_batch()
  loss = network.forward(data_batch)
  dx = network.backward()
  x += - learning_rate * dx
```

Training a neural network, main loop:

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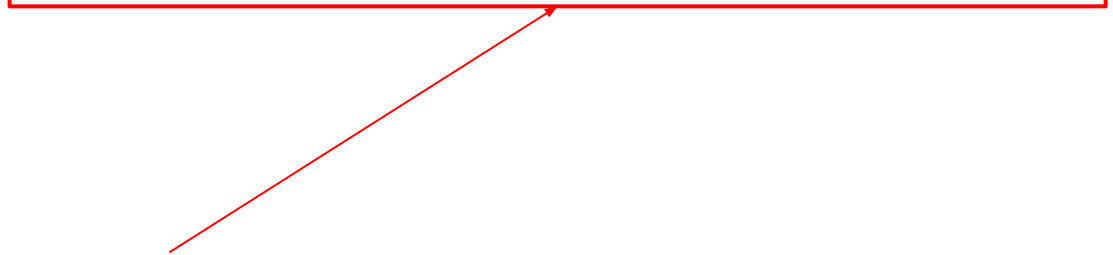


simple gradient descent update
now: complicate.

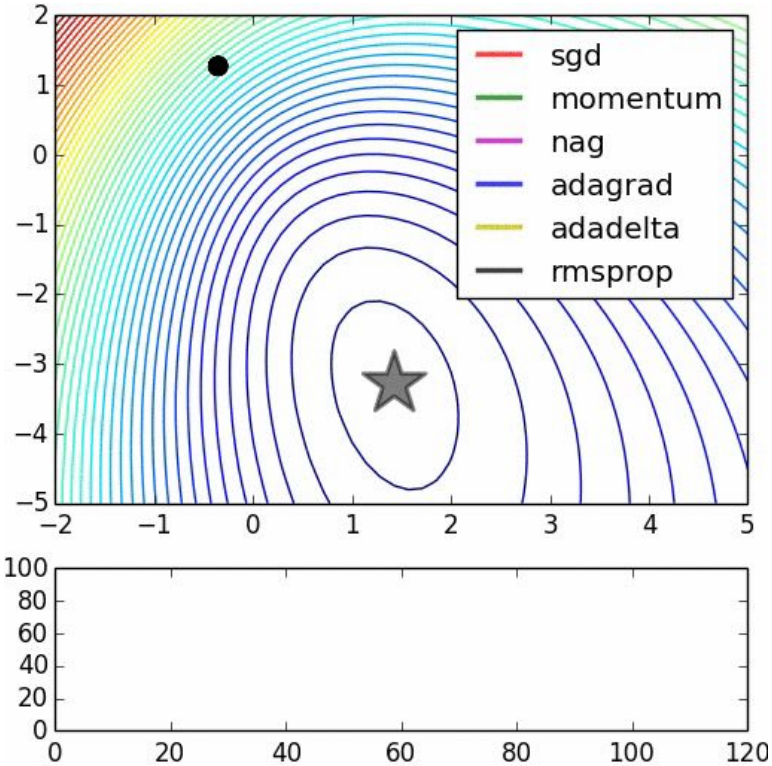
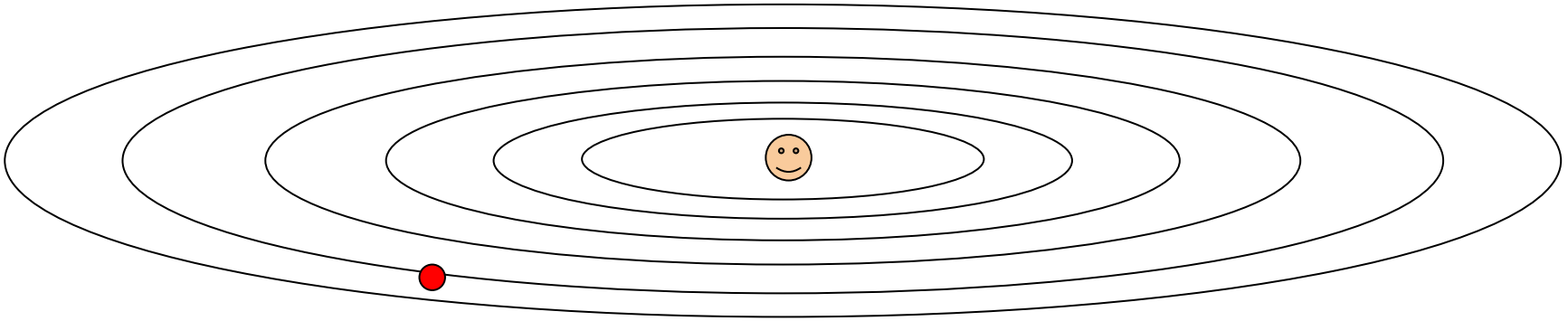


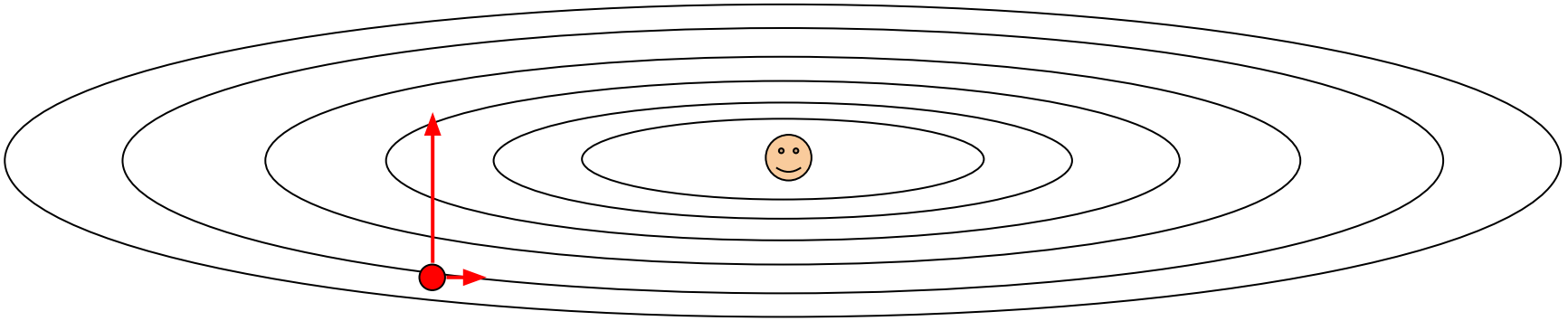
Image credits: Alec Radford

Suppose loss function is steep vertically but shallow horizontally:



Q: What is the trajectory along which we converge towards the minimum with SGD?

Suppose loss function is steep vertically but shallow horizontally:



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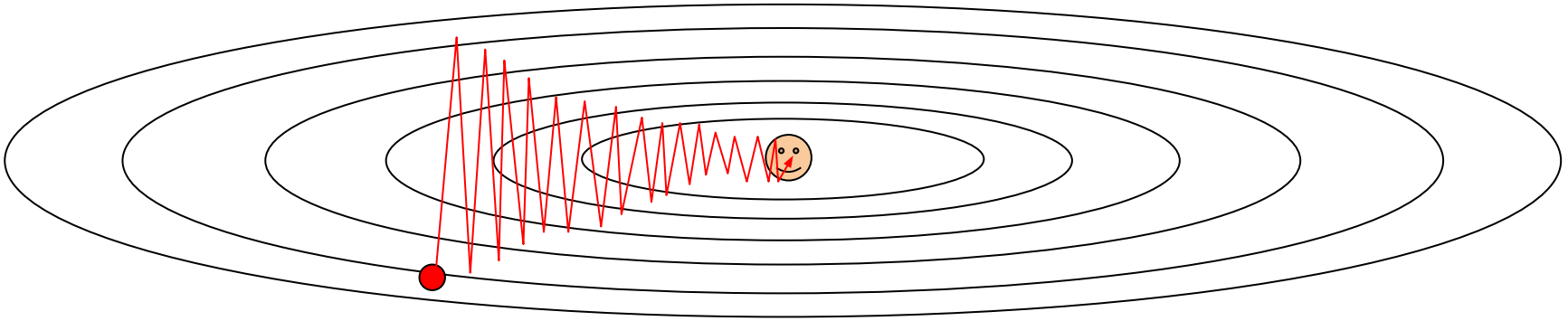


Q: What is the trajectory along which we converge towards the minimum with SGD? very slow progress along flat direction, jitter along steep one

Momentum update

```
# Gradient descent update
x += - learning_rate * dx
```

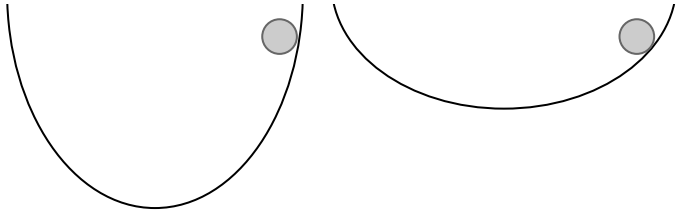


```
# Momentum update
v = mu * v - learning_rate * dx # integrate velocity
x += v # integrate position
```

- Physical interpretation as ball rolling down the loss function + friction (mu coefficient).
- mu = usually ~0.5, 0.9, or 0.99 (Sometimes annealed over time, e.g. from 0.5 -> 0.99)

Momentum update

```
# Gradient descent update
x += - learning_rate * dx
```



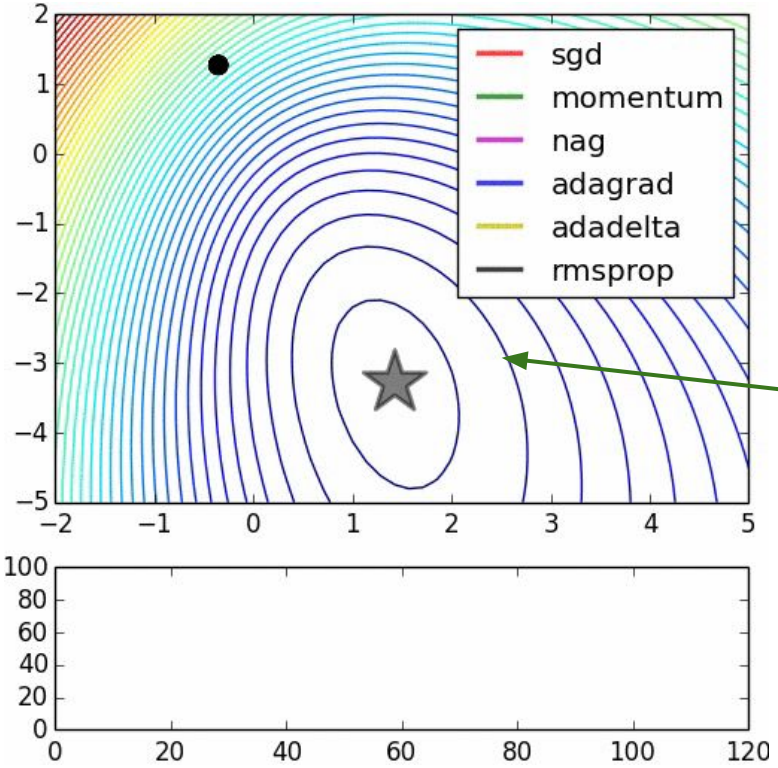
```
# Momentum update
v = mu * v - learning_rate * dx # integrate velocity
x += v # integrate position
```

- Allows a velocity to “build up” along shallow directions
- Velocity becomes damped in steep direction due to quickly changing sign

SGD

vs

Momentum

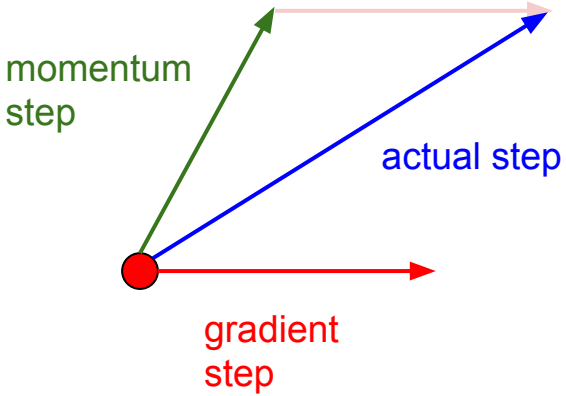


notice momentum overshooting the target, but overall getting to the minimum much faster.

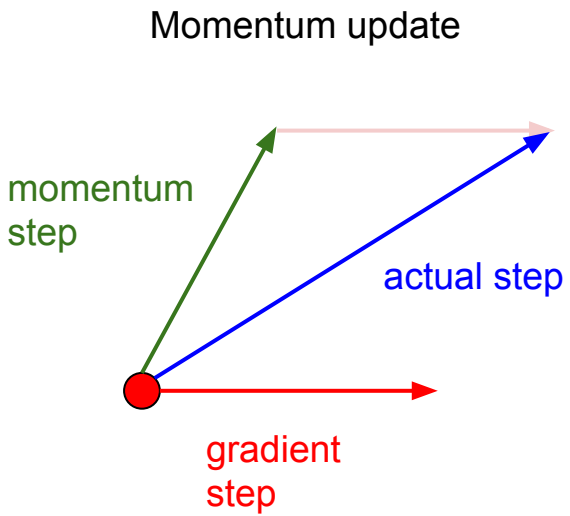
Nesterov Momentum update

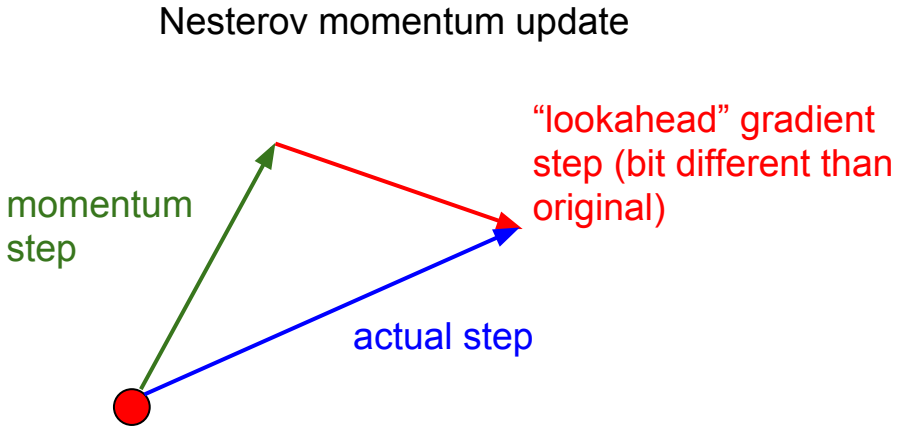
```
# Momentum update
v = mu * v - learning_rate * dx # integrate velocity
x += v # integrate position
```

Ordinary momentum update:

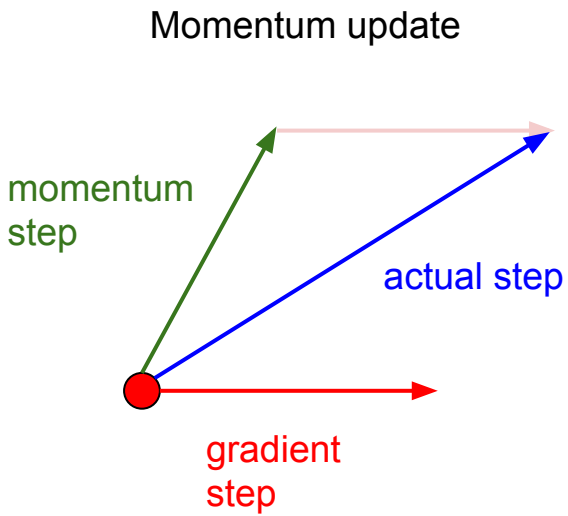


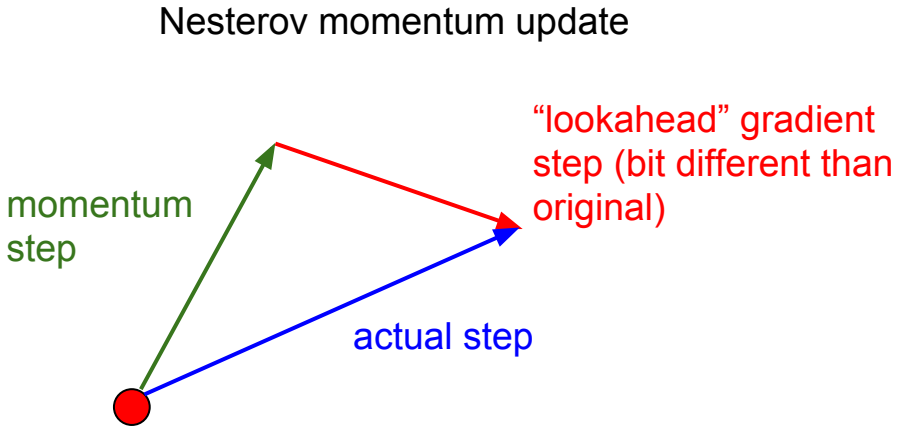
Nesterov Momentum update





Nesterov Momentum update





Nesterov: the only difference...

$$v_t = \mu v_{t-1} - \epsilon \nabla f(\theta_{t-1} + \mu v_{t-1})$$

$$\theta_t = \theta_{t-1} + v_t$$

Nesterov Momentum update

$$v_t = \mu v_{t-1} - \epsilon \nabla f(\theta_{t-1} + \mu v_{t-1})$$

$$\theta_t = \theta_{t-1} + v_t$$

Slightly inconvenient…
usually we have :

$$\theta_{t-1}, \nabla f(\theta_{t-1})$$

Nesterov Momentum update

$$v_t = \mu v_{t-1} - \epsilon \nabla f(\theta_{t-1} + \mu v_{t-1})$$

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$$\theta_{t-1}, \nabla f(\theta_{t-1})$$

Variable transform and rearranging saves the day:

$$\phi_{t-1} = \theta_{t-1} + \mu v_{t-1}$$

Nesterov Momentum update

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usually we have :

$$\theta_{t-1}, \nabla f(\theta_{t-1})$$

Variable transform and rearranging saves the day:

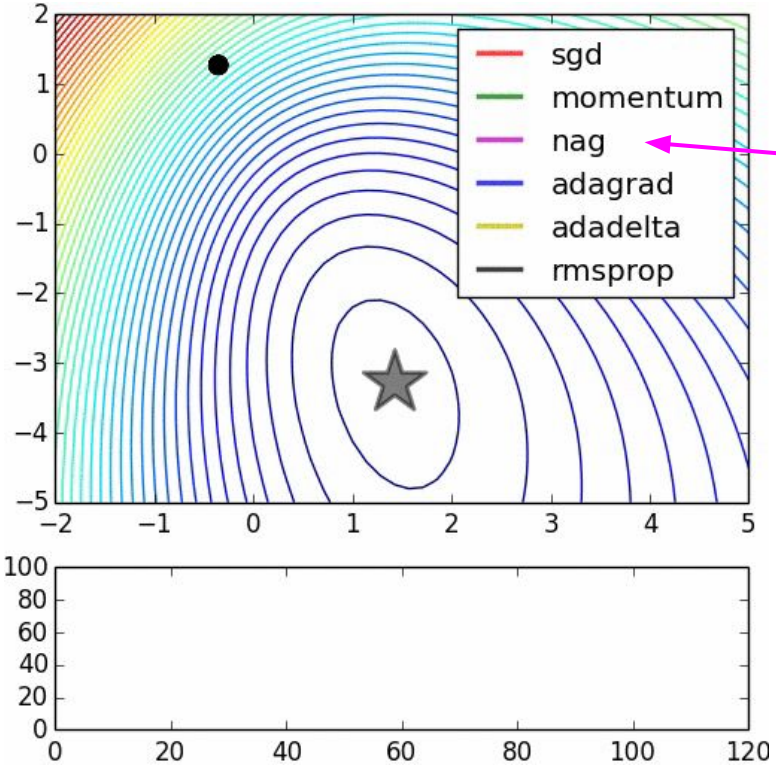
$$\phi_{t-1} = \theta_{t-1} + \mu v_{t-1}$$

Replace all thetas with phis, rearrange and obtain:

$$v_t = \mu v_{t-1} - \epsilon \nabla f(\phi_{t-1})$$

$$\phi_t = \phi_{t-1} - \mu v_{t-1} + (1 + \mu) v_t$$

```
# Nesterov momentum update rewrite
v_prev = v
v = mu * v - learning_rate * dx
x += -mu * v_prev + (1 + mu) * v
```



nag =
Nesterov
Accelerated
Gradient

AdaGrad update

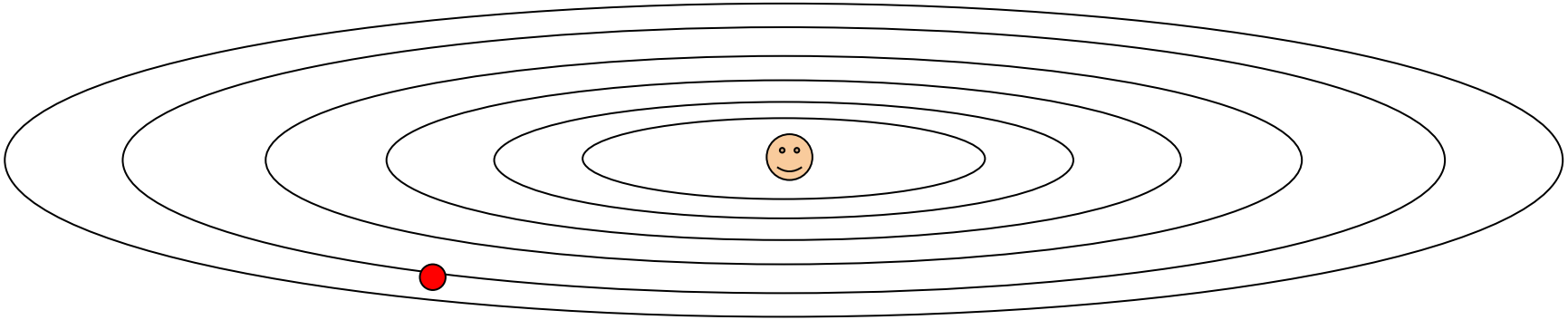
[Duchi et al., 2011]

```
# Adagrad update
cache += dx**2
x += - learning_rate * dx / (np.sqrt(cache) + 1e-7)
```

Added element-wise scaling of the gradient based on the historical sum of squares in each dimension

AdaGrad update

```
# Adagrad update
cache += dx**2
x += - learning_rate * dx / (np.sqrt(cache) + 1e-7)
```



Q: What happens with AdaGrad?

AdaGrad update

```
# Adagrad update
cache += dx**2
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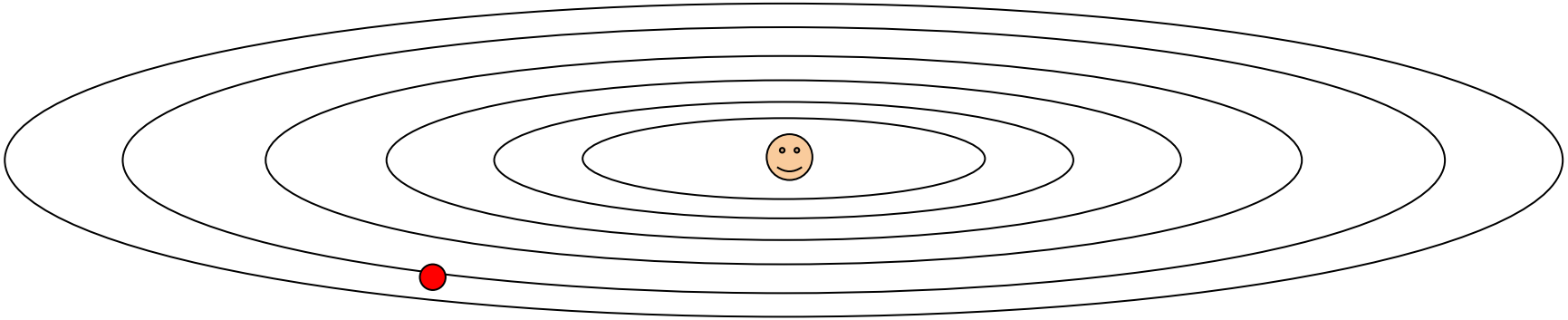
```



Q2: What happens to the step size over long time?

RMSProp update

[Tieleman and Hinton, 2012]

```
# Adagrad update
cache += dx**2
x += - learning_rate * dx / (np.sqrt(cache) + 1e-7)
```



```
# RMSProp
cache = decay_rate * cache + (1 - decay_rate) * dx**2
x += - learning_rate * dx / (np.sqrt(cache) + 1e-7)
```

rmsprop: A mini-batch version of rprop

- rprop is equivalent to using the gradient but also dividing by the size of the gradient.
  - The problem with mini-batch rprop is that we divide by a different number for each mini-batch. So why not force the number we divide by to be very similar for adjacent mini-batches?
- rmsprop: Keep a moving average of the squared gradient for each weight

$$MeanSquare(w,t) = 0.9\, MeanSquare(w,\ t-1) + 0.1\left(\partial E / \partial w(t)\right)^2$$

- Dividing the gradient by $\sqrt{MeanSquare(w,\ t)}$ makes the learning work much better (Tijmen Tieleman, unpublished).

Introduced in a slide in Geoff Hinton's Coursera class, lecture 6

rmsprop: A mini-batch version of rprop

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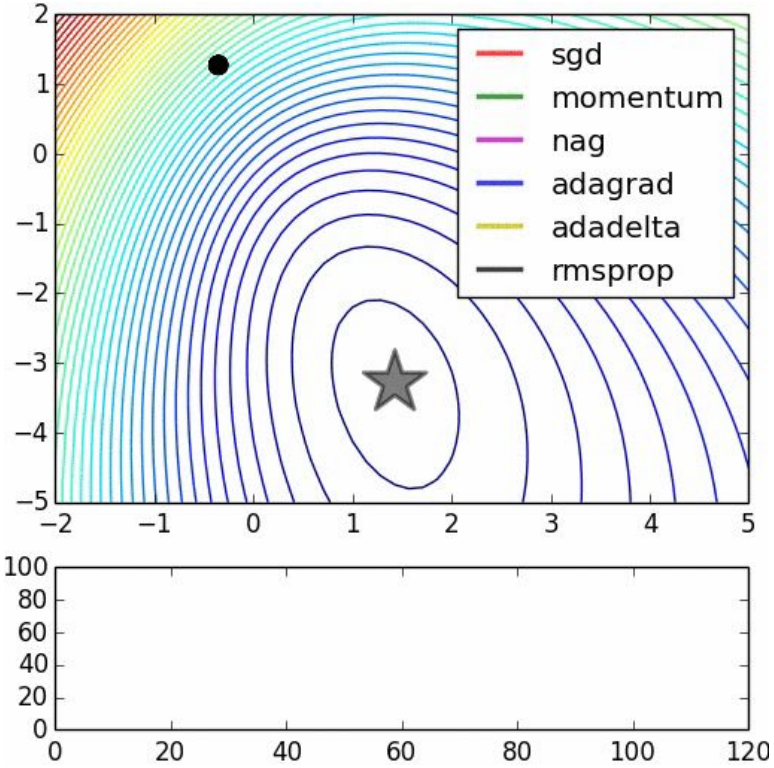
Introduced in a slide in Geoff Hinton's Coursera class, lecture 6

Cited by several papers as:

[52] T. Tieleman and G. E. Hinton. Lecture 6.5-rmsprop: Divide the gradient by a running average of its recent magnitude., 2012.



adagrad
rmsprop

Adam update

[Kingma and Ba, 2014]

(incomplete, but close)

```
# Adam
m = beta1*m + (1-beta1)*dx # update first moment
v = beta2*v + (1-beta2)*(dx**2) # update second moment
x += - learning_rate * m / (np.sqrt(v) + 1e-7)
```

Adam update

[Kingma and Ba, 2014]

(incomplete, but close)

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# Adam
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```

momentum

RMSProp-like

Looks a bit like RMSProp with momentum

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[Kingma and Ba, 2014]

(incomplete, but close)

```
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```

momentum

RMSProp-like

Looks a bit like RMSProp with momentum

```
# RMSProp
cache = decay_rate * cache + (1 - decay_rate) * dx**2
x += - learning_rate * dx / (np.sqrt(cache) + 1e-7)
```

Adam update

[Kingma and Ba, 2014]

```
# Adam
m,v = #... initialize caches to zeros
for t in xrange(1, big_number):
  dx = # ... evaluate gradient
  m = beta1*m + (1-beta1)*dx # update first moment
  v = beta2*v + (1-beta2)*(dx**2) # update second moment
  mb = m/(1-beta1**t) # correct bias
  vb = v/(1-beta2**t) # correct bias
  x += - learning_rate * mb / (np.sqrt(vb) + 1e-7)
```

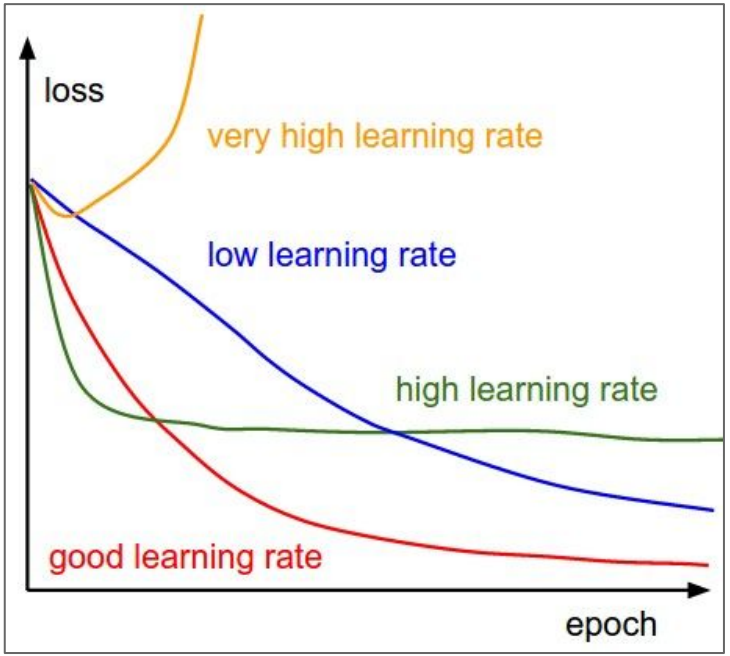
momentum

bias correction
(only relevant in first few iterations when t is small)

RMSProp-like

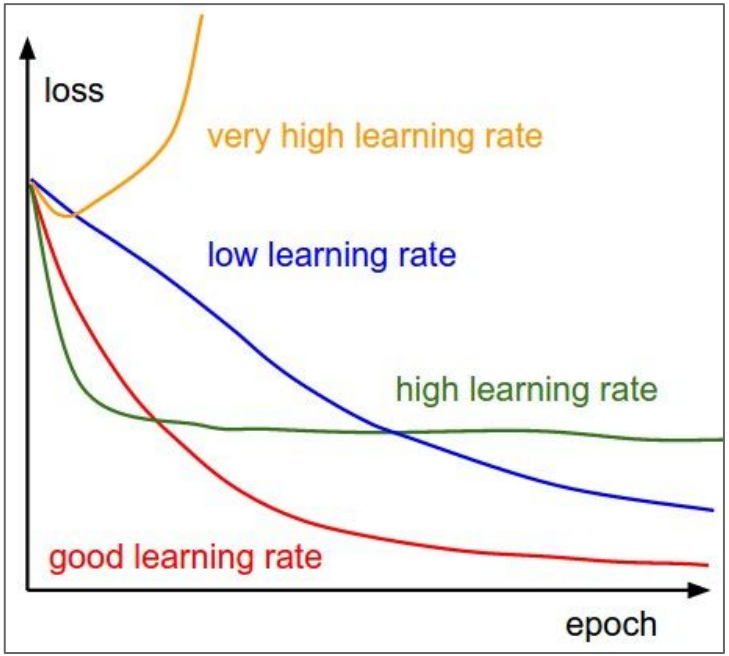
The bias correction compensates for the fact that m,v are initialized at zero and need some time to “warm up”.

SGD, SGD+Momentum, Adagrad, RMSProp, Adam all have **learning rate** as a hyperparameter.



Q: Which one of these learning rates is best to use?

SGD, SGD+Momentum, Adagrad, RMSProp, Adam all have **learning rate** as a hyperparameter.



=> Learning rate decay over time!

step decay:
e.g. decay learning rate by half every few epochs.

exponential decay:

$$\alpha = \alpha_0 e^{-kt}$$

1/t decay:

$$\alpha = \alpha_0 / (1 + kt)$$

Second order optimization methods

second-order Taylor expansion:

$$J(\boldsymbol{\theta}) \approx J(\boldsymbol{\theta}_0) + (\boldsymbol{\theta} - \boldsymbol{\theta}_0)^\top \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}_0) + \frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\theta}_0)^\top \boldsymbol{H}(\boldsymbol{\theta} - \boldsymbol{\theta}_0)$$

Solving for the critical point we obtain the Newton parameter update:

$$\boldsymbol{\theta}^* = \boldsymbol{\theta}_0 - \boldsymbol{H}^{-1} \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}_0)$$

Q: what is nice about this update?

Second order optimization methods

second-order Taylor expansion:

$$J(\boldsymbol{\theta}) \approx J(\boldsymbol{\theta}_0) + (\boldsymbol{\theta} - \boldsymbol{\theta}_0)^\top \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}_0) + \frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\theta}_0)^\top \boldsymbol{H}(\boldsymbol{\theta} - \boldsymbol{\theta}_0)$$

Solving for the critical point we obtain the Newton parameter update:

$$\boldsymbol{\theta}^* = \boldsymbol{\theta}_0 - \boldsymbol{H}^{-1} \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}_0)$$

notice:
no hyperparameters! (e.g. learning rate)

Q2: why is this impractical for training Deep Neural Nets?

Second order optimization methods

$$\theta^* = \theta_0 - \boldsymbol{H}^{-1} \nabla_\theta J(\theta_0)$$

- Quasi-Newton methods (**BGFS** most popular):
  instead of inverting the Hessian (O(n^3)), approximate inverse Hessian with rank 1 updates over time (O(n^2) each).

- **L-BFGS** (Limited memory BFGS):
  Does not form/store the full inverse Hessian.

L-BFGS

- **Usually works very well in full batch, deterministic mode** i.e. if you have a single, deterministic f(x) then L-BFGS will probably work very nicely

- **Does not transfer very well to mini-batch setting**. Gives bad results. Adapting L-BFGS to large-scale, stochastic setting is an active area of research.

In practice:

- **Adam** is a good default choice in most cases

- If you can afford to do full batch updates then try out **L-BFGS** (and don't forget to disable all sources of noise)

Evaluation:

Model Ensembles

1. Train multiple independent models
2. At test time average their results

Enjoy 2% extra performance

Fun Tips/Tricks:

- can also get a small boost from averaging multiple model checkpoints of a single model.

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- can also get a small boost from averaging multiple model checkpoints of a single model.
- keep track of (and use at test time) a running average parameter vector:

```
while True:
  data_batch = dataset.sample_data_batch()
  loss = network.forward(data_batch)
  dx = network.backward()
  x += - learning_rate * dx
  x_test = 0.995*x_test + 0.005*x # use for test set
```