Lecture 7: Training Neural Networks, Part II

Administrative: Assignment 2

Has been released

Due 10/22 11:59pm

- Multi-layer Neural Networks,
- Image Features,
- Optimizers

Administrative: Course Project

Groups assigned

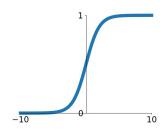
Proposal due 2/29

Come to OH to talk about projects

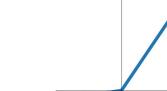
Last time: Activation Functions

Sigmoid

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

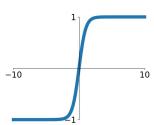


Leaky ReLU $\max(0.1x, x)$



tanh

tanh(x)

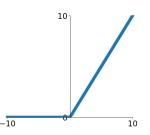


Maxout

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

ReLU

 $\max(0,x)$

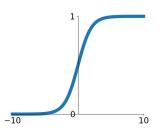


$$\begin{cases} x & x \ge 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$

Last time: Activation Functions

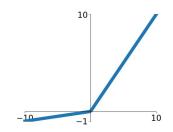
Sigmoid

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



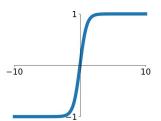
Leaky ReLU

 $\max(0.1x, x)$



tanh

tanh(x)



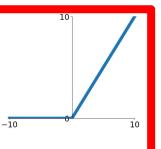
Maxout

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

ReLU

 $\max(0, x)$

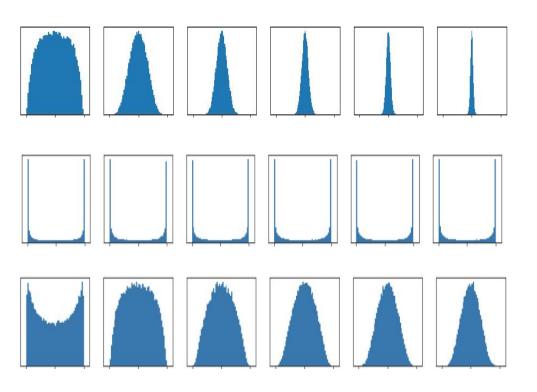
Good default choice



ELU

$$\begin{cases} x & x \ge 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$

Last time: Weight Initialization



Initialization too small:

Activations go to zero, gradients also zero, No learning =(

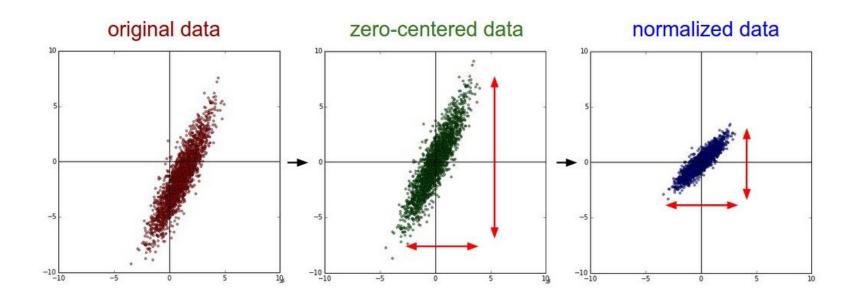
Initialization too big:

Activations saturate (for tanh), Gradients zero, no learning =(

Initialization just right:

Nice distribution of activations at all layers, Learning proceeds nicely =)

Last time: Data Preprocessing



Last Time: Batch Normalization

[loffe and Szegedy, 2015]

Input: $x: N \times D$

$$\mu_j = \frac{1}{N} \sum_{i=1}^N x_{i,j} \quad \text{Per-channel mean,} \\ \text{shape is D}$$

Learnable scale and shift parameters:

$$\gamma, \beta: D$$

Learning $\gamma = \sigma$, $\beta = \mu$ will recover the identity function!

$$\sigma_j^2 = \frac{1}{N} \sum_{i=1}^N (x_{i,j} - \mu_j)^2 \quad \mbox{Per-channel var,} \\ \mbox{shape is D}$$

$$\hat{x}_{i,j} = \frac{x_{i,j} - \mu_j}{\sqrt{\sigma_j^2 + \varepsilon}} \qquad \text{Normalized x,} \\ \text{Shape is N x D}$$

$$y_{i,j} = \gamma_j \hat{x}_{i,j} + \beta_j$$
 Output, Shape is N x D

Batch Normalization: Test-Time

Input: $x: N \times D$

$$\mu_j = {}^{ ext{(Running)}} \, {}_{ ext{values seen during training}}$$

Per-channel mean, shape is D

Per-channel var,

Learnable scale and shift parameters:

$$\gamma, \beta: D$$

During testing batchnorm becomes a linear operator!
Can be fused with the previous fully-connected or conv layer

$$\sigma_j^2 = \text{ (Running) average of values seen during training}$$

training shape is D

Normalized x,

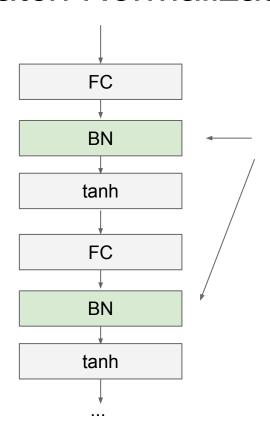
$$\hat{x}_{i,j} = \frac{x_{i,j} - \mu_j}{\sqrt{\sigma_j^2 + \varepsilon}}$$

$$y_{i,j} = \gamma_j \hat{x}_{i,j} + \beta_j$$
 Output

Output, Shape is N x D

Shape is N x D

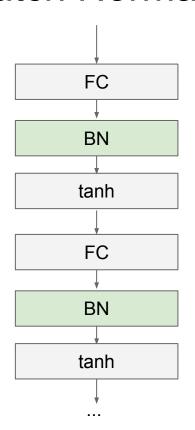
Batch Normalization



Usually inserted after Fully Connected or Convolutional layers, and before nonlinearity.

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

Batch Normalization



- Makes deep networks much easier to train!
- Improves gradient flow
- Allows higher learning rates, faster convergence
- Networks become more robust to initialization
- Acts as regularization during training
- Zero overhead at test-time: can be fused with conv!
- Behaves differently during training and testing: this
 is a very common source of bugs!

Batch Normalization for ConvNets

Batch Normalization for **fully-connected** networks

$$x: N \times D$$
Normalize
$$\mu, \sigma: 1 \times D$$

$$y, \beta: 1 \times D$$

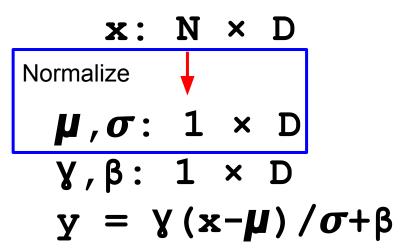
$$y = \frac{y(x-\mu)}{\sigma+\beta}$$

Batch Normalization for **convolutional** networks (Spatial Batchnorm, BatchNorm2D)

Normalize
$$\mathbf{x}: \mathbf{N} \times \mathbf{C} \times \mathbf{H} \times \mathbf{W}$$
 $\mu, \sigma: \mathbf{1} \times \mathbf{C} \times \mathbf{1} \times \mathbf{1}$
 $\gamma, \beta: \mathbf{1} \times \mathbf{C} \times \mathbf{1} \times \mathbf{1}$
 $\gamma = \gamma(\mathbf{x} - \mu) / \sigma + \beta$

Layer Normalization

Batch Normalization for fully-connected networks



Layer Normalization for fully-connected networks
Same behavior at train and test!
Can be used in recurrent networks

Normalize
$$\mu, \sigma: N \times D$$

$$\psi, \sigma: N \times 1$$

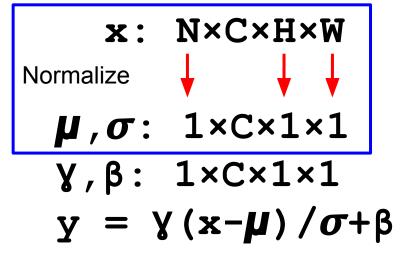
$$\psi, \beta: 1 \times D$$

$$\psi = \psi(x-\mu)/\sigma + \beta$$

Ba, Kiros, and Hinton, "Layer Normalization", arXiv 2016

Instance Normalization

Batch Normalization for convolutional networks

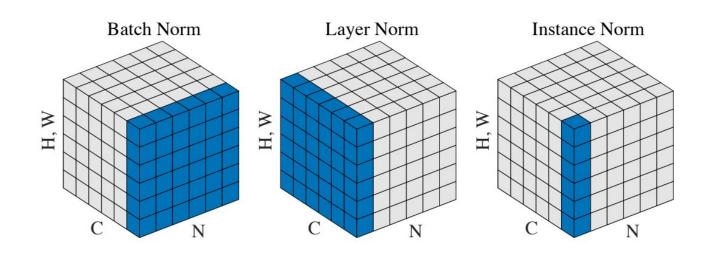


Instance Normalization for convolutional networks
Same behavior at train / test!

$$x: N \times C \times H \times W$$
Normalize
 $\mu, \sigma: N \times C \times 1 \times 1$
 $y, \beta: 1 \times C \times 1 \times 1$
 $y = y(x-\mu)/\sigma + \beta$

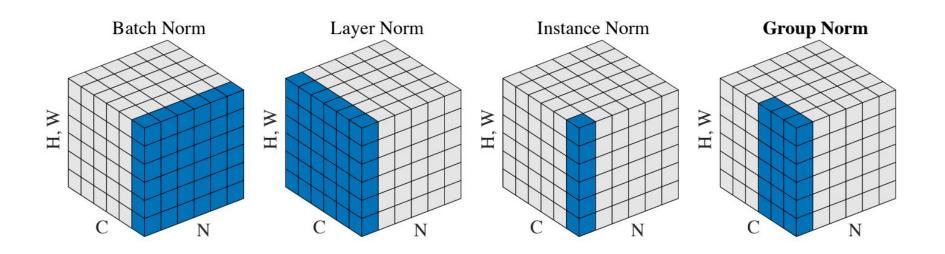
Ulyanov et al, Improved Texture Networks: Maximizing Quality and Diversity in Feed-forward Stylization and Texture Synthesis, CVPR 2017

Comparison of Normalization Layers



Wu and He, "Group Normalization", ECCV 2018

Group Normalization



Wu and He, "Group Normalization", ECCV 2018

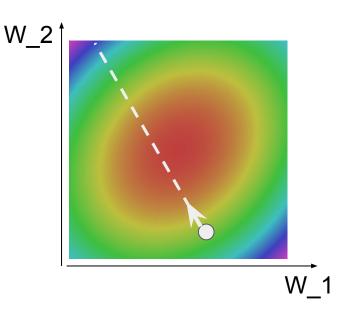
Today

- Improve your training error:
 - (Fancier) Optimizers
 - Learning rate schedules
- Improve your test error:
 - Regularization
 - Choosing Hyperparameters

(Fancier) Optimizers

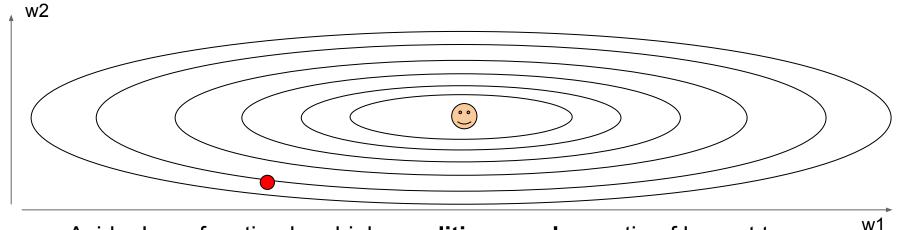
Optimization

```
# Vanilla Gradient Descent
while True:
   weights_grad = evaluate_gradient(loss_fun, data, weights)
   weights += - step_size * weights_grad # perform parameter update
```



Optimization: Problem #1 with SGD

What if loss changes quickly in one direction and slowly in another? What does gradient descent do?



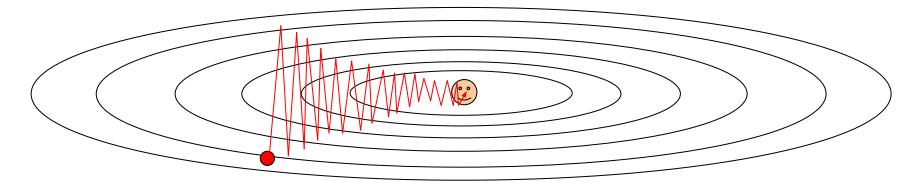
Aside: Loss function has high **condition number**: ratio of largest to smallest singular value of the Hessian matrix is large

VV I

Optimization: Problem #1 with SGD

What if loss changes quickly in one direction and slowly in another? What does gradient descent do?

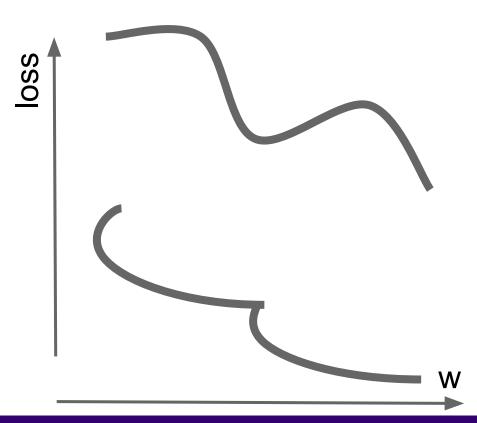
Very slow progress along shallow dimension, jitter along steep direction



Loss function has high **condition number**: ratio of largest to smallest singular value of the Hessian matrix is large

Optimization: Problem #2 with SGD

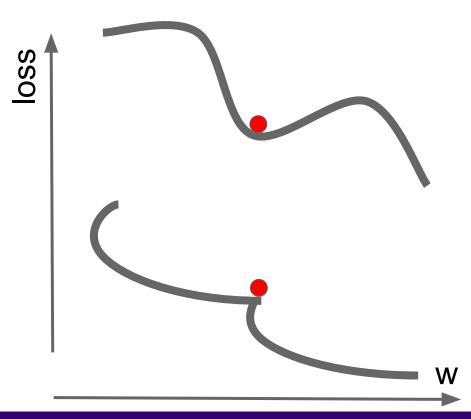
What if the loss function has a local minima or saddle point?



Optimization: Problem #2 with SGD

What if the loss function has a local minima or saddle point?

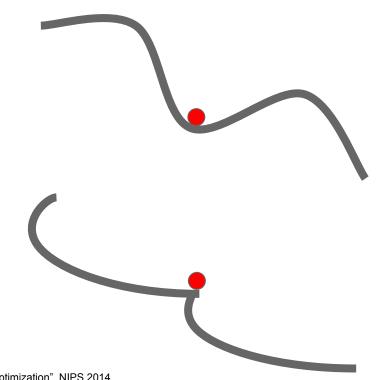
Zero gradient, gradient descent gets stuck



Optimization: Problem #2 with SGD

What if the loss function has a local minima or saddle point?

Saddle points much more common in high dimension



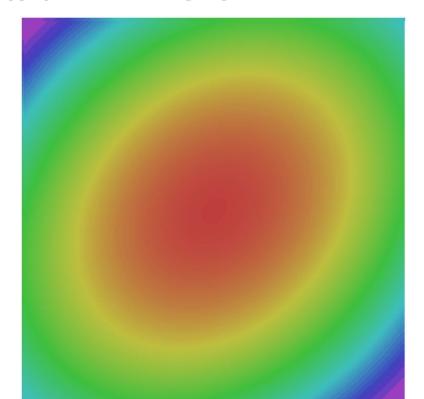
Dauphin et al. "Identifying and attacking the saddle point problem in high-dimensional non-convex optimization". NIPS 2014

Optimization: Problem #3 with SGD

Our gradients come from minibatches so they can be noisy!

$$L(W) = \frac{1}{N} \sum_{i=1}^{N} L_i(x_i, y_i, W)$$

$$\nabla_W L(W) = \frac{1}{N} \sum_{i=1}^{N} \nabla_W L_i(x_i, y_i, W)$$

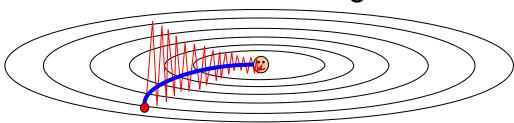


SGD + Momentum

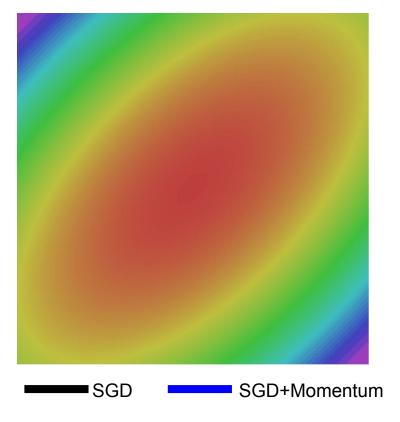
Local Minima Saddle points



Poor Conditioning



Gradient Noise



SGD: the simple two line update code

SGD

```
x_{t+1} = x_t - \alpha \nabla f(x_t)
```

```
while True:
    dx = compute_gradient(x)
    x -= learning_rate * dx
```

SGD + Momentum:

continue moving in the general direction as the previous iterations

SGD

$$x_{t+1} = x_t - \alpha \nabla f(x_t)$$

```
while True:
   dx = compute_gradient(x)
   x -= learning_rate * dx
```

SGD+Momentum

```
v_{t+1} = \rho v_t + \nabla f(x_t)x_{t+1} = x_t - \alpha v_{t+1}
```

- Build up "velocity" as a running mean of gradients
- Rho gives "friction"; typically rho=0.9 or 0.99

Sutskever et al, "On the importance of initialization and momentum in deep learning", ICML 2013

SGD + Momentum:

continue moving in the general direction as the previous iterations

SGD

$$x_{t+1} = x_t - \alpha \nabla f(x_t)$$

```
while True:
   dx = compute_gradient(x)
   x -= learning_rate * dx
```

SGD+Momentum

```
v_{t+1} = \rho v_t + \nabla f(x_t)x_{t+1} = x_t - \alpha v_{t+1}
```

```
vx = 0
while True:
    dx = compute_gradient(x)
    vx = rho * vx + dx
    x -= learning_rate * vx
```

- Build up "velocity" as a running mean of gradients
- Rho gives "friction"; typically rho=0.9 or 0.99

Sutskever et al, "On the importance of initialization and momentum in deep learning", ICML 2013

SGD + Momentum:

alternative equivalent formulation

SGD+Momentum

```
v_{t+1} = \rho v_t - \alpha \nabla f(x_t)x_{t+1} = x_t + v_{t+1}
```

```
vx = 0
while True:
    dx = compute_gradient(x)
    vx = rho * vx - learning_rate * dx
    x += vx
```

SGD+Momentum

```
v_{t+1} = \rho v_t + \nabla f(x_t)x_{t+1} = x_t - \alpha v_{t+1}
```

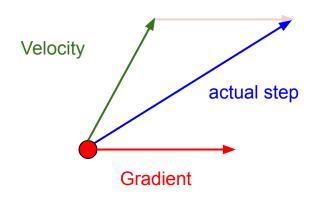
```
vx = 0
while True:
    dx = compute_gradient(x)
    vx = rho * vx + dx
    x -= learning_rate * vx
```

You may see SGD+Momentum formulated different ways, but they are equivalent - give same sequence of x

Sutskever et al, "On the importance of initialization and momentum in deep learning", ICML 2013

SGD+Momentum

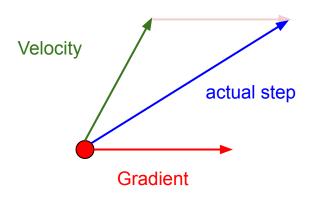
Momentum update:



Combine gradient at current point with velocity to get step used to update weights

Nesterov, "A method of solving a convex programming problem with convergence rate O(1/k^2)", 1983 Nesterov, "Introductory lectures on convex optimization: a basic course", 2004 Sutskever et al, "On the importance of initialization and momentum in deep learning", ICML 2013

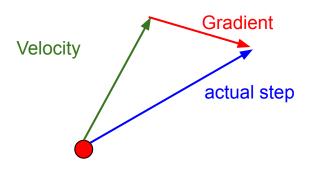
Momentum update:



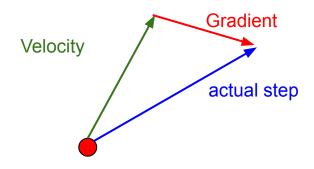
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Nesterov Momentum

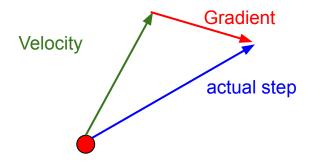


$$v_{t+1} = \rho v_t - \alpha \nabla f(x_t + \rho v_t)$$
$$x_{t+1} = x_t + v_{t+1}$$



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$$x_{t+1} = x_t + v_{t+1}$$

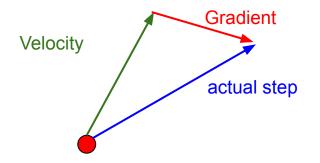
Annoying, usually we want update in terms of $x_t, \nabla f(x_t)$



$$v_{t+1} = \rho v_t - \alpha \nabla f(x_t + \rho v_t)$$
$$x_{t+1} = x_t + v_{t+1}$$

Change of variables $\tilde{x}_t = x_t + \rho v_t$ and rearrange:

Annoying, usually we want update in terms of $x_t, \nabla f(x_t)$



$$v_{t+1} = \rho v_t - \alpha \nabla f(x_t + \rho v_t)$$
$$x_{t+1} = x_t + v_{t+1}$$

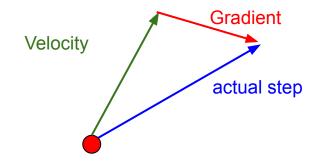
Change of variables $\tilde{x}_t = x_t + \rho v_t$ and rearrange:

$$v_{t+1} = \rho v_t - \alpha \nabla f(\tilde{x}_t)$$

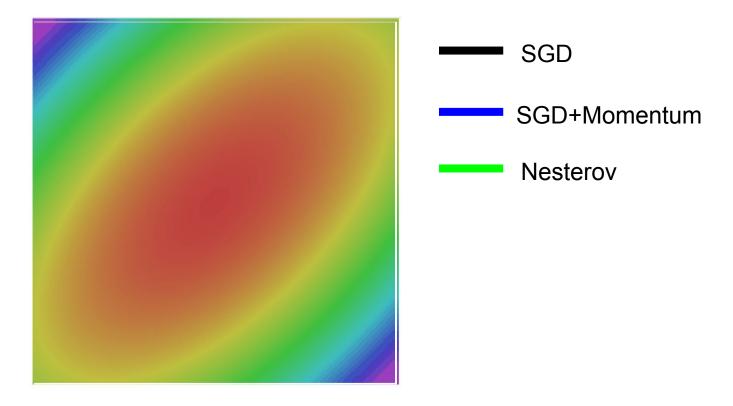
$$\tilde{x}_{t+1} = \tilde{x}_t - \rho v_t + (1+\rho)v_{t+1}$$

$$= \tilde{x}_t + v_{t+1} + \rho(v_{t+1} - v_t)$$

Annoying, usually we want update in terms of $x_t, \nabla f(x_t)$



Nesterov Momentum



```
grad_squared = 0
while True:
    dx = compute_gradient(x)
    grad_squared += dx * dx
x -= learning_rate * dx / (np.sqrt(grad_squared) + 1e-7)
```

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

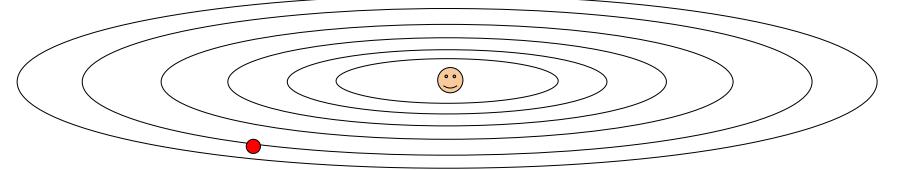
"Per-parameter learning rates" or "adaptive learning rates"

Duchi et al, "Adaptive subgradient methods for online learning and stochastic optimization", JMLR 2011

```
grad_squared = 0
while True:
  dx = compute\_gradient(x)
  grad_squared += dx * dx
 x -= learning_rate * dx / (np.sqrt(grad_squared) + 1e-7)
```

Q: What happens with AdaGrad?

```
grad_squared = 0
while True:
    dx = compute_gradient(x)
    grad_squared += dx * dx
    x -= learning_rate * dx / (np.sqrt(grad_squared) + 1e-7)
```



Q: What happens with AdaGrad?

Progress along "steep" directions is damped; progress along "flat" directions is accelerated

```
grad_squared = 0
while True:
  dx = compute\_gradient(x)
  grad_squared += dx * dx
 x -= learning_rate * dx / (np.sqrt(grad_squared) + 1e-7)
```

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

```
grad_squared = 0
while True:
  dx = compute\_gradient(x)
  grad_squared += dx * dx
 x -= learning_rate * dx / (np.sqrt(grad_squared) + 1e-7)
```

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

RMSProp: "Leaky AdaGrad"

AdaGrad

```
grad_squared = 0
while True:
    dx = compute_gradient(x)
    grad_squared += dx * dx
    x -= learning_rate * dx / (np.sqrt(grad_squared) + 1e-7)
```

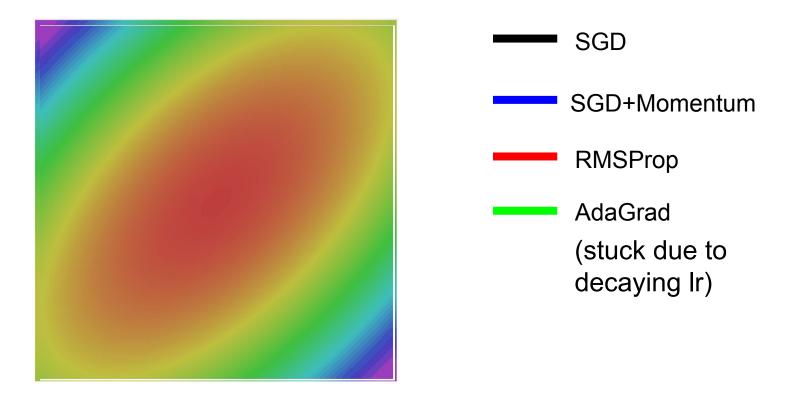


RMSProp

```
grad_squared = 0
while True:
    dx = compute_gradient(x)
    grad_squared = decay_rate * grad_squared + (1 - decay_rate) * dx * dx
    x -= learning_rate * dx / (np.sqrt(grad_squared) + 1e-7)
```

Tieleman and Hinton, 2012

RMSProp



Adam (almost)

```
first_moment = 0
second_moment = 0
while True:
    dx = compute_gradient(x)
    first_moment = beta1 * first_moment + (1 - beta1) * dx
    second_moment = beta2 * second_moment + (1 - beta2) * dx * dx
    x -= learning_rate * first_moment / (np.sqrt(second_moment) + 1e-7))
```

Adam (almost)

```
first moment = 0
second moment = 0
while True:
  dx = compute\_gradient(x)
 first_moment = beta1 * first_moment + (1 - beta1) * dx
 second_moment = beta2 * second_moment + (1 - beta2) * dx * dx
 x -= learning_rate * first_moment / (np.sqrt(second_moment) + 1e-7))
```

Momentum

AdaGrad / RMSProp

Sort of like RMSProp with momentum

Q: What happens at first timestep?

Adam (full form)

```
first_moment = 0
second_moment = 0
for t in range(1, num_iterations):
    dx = compute_gradient(x)
    first_moment = beta1 * first_moment + (1 - beta1) * dx

    second_moment = beta2 * second_moment + (1 - beta2) * dx * dx

first_unbias = first_moment / (1 - beta1 ** t)
    second_unbias = second_moment / (1 - beta2 ** t)

x -= learning_rate * first_unbias / (np.sqrt(second_unbias) + 1e-7))

AdaGrad / RMSProp
```

Bias correction for the fact that first and second moment estimates start at zero

Adam (full form)

```
first moment = 0
second moment = 0
for t in range(1, num_iterations):
  dx = compute\_gradient(x)
  first_moment = beta1 * first_moment + (1 - beta1) * dx
  second_moment = beta2 * second_moment + (1 - beta2) * dx * dx
  first_unbias = first_moment / (1 - beta1 ** t)
  second_unbias = second_moment / (1 - beta2 ** t)
  x -= learning_rate * first_unbias / (np.sqrt(second_unbias) + 1e-7))
```

Momentum

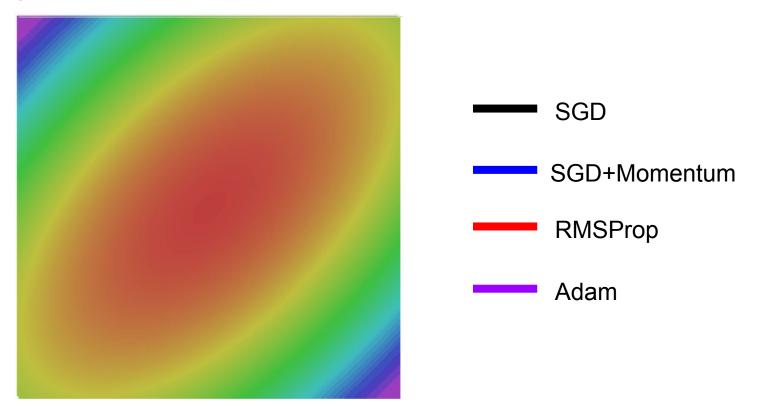
Bias correction

AdaGrad / RMSProp

Bias correction for the fact that first and second moment estimates start at zero

Adam with beta 1 = 0.9. beta2 = 0.999, and learning rate = 1e-3 or 5e-4 is a great starting point for many models!

Adam



L2 Regularization vs Weight Decay

Optimization Algorithm

$$\begin{split} L(w) &= L_{data}(w) + L_{reg}(w) \\ g_t &= \nabla L(w_t) \\ s_t &= optimizer(g_t) \\ w_{t+1} &= w_t - \alpha s_t \end{split}$$

L2 Regularization

$$L(w) = L_{data}(w) + \lambda |w|^{2}$$

$$g_{t} = \nabla L(w_{t}) = \nabla L_{data}(w_{t}) + 2\lambda w_{t}$$

$$s_{t} = optimizer(g_{t})$$

$$w_{t+1} = w_{t} - \alpha s_{t}$$

L2 Regularization vs Weight Decay

Optimization Algorithm

$$L(w) = L_{data}(w) + L_{reg}(w)$$

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L2 Regularization and Weight Decay are equivalent for SGD, SGD+Momentum so people often use the terms interchangeably!

L2 Regularization

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$$g_{t} = \nabla L(w_{t}) = \nabla L_{data}(w_{t}) + 2\lambda w_{t}$$

$$s_{t} = optimizer(g_{t})$$

$$w_{t+1} = w_{t} - \alpha s_{t}$$

Weight Decay

$$\begin{split} L(w) &= L_{data}(w) \\ g_t &= \nabla L_{data}(w_t) \\ s_t &= optimizer(g_t) + 2\lambda w_t \\ w_{t+1} &= w_t - \alpha s_t \end{split}$$

L2 Regularization vs Weight Decay

Optimization Algorithm

$$L(w) = L_{data}(w) + L_{reg}(w)$$

$$g_t = \nabla L(w_t)$$

$$s_t = optimizer(g_t)$$

$$w_{t+1} = w_t - \alpha s_t$$

L2 Regularization and Weight Decay are equivalent for SGD, SGD+Momentum so people often use the terms interchangeably!

But they are not the same for adaptive methods (AdaGrad, RMSProp, Adam, etc)

L2 Regularization

$$L(w) = L_{data}(w) + \lambda |w|^{2}$$

$$g_{t} = \nabla L(w_{t}) = \nabla L_{data}(w_{t}) + 2\lambda w_{t}$$

$$s_{t} = optimizer(g_{t})$$

$$w_{t+1} = w_{t} - \alpha s_{t}$$

Weight Decay

$$\begin{split} L(w) &= L_{data}(w) \\ g_t &= \nabla L_{data}(w_t) \\ s_t &= optimizer(g_t) + 2\lambda w_t \\ w_{t+1} &= w_t - \alpha s_t \end{split}$$

AdamW: Decoupled Weight Decay

Algorithm 2 Adam with L₂ regularization and Adam with decoupled weight decay (AdamW)

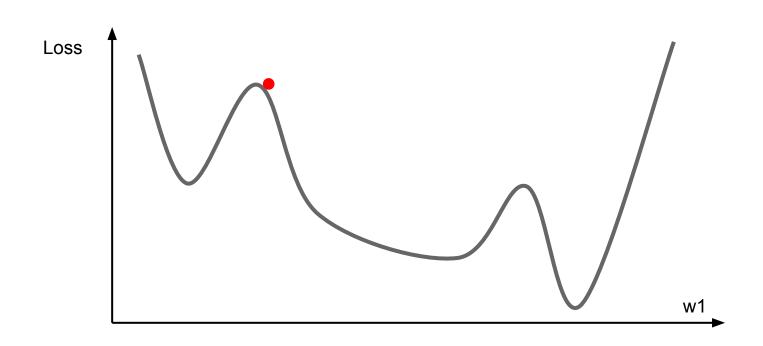
```
1: given \alpha = 0.001, \beta_1 = 0.9, \beta_2 = 0.999, \epsilon = 10^{-8}, \lambda \in \mathbb{R}
 2: initialize time step t \leftarrow 0, parameter vector \boldsymbol{\theta}_{t=0} \in \mathbb{R}^n, first moment vector \boldsymbol{m}_{t=0} \leftarrow \boldsymbol{0}, second moment
       vector \mathbf{v}_{t=0} \leftarrow \mathbf{0}, schedule multiplier \eta_{t=0} \in \mathbb{R}
 3: repeat
          t \leftarrow t + 1
        \nabla f_t(\boldsymbol{\theta}_{t-1}) \leftarrow \text{SelectBatch}(\boldsymbol{\theta}_{t-1})
                                                                                                            > select batch and return the corresponding gradient
        \boldsymbol{g}_t \leftarrow \nabla f_t(\boldsymbol{\theta}_{t-1}) + \lambda \boldsymbol{\theta}_{t-1}
         \boldsymbol{m}_t \leftarrow \beta_1 \boldsymbol{m}_{t-1} + (1 - \beta_1) \boldsymbol{g}_t
                                                                                                                  ▶ here and below all operations are element-wise
         \mathbf{v}_{t} \leftarrow \beta_{2} \mathbf{v}_{t-1} + (1 - \beta_{2}) \mathbf{g}_{t}^{2}
         \hat{\boldsymbol{m}}_t \leftarrow \boldsymbol{m}_t/(1-\beta_1^t)
                                                                                                                                                     \triangleright \beta_1 is taken to the power of t
         \hat{\mathbf{v}}_t \leftarrow \mathbf{v}_t/(1-\beta_2^t)
10:
                                                                                                                                                     \triangleright \beta_2 is taken to the power of t

    ▷ can be fixed, decay, or also be used for warm restarts

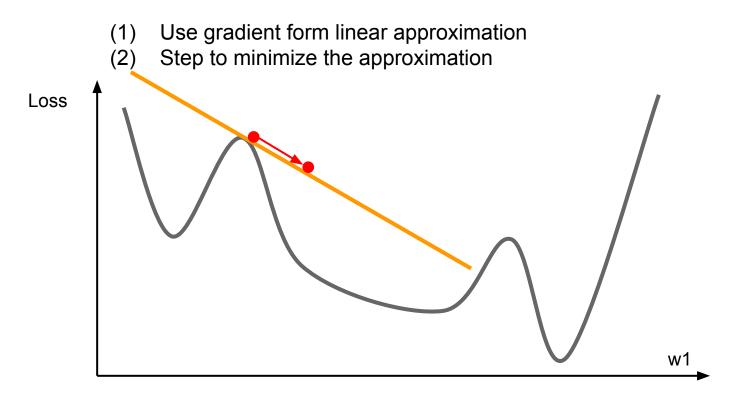
11:
         \eta_t \leftarrow \text{SetScheduleMultiplier}(t)
           \boldsymbol{\theta}_t \leftarrow \boldsymbol{\theta}_{t-1} - \eta_t \left( \alpha \hat{\boldsymbol{m}}_t / (\sqrt{\hat{\boldsymbol{v}}_t} + \epsilon) + \lambda \boldsymbol{\theta}_{t-1} \right)
13: until stopping criterion is met
```

14: **return** optimized parameters θ_t

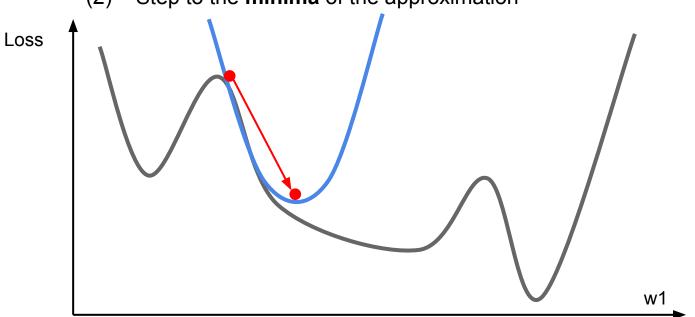
First-Order Optimization



First-Order Optimization



- (1) Use gradient and Hessian to form quadratic approximation
- (2) Step to the **minima** of the approximation



second-order Taylor expansion:

$$L(\theta) \approx L(\theta_0) + (\theta - \theta_0)^T \nabla_{\theta} L(\theta_0) + \frac{1}{2} (\theta - \theta_0)^T H(\theta - \theta_0)$$

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

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

Q: Why is this bad for deep learning?

second-order Taylor expansion:

$$L(\theta) \approx L(\theta_0) + (\theta - \theta_0)^T \nabla_{\theta} L(\theta_0) + \frac{1}{2} (\theta - \theta_0)^T H(\theta - \theta_0)$$

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

$$\theta^* = \theta_0 - H^{-1} \nabla_\theta L(\theta_0) \quad \begin{array}{l} \text{Hessian has O(N^2) elements} \\ \text{Inverting takes O(N^3)} \\ \text{N = (Tens or Hundreds of) Millions} \end{array}$$

Q: Why is this bad for deep learning?

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

- 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 second-order methods to large-scale, stochastic setting is an active area of research.

Le et al, "On optimization methods for deep learning, ICML 2011"

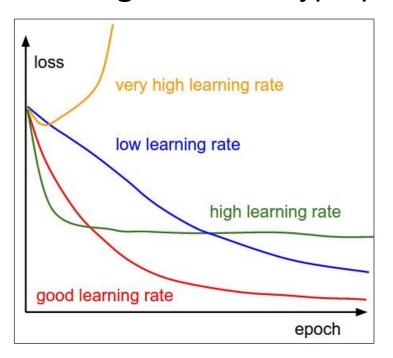
Ba et al, "Distributed second-order optimization using Kronecker-factored approximations", ICLR 2017

In practice:

- AdamW should probably be your "default" optimizer for new problems
- Adam is a good second choice in many cases; it often works ok even with constant learning rate
- SGD+Momentum can outperform Adam but may require more tuning of LR and schedule
 - Try cosine schedule, very few hyperparameters!

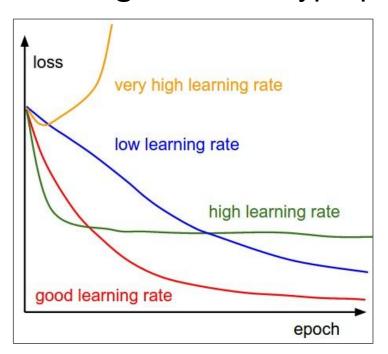
Learning rate schedules

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



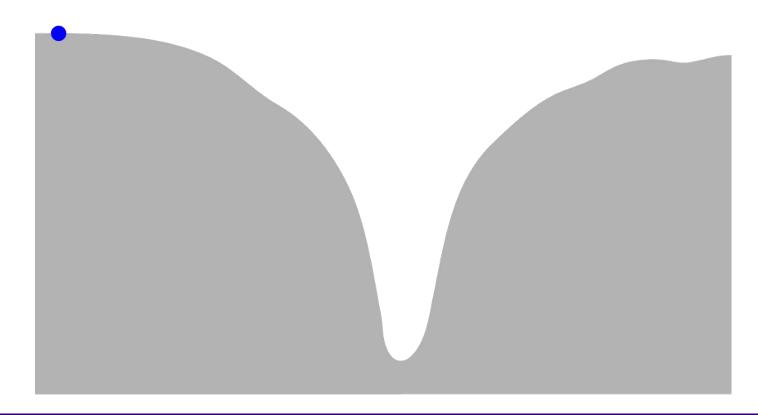
Q: Which one of these learning rates is best to use?

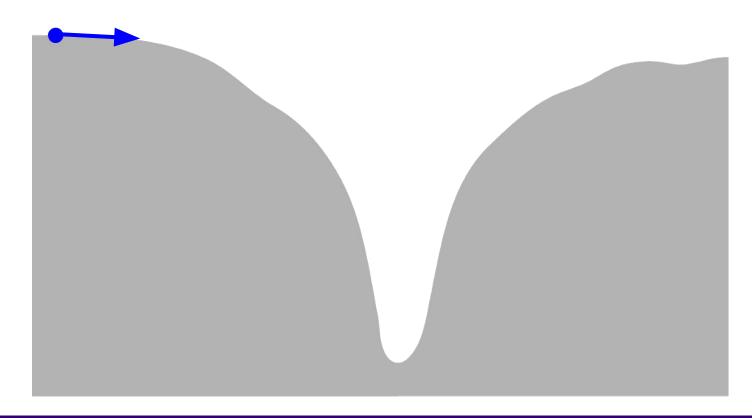
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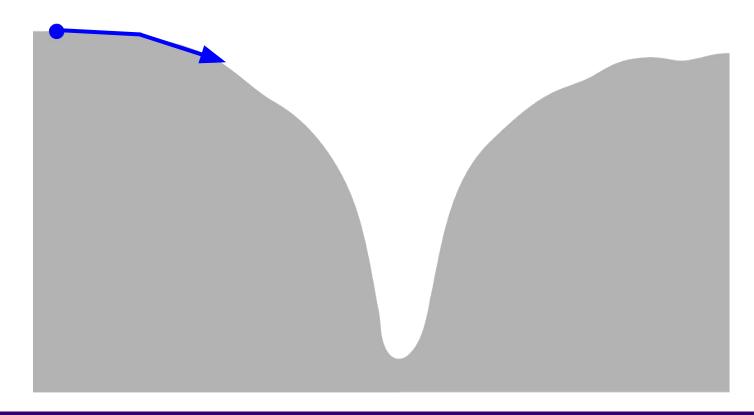


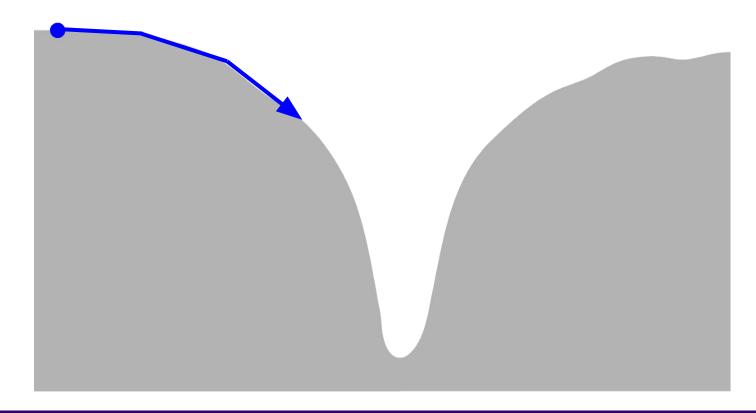
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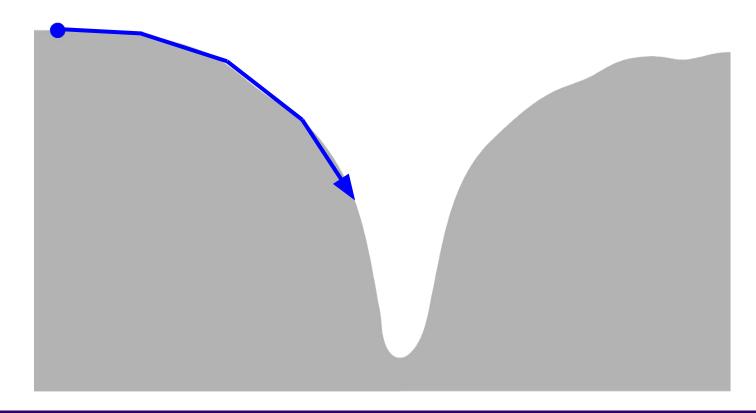
A: In reality, all of these are good learning rates.

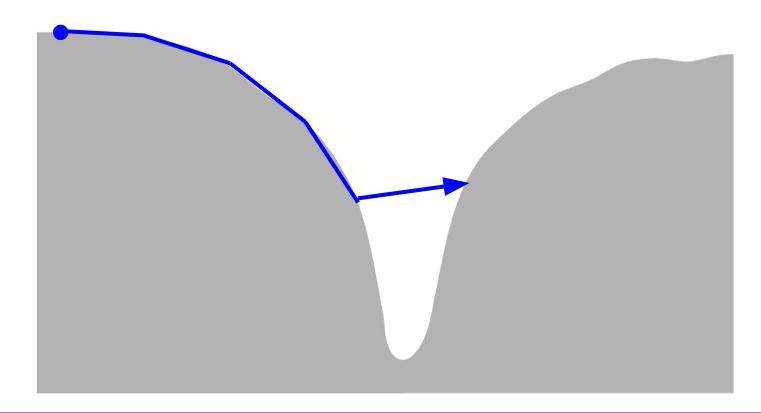


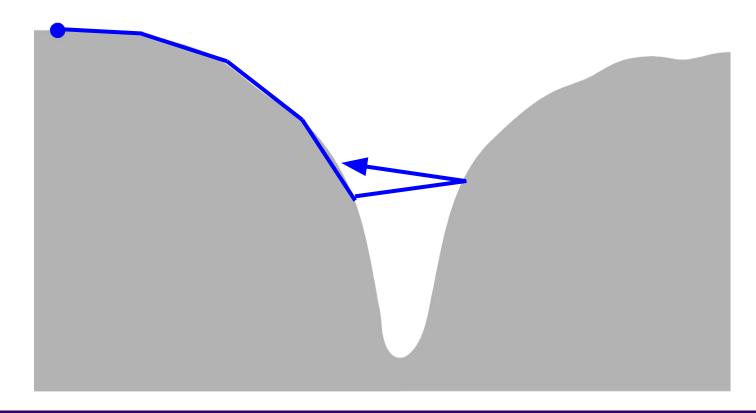


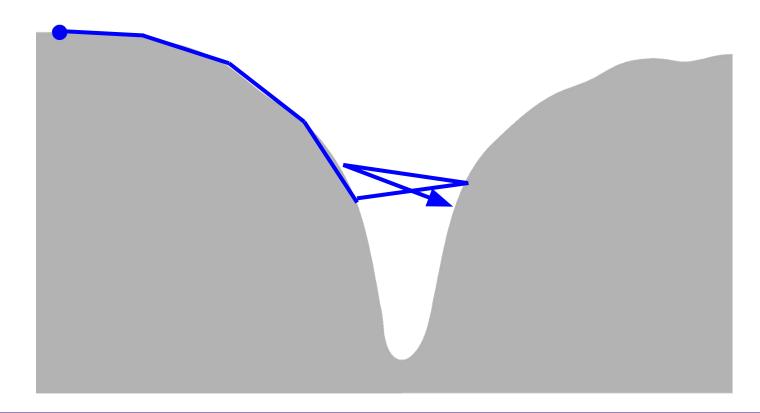




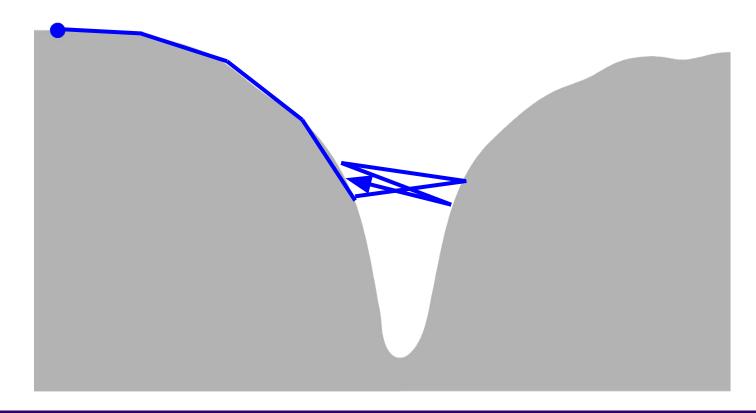




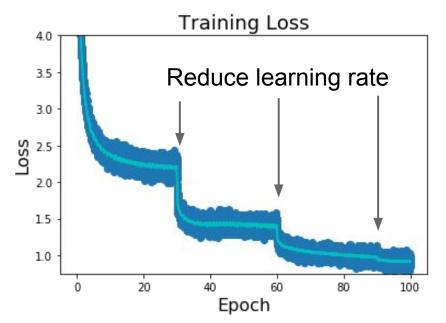




Phases of learning...

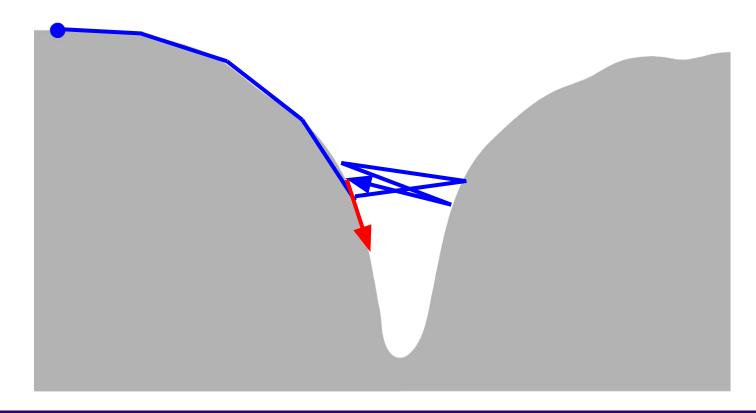


Learning rate decays over time

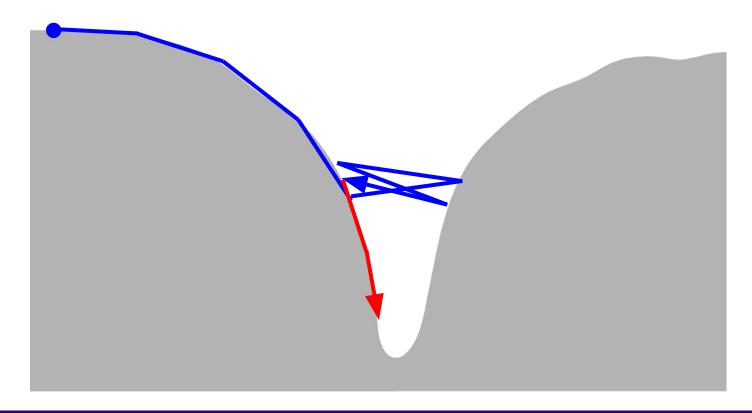


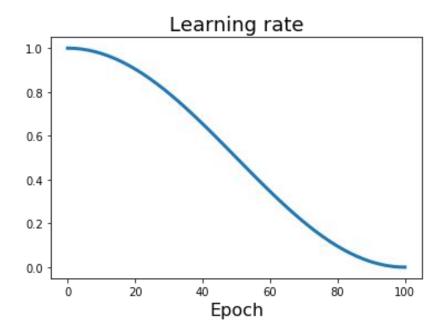
Step: Reduce learning rate at a few fixed points. E.g. for ResNets, multiply LR by 0.1 after epochs 30, 60, and 90.

Phases of learning...



Phases of learning...





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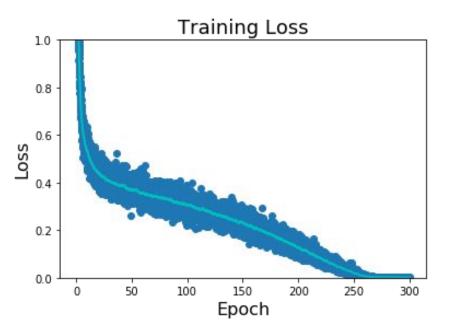
Cosine:
$$\alpha_t = \frac{1}{2}\alpha_0 \left(1 + \cos(t\pi/T)\right)$$

Loshchilov and Hutter, "SGDR: Stochastic Gradient Descent with Warm Restarts", ICLR 2017 Radford et al, "Improving Language Understanding by Generative Pre-Training", 2018 Feichtenhofer et al, "SlowFast Networks for Video Recognition", arXiv 2018 Child at al, "Generating Long Seguences with Sparse Transformers", arXiv 2019

 $lpha_0$: Initial learning rate

 $lpha_t$: Learning rate at epoch t

T: Total number of epochs



Step: Reduce learning rate at a few fixed points. E.g. for ResNets, multiply LR by 0.1 after epochs 30, 60, and 90.

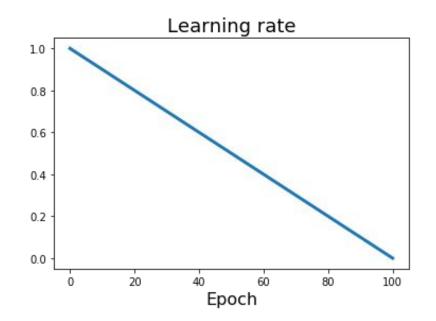
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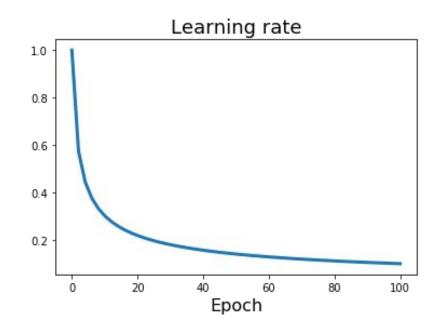
Linear:
$$\alpha_t = \alpha_0(1 - t/T)$$

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Devlin et al, "BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding", 2018



Step: Reduce learning rate at a few fixed points. E.g. for ResNets, multiply LR by 0.1 after epochs 30, 60, and 90.

Cosine:
$$\alpha_t = \frac{1}{2}\alpha_0 \left(1 + \cos(t\pi/T)\right)$$

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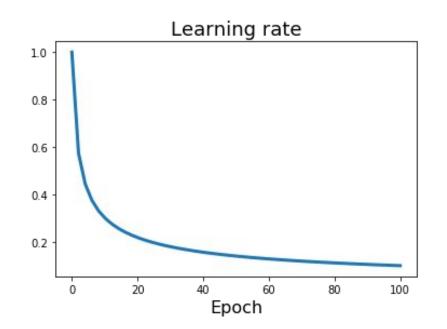
Inverse sqrt:
$$\alpha_t = \alpha_0/\sqrt{t}$$

 $lpha_0$: Initial learning rate

 $lpha_t$: Learning rate at epoch t

T: Total number of epochs

Vaswani et al, "Attention is all you need", NIPS 2017



Step: Reduce learning rate at a few fixed points. E.g. for ResNets, multiply LR by 0.1 after epochs 30, 60, and 90.

Cosine:
$$\alpha_t = \frac{1}{2}\alpha_0 \left(1 + \cos(t\pi/T)\right)$$

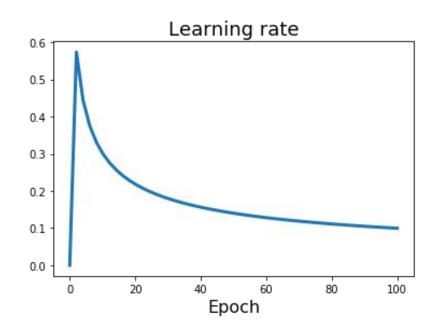
Linear:
$$\alpha_t = \alpha_0(1 - t/T)$$

Inverse sqrt:
$$\alpha_t = \alpha_0/\sqrt{t}$$

Constant:
$$\alpha_t = \alpha_0$$

Vaswani et al, "Attention is all you need", NIPS 2017

Learning Rate Decay: Linear Warmup

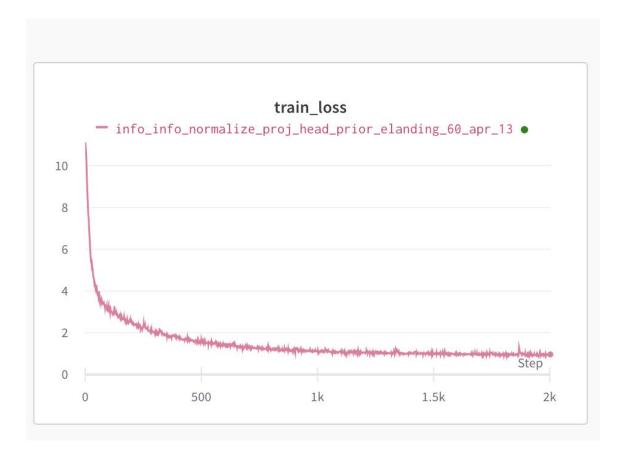


High initial learning rates can make loss explode; linearly increasing learning rate from 0 over the first ~5000 iterations can prevent this

Empirical rule of thumb: If you increase the batch size by N, also scale the initial learning rate by N

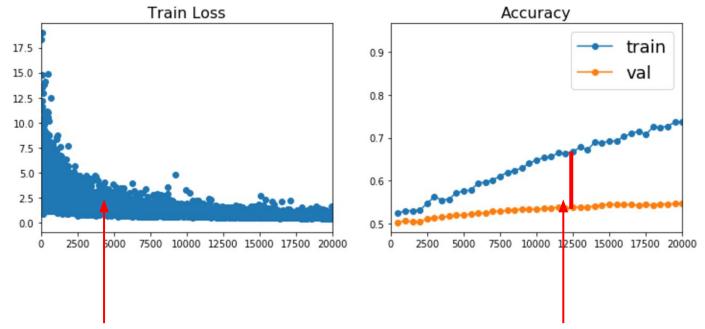
Goyal et al, "Accurate, Large Minibatch SGD: Training ImageNet in 1 Hour", arXiv 2017

with cosine and warmup



Improve test error

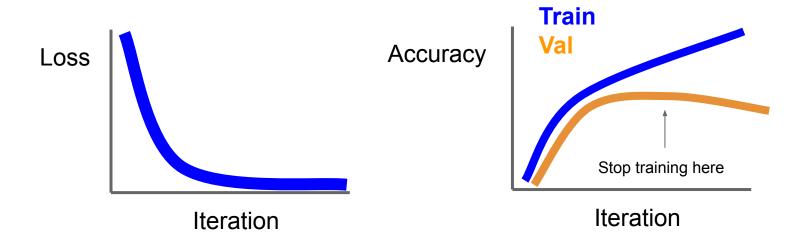
Beyond Training Error



Better optimization algorithms help reduce training loss

But we really care about error on new data - how to reduce the gap?

Early Stopping: Always do this



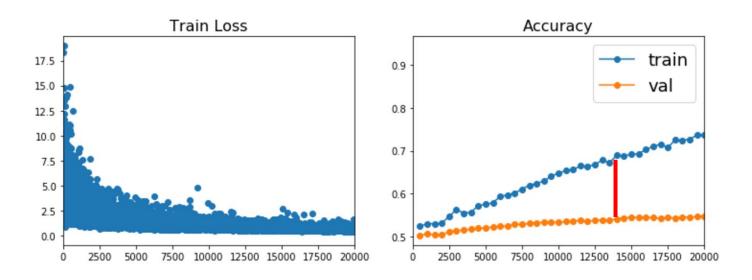
Stop training the model when accuracy on the validation set decreases Or train for a long time, but always keep track of the model snapshot that worked best on val

Model Ensembles

- 1. Train multiple independent models
- 2. At test time average their results (Take average of predicted probability distributions, then choose argmax)

Enjoy 2% extra performance

How to improve single-model performance?



Regularization

Regularization: Add term to loss

$$L=rac{1}{N}\sum_{i=1}^{N}\sum_{j
eq y_i}\max(0,f(x_i;W)_j-f(x_i;W)_{y_i}+1)+\lambda R(W)$$

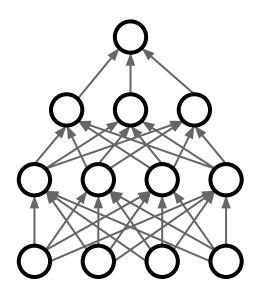
In common use:

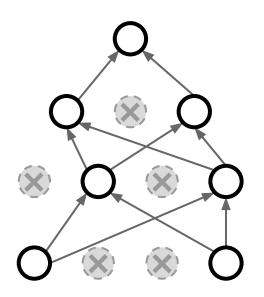
L2 regularization
$$R(W) = \sum_{k} \sum_{l} W_{k,l}^2$$
 (Weight decay)

L1 regularization
$$R(W) = \sum_{k} \sum_{l} |W_{k,l}|$$

Elastic net (L1 + L2)
$$R(W) = \sum_{k} \sum_{l} \beta W_{k,l}^{2} + |W_{k,l}|$$

In each forward pass, randomly set some neurons to zero Probability of dropping is a hyperparameter; 0.5 is common

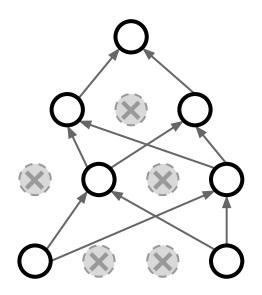




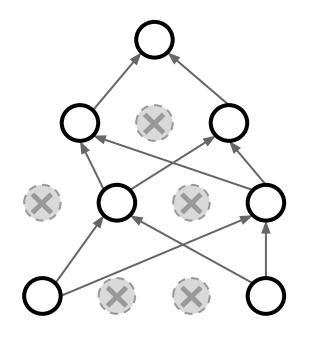
Srivastava et al, "Dropout: A simple way to prevent neural networks from overfitting", JMLR 2014

```
p = 0.5 # probability of keeping a unit active. higher = less dropout
def train_step(X):
  """ X contains the data """
  # forward pass for example 3-layer neural network
  H1 = np.maximum(0, np.dot(W1, X) + b1)
  U1 = np.random.rand(*H1.shape) < p # first dropout mask
  H1 *= U1 # drop!
  H2 = np.maximum(0, np.dot(W2, H1) + b2)
  U2 = np.random.rand(*H2.shape) < p # second dropout mask
  H2 *= U2 # drop!
  out = np.dot(W3, H2) + b3
  # backward pass: compute gradients... (not shown)
  # perform parameter update... (not shown)
```

Example forward pass with a 3-layer network using dropout



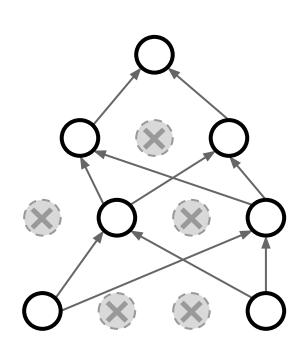
How can this possibly be a good idea?



Forces the network to have a redundant representation; Prevents co-adaptation of features



How can this possibly be a good idea?



Another interpretation:

Dropout is training a large **ensemble** of models (that share parameters).

Each binary mask is one model

An FC layer with 4096 units has $2^{4096} \sim 10^{1233}$ possible masks! Only $\sim 10^{82}$ atoms in the universe...

Dropout makes our output random!

Output Input (label) (image)
$$y = f_W(x,z) \quad \text{Random} \quad \text{mask}$$

Want to "average out" the randomness at test-time

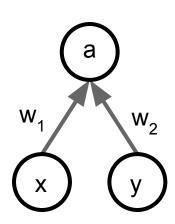
$$y = f(x) = E_z[f(x,z)] = \int p(z)f(x,z)dz$$

But this integral seems hard ...

Want to approximate the integral

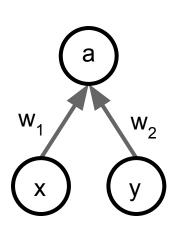
$$y = f(x) = E_z[f(x,z)] = \int p(z)f(x,z)dz$$

Consider a single neuron.



Want to approximate the integral

$$y = f(x) = E_z[f(x,z)] = \int p(z)f(x,z)dz$$

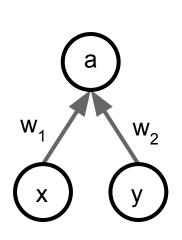


Consider a single neuron.

At test time we have: $E[a] = w_1x + w_2y$

Want to approximate the integral

$$y = f(x) = E_z[f(x,z)] = \int p(z)f(x,z)dz$$



Consider a single neuron.

At test time we have: $E[a] = w_1x + w_2y$

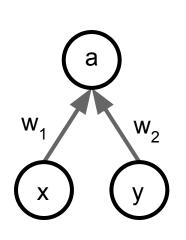
During training we have: $E[a] = \frac{1}{4}(w_1x + w_2y) + \frac{1}{4}(w_1x + w_20)$

$$+\frac{1}{4}(w_10+w_20)+\frac{1}{4}(w_10+w_2y)$$

$$= \frac{1}{2}(w_1x + w_2y)$$

Want to approximate the integral

$$y = f(x) = E_z[f(x,z)] = \int p(z)f(x,z)dz$$



Consider a single neuron.

At test time we have: $E[a] = w_1x + w_2y$

During training we have: $E[a] = \frac{1}{4}(w_1x + w_2y) + \frac{1}{4}(w_1x + w_20)$

At test time, **multiply** by dropout probability

$$+\frac{1}{4}(w_10+w_20)+\frac{1}{4}(w_10+w_2y)$$

$$= \frac{1}{2}(w_1x + w_2y)$$

```
def predict(X):
    # ensembled forward pass
H1 = np.maximum(0, np.dot(W1, X) + b1) * p # NOTE: scale the activations
H2 = np.maximum(0, np.dot(W2, H1) + b2) * p # NOTE: scale the activations
out = np.dot(W3, H2) + b3
```

At test time all neurons are active always => We must scale the activations so that for each neuron: output at test time = expected output at training time

```
Vanilla Dropout: Not recommended implementation (see notes below)
p = 0.5 # probability of keeping a unit active, higher = less dropout
def train step(X):
  """ X contains the data """
 # forward pass for example 3-layer neural network
 H1 = np.maximum(0, np.dot(W1, X) + b1)
 U1 = np.random.rand(*H1.shape) < p # first dropout mask
 H1 *= U1 # drop!
 H2 = np.maximum(0, np.dot(W2, H1) + b2)
 U2 = np.random.rand(*H2.shape) < p # second dropout mask
 H2 *= U2 # drop!
 out = np.dot(W3, H2) + b3
 # backward pass: compute gradients... (not shown)
 # perform parameter update... (not shown)
def predict(X):
 # ensembled forward pass
 H1 = np.maximum(0, np.dot(W1, X) + b1) * p # NOTE: scale the activations
 H2 = np.maximum(0, np.dot(W2, H1) + b2) * p # NOTE: scale the activations
 out = np.dot(W3, H2) + b3
```

Dropout Summary

drop in train time

scale at test time

More common: "Inverted dropout"

```
p = 0.5 # probability of keeping a unit active. higher = less dropout
def train step(X):
  # forward pass for example 3-layer neural network
  H1 = np.maximum(0, np.dot(W1, X) + b1)
 U1 = (np.random.rand(*H1.shape) < p) / p # first dropout mask. Notice /p!
  H1 *= U1 # drop!
 H2 = np.maximum(0, np.dot(W2, H1) + b2)
 U2 = (np.random.rand(*H2.shape) < p) / p # second dropout mask. Notice /p!
 H2 *= U2 # drop!
  out = np.dot(W3, H2) + b3
 # backward pass: compute gradients... (not shown)
  # perform parameter update... (not shown)
                                                                      test time is unchanged!
def predict(X):
 # ensembled forward pass
 H1 = np.maximum(0, np.dot(W1, X) + b1) # no scaling necessary
 H2 = np.maximum(0, np.dot(W2, H1) + b2)
 out = np.dot(W3, H2) + b3
```

Regularization: A common pattern

Training: Add some kind of randomness

$$y = f_W(x, z)$$

Testing: Average out randomness (sometimes approximate)

$$y = f(x) = E_z[f(x,z)] = \int p(z)f(x,z)dz$$

Regularization: A common pattern

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$$y = f_W(x, z)$$

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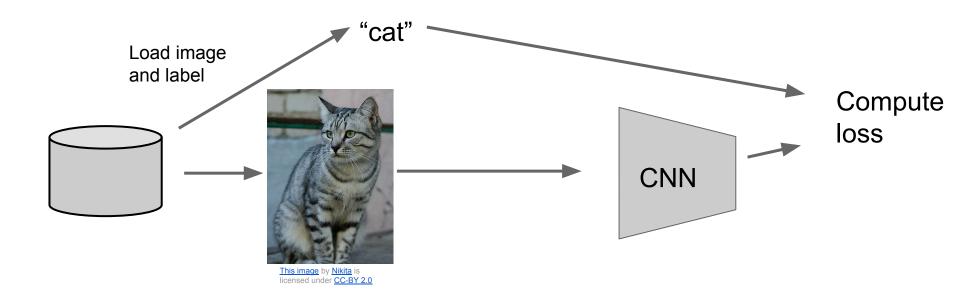
$$y = f(x) = E_z[f(x,z)] = \int p(z)f(x,z)dz$$

Example: Batch Normalization

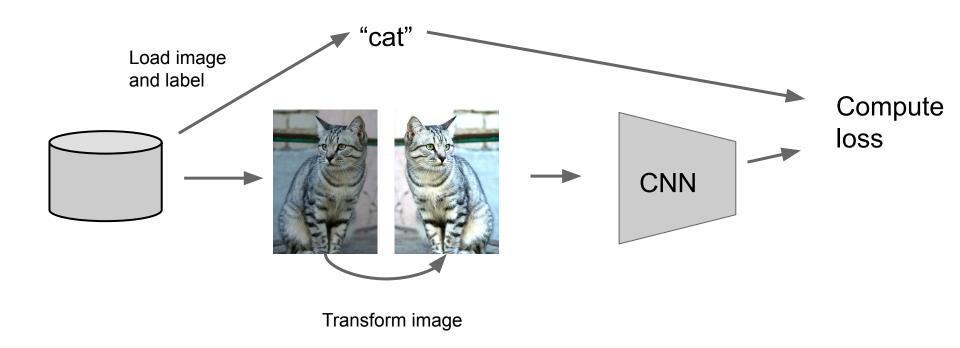
Training:
Normalize using
stats from random
minibatches

Testing: Use fixed stats to normalize

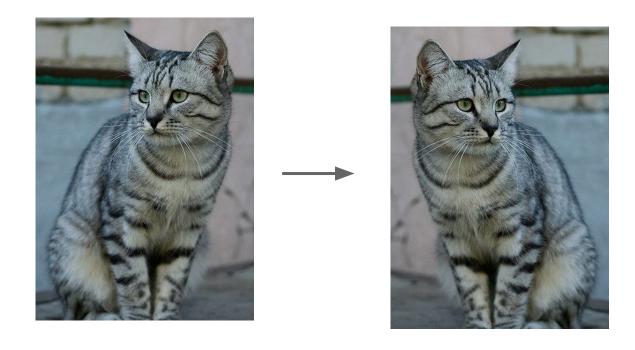
Regularization: Data Augmentation



Regularization: Data Augmentation



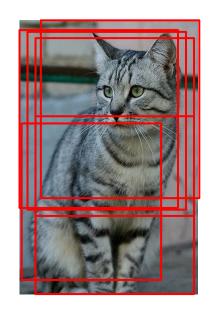
Data Augmentation Horizontal Flips



Data Augmentation Random crops and scales

Training: sample random crops / scales ResNet:

- 1. Pick random L in range [256, 480]
- 2. Resize training image, short side = L
- 3. Sample random 224 x 224 patch

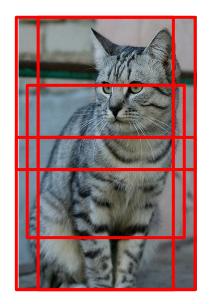


Data Augmentation Random crops and scales

Training: sample random crops / scales

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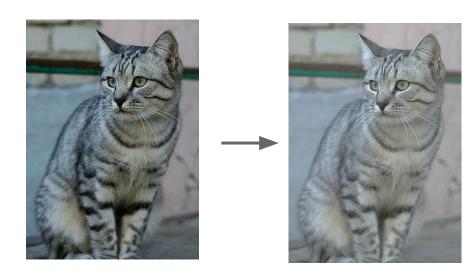
Testing: average a fixed set of crops

ResNet:

- 1. Resize image at 5 scales: {224, 256, 384, 480, 640}
- 2. For each size, use 10 224 x 224 crops: 4 corners + center, + flips

Data Augmentation Color Jitter

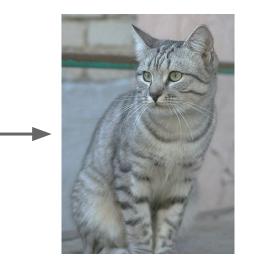
Simple: Randomize contrast and brightness



Data Augmentation Color Jitter

Simple: Randomize contrast and brightness





More Complex:

- 1. Apply PCA to all [R, G, B] pixels in training set
- 2. Sample a "color offset" along principal component directions
- Add offset to all pixels of a training image

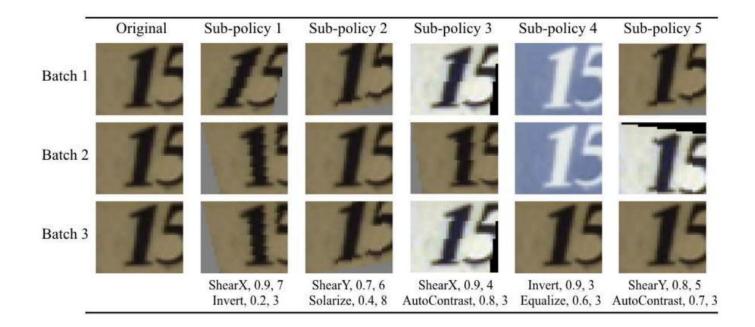
(As seen in [Krizhevsky et al. 2012], ResNet, etc)

Data Augmentation Get creative for your problem!

Examples of data augmentations:

- translation
- rotation
- stretching
- shearing,
- lens distortions, ... (go crazy)

Automatic Data Augmentation



Cubuk et al., "AutoAugment: Learning Augmentation Strategies from Data", CVPR 2019

Regularization: A common pattern

Training: Add random noise

Testing: Marginalize over the noise

Examples:

Dropout

Batch Normalization

Data Augmentation

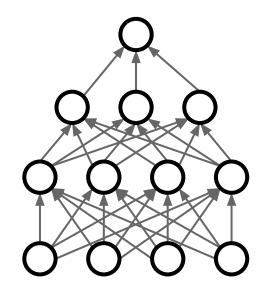
Regularization: DropConnect

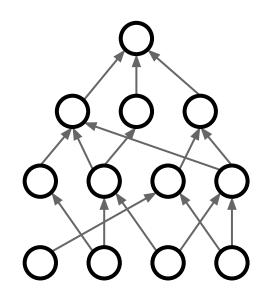
Training: Drop connections between neurons (set weights to 0)

Testing: Use all the connections

Examples:

Dropout
Batch Normalization
Data Augmentation
DropConnect





Wan et al, "Regularization of Neural Networks using DropConnect", ICML 2013

Regularization: Fractional Pooling

Training: Use randomized pooling regions

Testing: Average predictions from several regions

Examples:

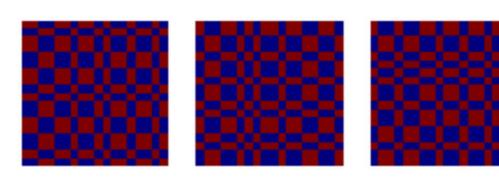
Dropout

Batch Normalization

Data Augmentation

DropConnect

Fractional Max Pooling



Graham, "Fractional Max Pooling", arXiv 2014

Regularization: Stochastic Depth

Training: Skip some layers in the network

Testing: Use all the layer

Examples:

Dropout

Batch Normalization

Data Augmentation

DropConnect

Fractional Max Pooling

Stochastic Depth (will become more

clear in next week's lecture)

Huang et al, "Deep Networks with Stochastic Depth", ECCV 2016

Regularization: Cutout

Training: Set random image regions to zero

Testing: Use full image

Examples:

Dropout

Batch Normalization

Data Augmentation

DropConnect

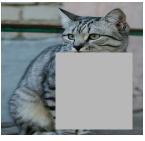
Fractional Max Pooling

Stochastic Depth

Cutout / Random Crop

DeVries and Taylor, "Improved Regularization of Convolutional Neural Networks with Cutout", arXiv 2017









Works very well for small datasets like CIFAR, less common for large datasets like ImageNet

Regularization: Mixup

Training: Train on random blends of images

Testing: Use original images

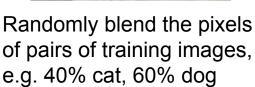
Examples:

Dropout
Batch Normalization
Data Augmentation
DropConnect
Fractional Max Pooling
Stochastic Depth
Cutout / Random Crop
Mixup









Target label: cat: 0.4 dog: 0.6

CNN

Zhang et al, "mixup: Beyond Empirical Risk Minimization", ICLR 2018

Regularization: CutMix

Training: Train on random blends of images

Testing: Use original images

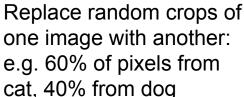
Examples:

Dropout
Batch Normalization
Data Augmentation
DropConnect
Fractional Max Pooling
Stochastic Depth
Cutout / Random Crop
Mixup









CNN Target label: cat: 0.4 dog: 0.6

Yun et al, "CutMix: Regularization Strategies to Train Strong Classifiers with Localizable Features", ICCV 2019

Regularization: Label Smoothing

Training: Change target distribution

Testing: Take argmax over predictions

Examples:

Dropout

Batch Normalization

Data Augmentation

DropConnect

Fractional Max Pooling

Stochastic Depth

Cutout / Random Crop

Mixup

Label Smoothing



<u>Standard Training:</u> <u>Label Smoothing:</u>

Cat: 100% Cat: 90% Dog: 5% Fish: 0% Fish: 5%

Set target distribution to be $1 - \frac{K-1}{K}\epsilon$ on the correct category and ϵ/K on all other categories, with K categories and $\epsilon \in 0,1$. Loss is cross-entropy between predicted and target distribution.

Szegedy et al, "Rethinking the Inception Architecture for Computer Vision". CVPR 2015

Regularization - In practice

Training: Add random noise

Testing: Marginalize over the noise

Examples:

Dropout

Batch Normalization

Data Augmentation

DropConnect

Fractional Max Pooling

Stochastic Depth

Cutout / Random Crop

Mixup

- Use dropout for large fully-connected layers
- Using **batchnorm** is always a good idea
- Try Cutout, MixUp, CutMix,
 Stochastic Depth, Label Smoothing
 to squeeze out a bit of extra
 performance

Choosing Hyperparameters: Grid Search

Choose several values for each hyperparameter (Often space choices log-linearly)

Example:

Weight decay: [1x10⁻⁴, 1x10⁻³, 1x10⁻², 1x10⁻¹]

Learning rate: $[1x10^{-4}, 1x10^{-3}, 1x10^{-2}, 1x10^{-1}]$

Evaluate all possible choices on this hyperparameter grid

Choosing Hyperparameters: Random search

Choose several values for each hyperparameter (Often space choices log-linearly)

Example:

Weight decay: **log-uniform** on [1x10⁻⁴, 1x10⁻¹]

Learning rate: **log-uniform** on [1x10⁻⁴, 1x10⁻¹]

Run many different trials

Random Search vs. Grid Search

Random Search for Hyper-Parameter Optimization Bergstra and Bengio, 2012

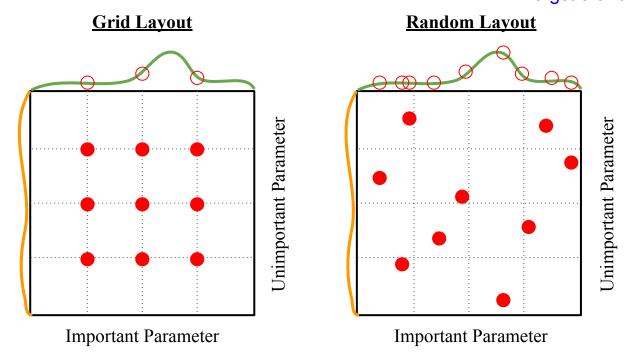


Illustration of Bergstra et al., 2012 by Shayne Longpre, copyright CS231n 2017

(without tons of GPUs)

Step 1: Check initial loss

Turn off weight decay, sanity check loss at initialization e.g. log(C) for softmax with C classes

Step 1: Check initial loss

Step 2: Overfit a small sample

Try to train to 100% training accuracy on a small sample of training data (~5-10 minibatches); fiddle with architecture, learning rate, weight initialization

Loss not going down? LR too low, bad initialization Loss explodes to Inf or NaN? LR too high, bad initialization

Step 1: Check initial loss

Step 2: Overfit a small sample

Step 3: Find LR that makes loss go down

Use the architecture from the previous step, use all training data, turn on small weight decay, find a learning rate that makes the loss drop significantly within ~100 iterations

Good learning rates to try: 1e-1, 1e-2, 1e-3, 1e-4

Step 1: Check initial loss

Step 2: Overfit a small sample

Step 3: Find LR that makes loss go down

Step 4: Coarse grid, train for ~1-5 epochs

Choose a few values of learning rate and weight decay around what worked from Step 3, train a few models for ~1-5 epochs.

Good weight decay to try: 1e-4, 1e-5, 0

Step 1: Check initial loss

Step 2: Overfit a small sample

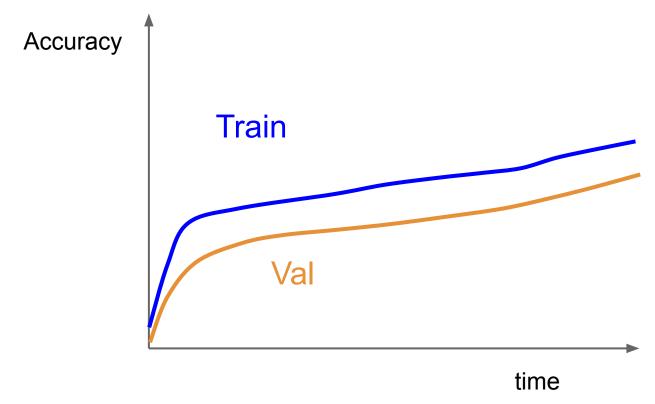
Step 3: Find LR that makes loss go down

Step 4: Coarse grid, train for ~1-5 epochs

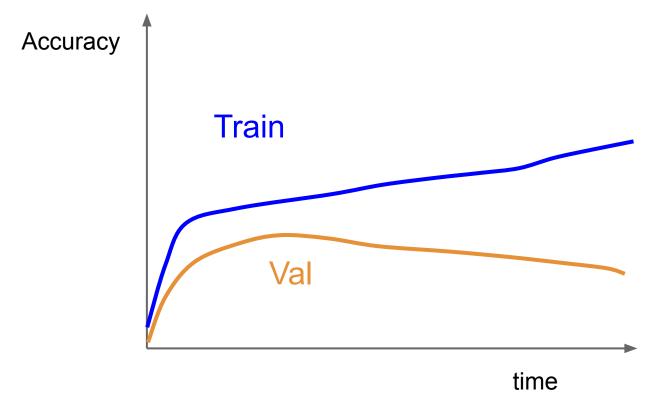
Step 5: Refine grid, train longer

Pick best models from Step 4, train them for longer (~10-20 epochs) without learning rate decay

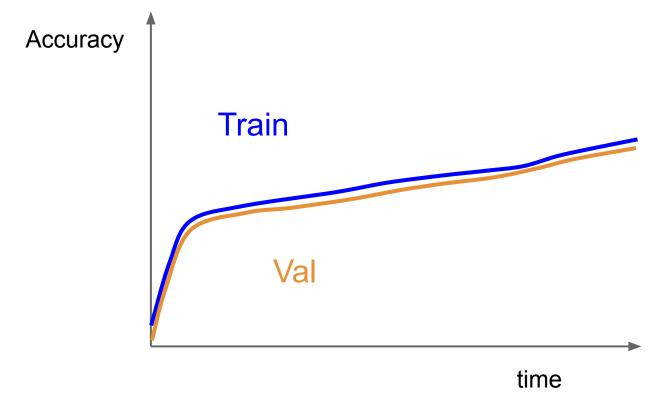
- Step 1: Check initial loss
- Step 2: Overfit a small sample
- Step 3: Find LR that makes loss go down
- Step 4: Coarse grid, train for ~1-5 epochs
- **Step 5**: Refine grid, train longer
- Step 6: Look at loss and accuracy curves



Q1. You see this. What should you do?

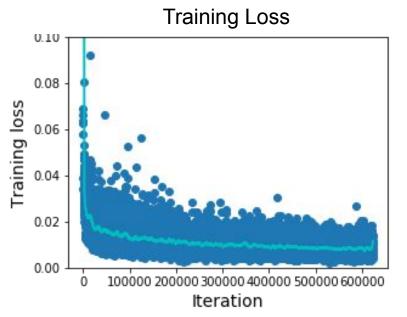


Q2. You see this. What should you do?

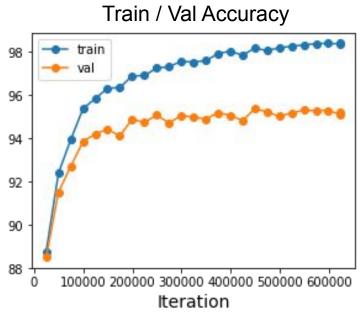


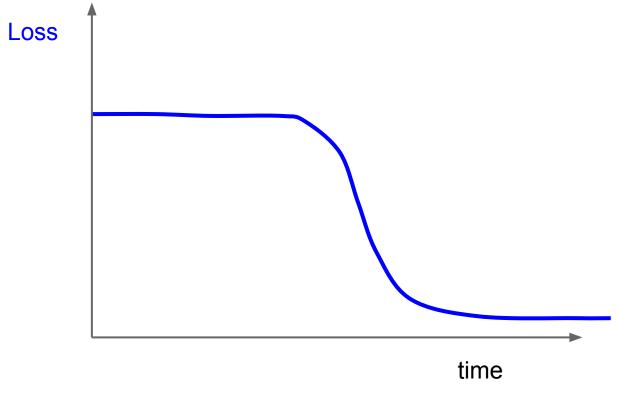
Q3. You see this. What should you do?

Look at learning curves!

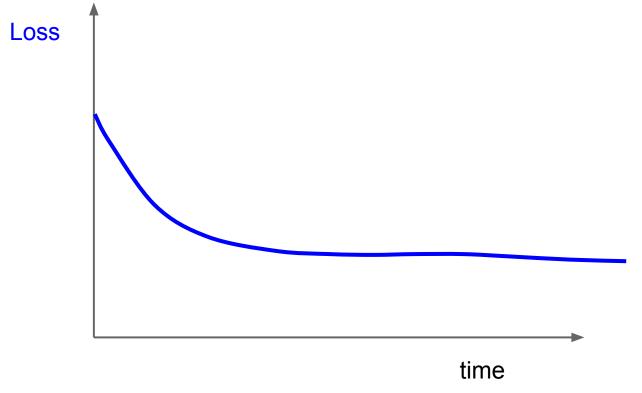


Losses may be noisy, use a scatter plot and also plot moving average to see trends better

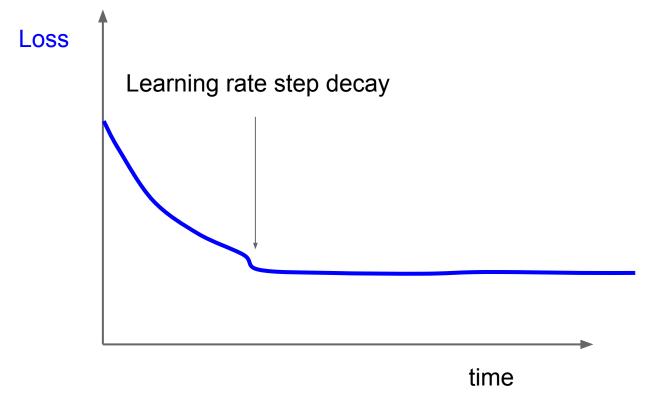




Q4. You see this. What should you do?



Q5. You see this. What should you do?



Q5. You see this. What should you do?

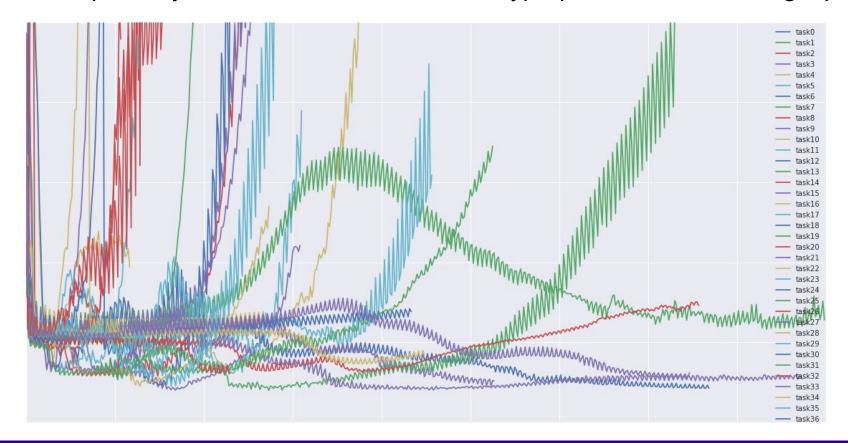
Cross-validation

We develop
"command centers"
to visualize all our
models training with
different
hyperparameters

check out <u>weights</u> and biases



You can plot all your loss curves for different hyperparameters on a single plot



- Step 1: Check initial loss
- Step 2: Overfit a small sample
- Step 3: Find LR that makes loss go down
- Step 4: Coarse grid, train for ~1-5 epochs
- **Step 5**: Refine grid, train longer
- **Step 6**: Look at loss and accuracy curves
- Step 7: GOTO step 5

Hyperparameters to play with:

- learning rate,
- Its decay schedule, update type
- regularization (L2/Dropout strength)

This image by Paolo Guereta is licensed under CC-BY 2.0

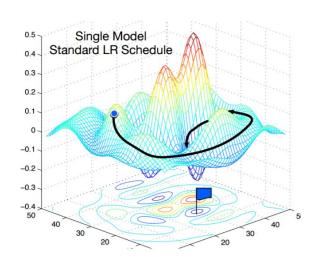
Summary

- Improve your training error:
 - Optimizers
 - Learning rate schedules
- Improve your test error:
 - Regularization
 - Choosing Hyperparameters

Next time: Visualizing and understanding neural networks

Model Ensembles: Tips and Tricks

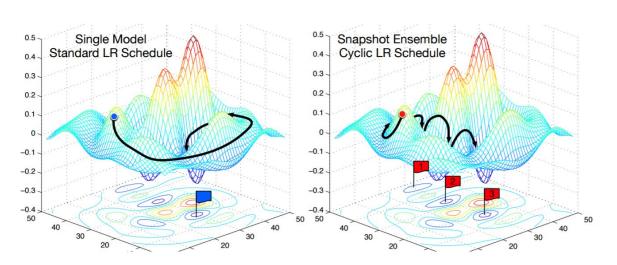
Instead of training independent models, use multiple snapshots of a single model during training!



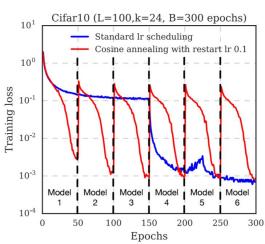
Loshchilov and Hutter, "SGDR: Stochastic gradient descent with restarts", arXiv 2016 Huang et al, "Snapshot ensembles: train 1, get M for free", ICLR 2017 Figures copyright Yixuan Li and Geoff Pleiss, 2017. Reproduced with permission.

Model Ensembles: Tips and Tricks

Instead of training independent models, use multiple snapshots of a single model during training!



Loshchilov and Hutter, "SGDR: Stochastic gradient descent with restarts", arXiv 2016 Huang et al, "Snapshot ensembles: train 1, get M for free", ICLR 2017 Figures copyright Yixuan Li and Geoff Pleiss. 2017. Reproduced with permission.



Cyclic learning rate schedules can make this work even better!

Model Ensembles: Tips and Tricks

Instead of using actual parameter vector, keep a moving average of the parameter vector and use that at test time (Polyak averaging)

```
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
```

Polyak and Juditsky, "Acceleration of stochastic approximation by averaging", SIAM Journal on Control and Optimization, 1992.

Track the ratio of weight updates / weight magnitudes:

```
# assume parameter vector W and its gradient vector dW
param_scale = np.linalg.norm(W.ravel())

update = -learning_rate*dW # simple SGD update

update_scale = np.linalg.norm(update.ravel())

W += update # the actual update

print update_scale / param_scale # want ~1e-3
```

ratio between the updates and values: ~ 0.0002 / 0.02 = 0.01 (about okay) want this to be somewhere around 0.001 or so