Lecture 7:

Optimizing Neural Networks

Administrative: Assignment 2

Due 1/2 11:59pm

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

Administrative: Course Project

Project proposal due 1/29 11:59pm

Submit to Gradescope (1 per group, add all group members)

Expectations on course website

Project can change between Proposal and Milestone

Administrative: Midterm

In class, Feb 5

Covers up to lecture 8

Allowed:

-1 double sided handwritten “cheat sheet”

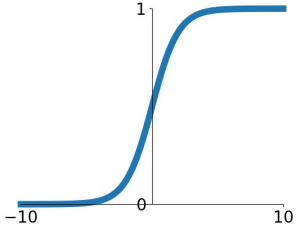
- 1 non-graphing calculator

Many practice exams in the Exam Archive

Last time: Activation Functions

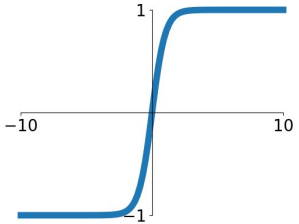
Sigmoid

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



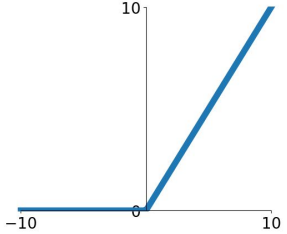
tanh

$$\tanh(x)$$



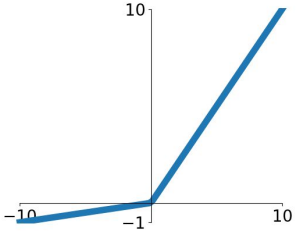
ReLU

$$\max(0, x)$$



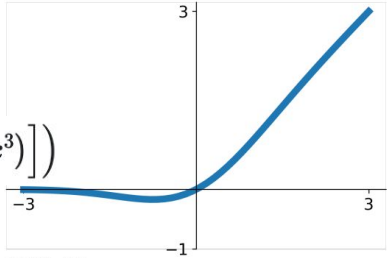
Leaky ReLU

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



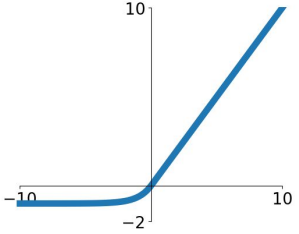
GeLU

$$0.5x\left(1+\tanh\left[\sqrt{2/\pi}\left(x+0.044715x^3\right)\right]\right)$$

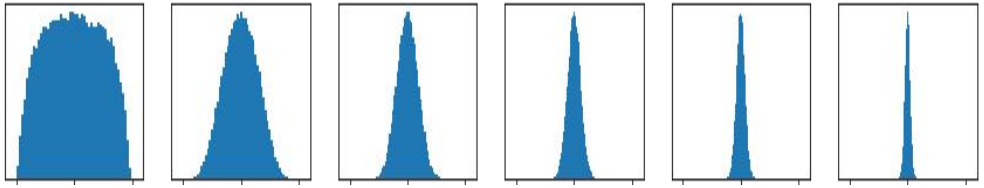


ELU

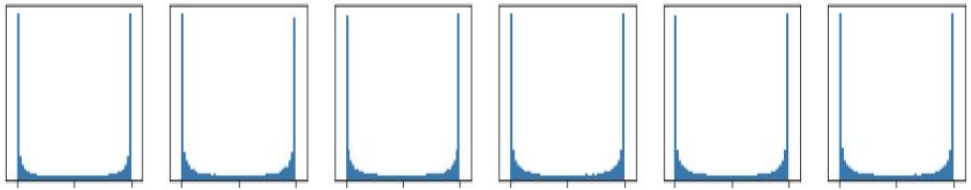
$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$



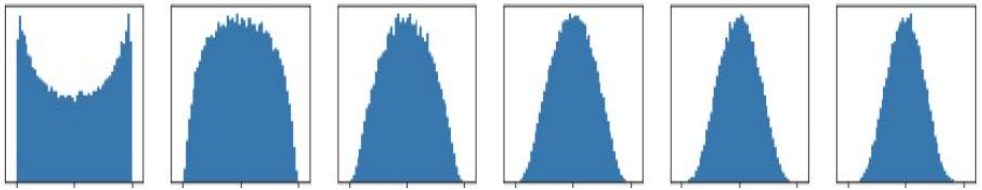
Last time: Weight Initialization



Initialization too small:
Activations go to zero, gradients also zero,
No learning =(

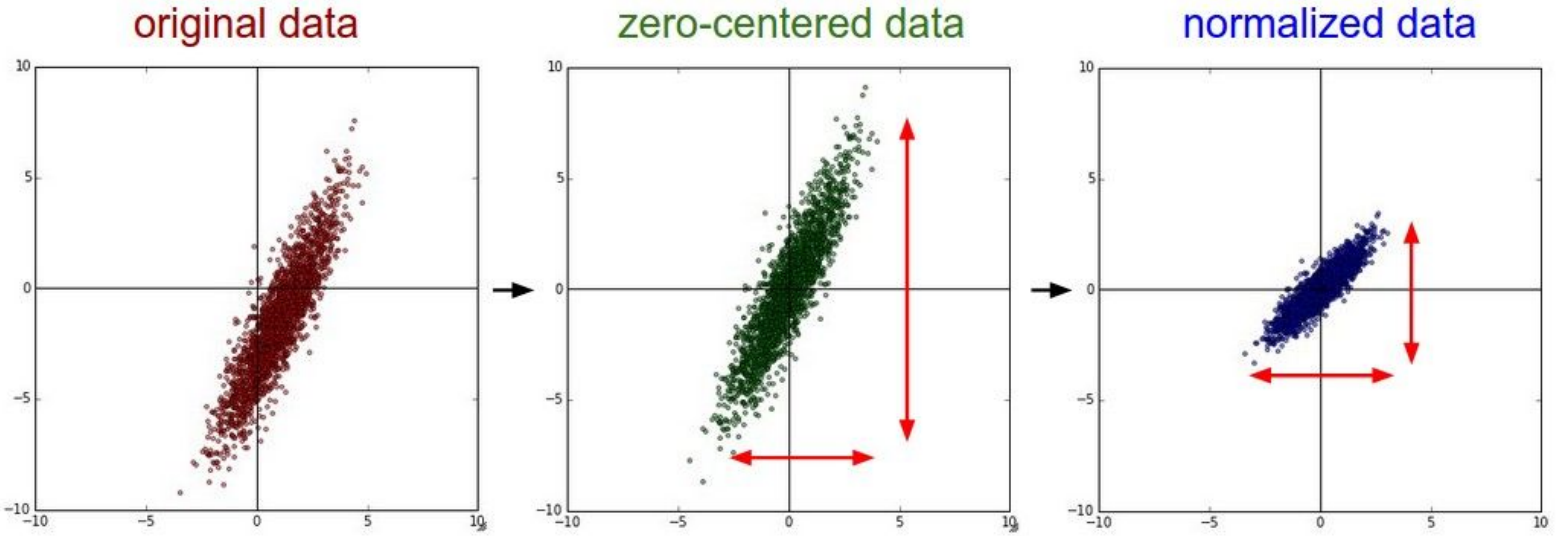


Initialization too big:
Activations saturate (for tanh),
Gradients zero, no learning =(



Initialization just right:
Nice distribution of activations at all layers,
Learning proceeds nicely =)

Last time: Data Preprocessing



Last Time: Batch Normalization

[Ioffe and Szegedy, 2015]

Input: $x : N \times D$

Learnable scale and shift parameters:

$$\gamma, \beta : D$$

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

$$\mu_j = \frac{1}{N} \sum_{i=1}^{N} x_{i,j}$$

Per-channel mean, shape is D

$$\sigma_j^2 = \frac{1}{N} \sum_{i=1}^{N} (x_{i,j} - \mu_j)^2$$

Per-channel var, shape is D

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

Normalized x, Shape is N x D

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

Output, Shape is N x D

Today

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

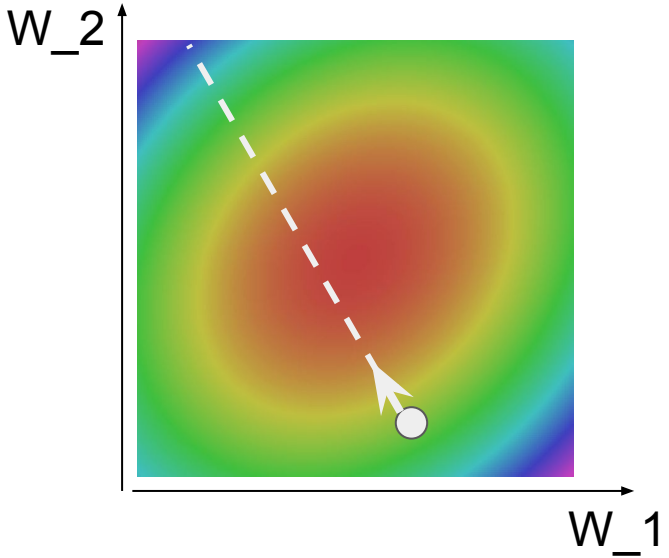
(Fancier) Optimizers

Can we do better than SGD?

Vanilla SGD

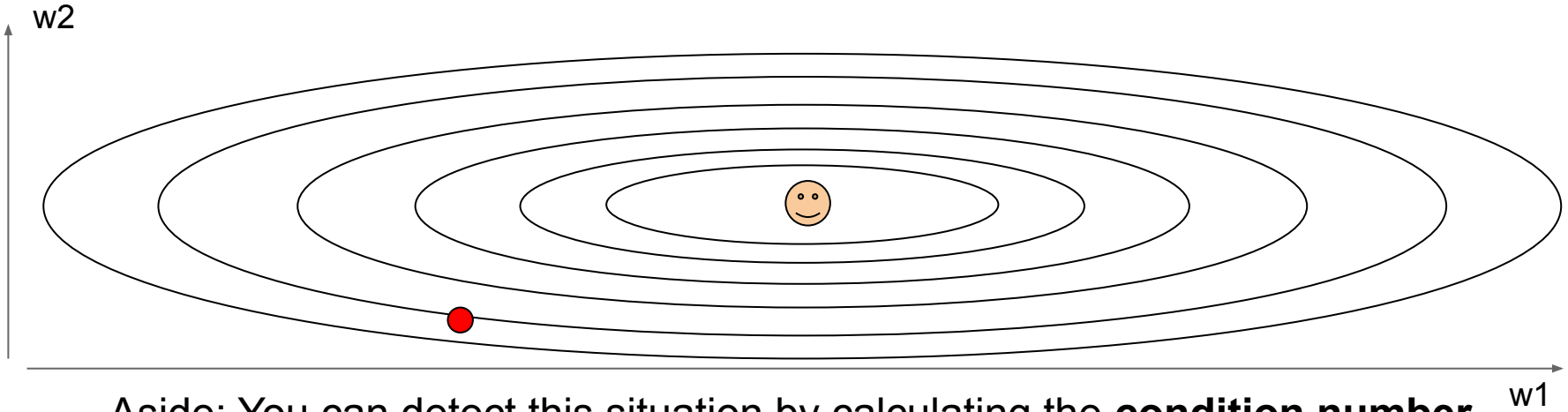
```
# Vanilla Gradient Descent

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



Optimization: Problem #1 with SGD

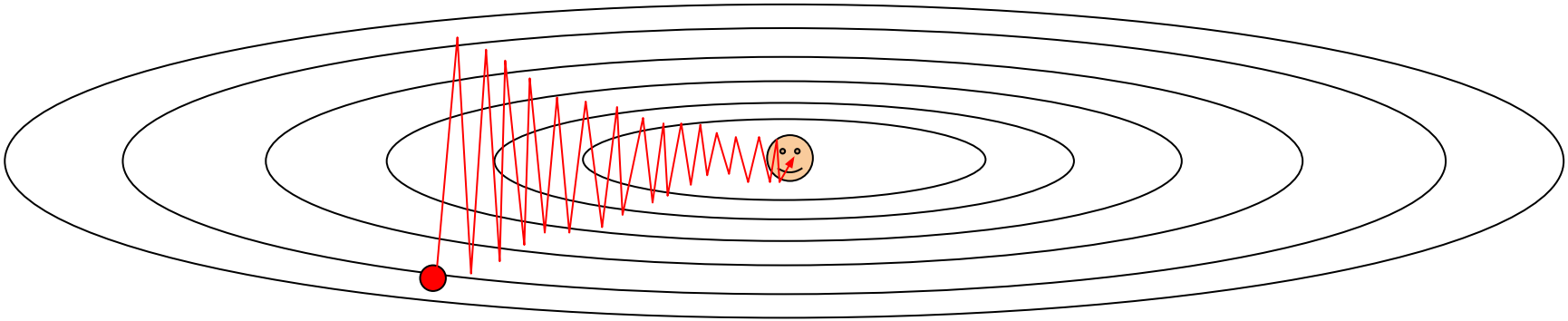
What if loss changes quickly in one direction and slowly in another?
What does gradient descent do?



Aside: You can detect this situation by calculating the **condition number**, which is the ratio of largest to smallest singular value of the Hessian matrix
Large ratio implies high condition number implies the loss is uneven

Optimization: Problem #1 with SGD

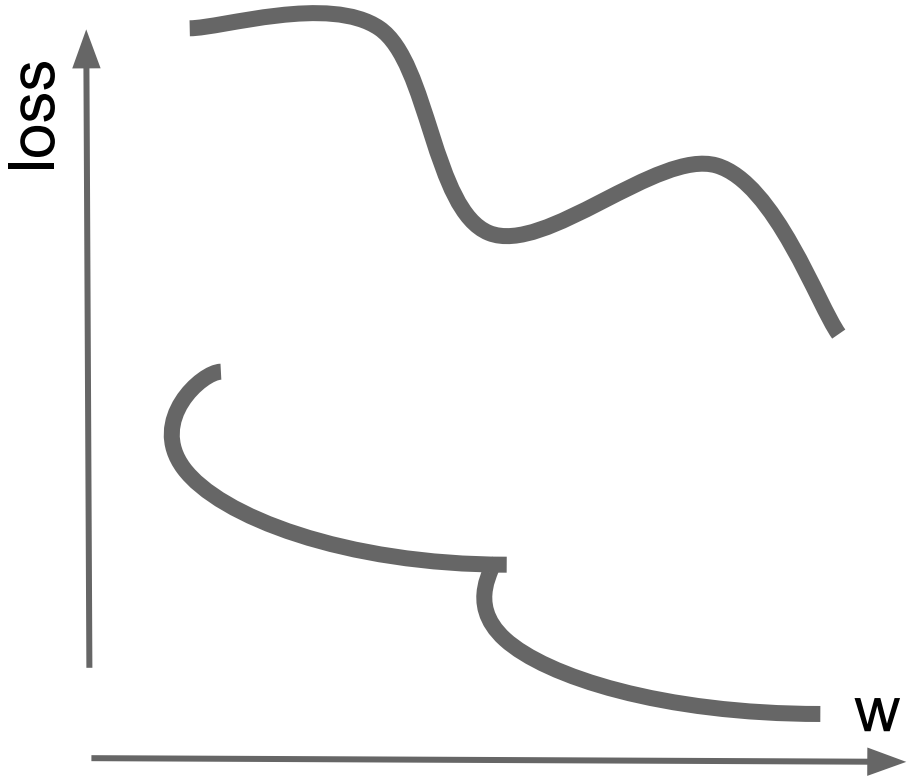
What if loss changes quickly in one direction and slowly in another?
What does gradient descent do?
Very slow progress along shallow dimension, jitter along steep direction



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

Optimization: Problem #2 with SGD

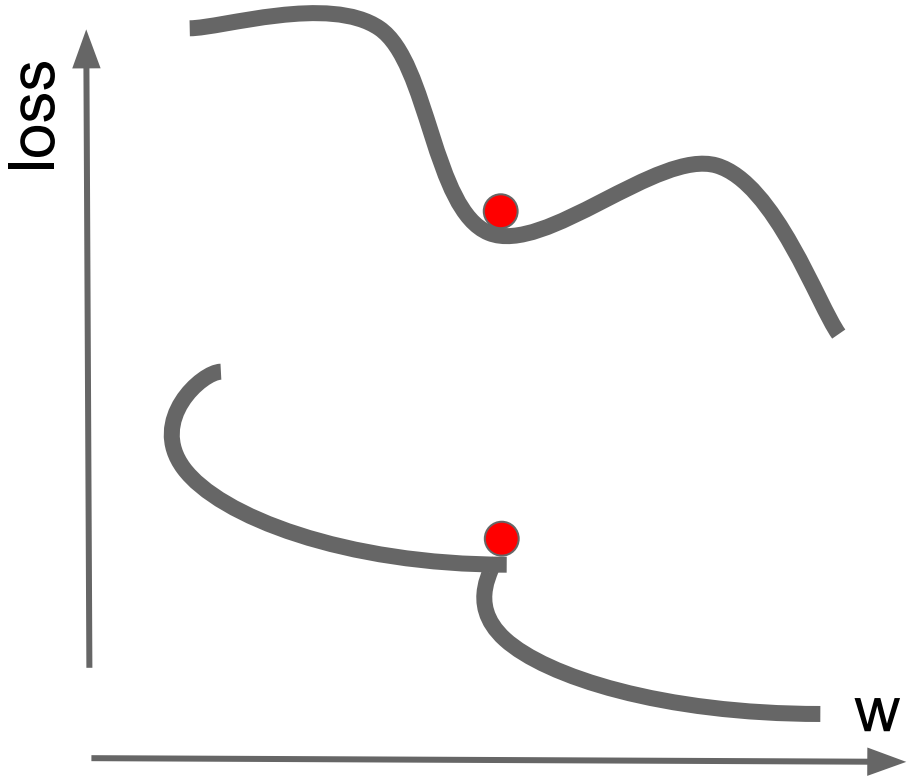
What if the loss function has a **local minima** or **saddle point**?



Optimization: Problem #2 with SGD

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

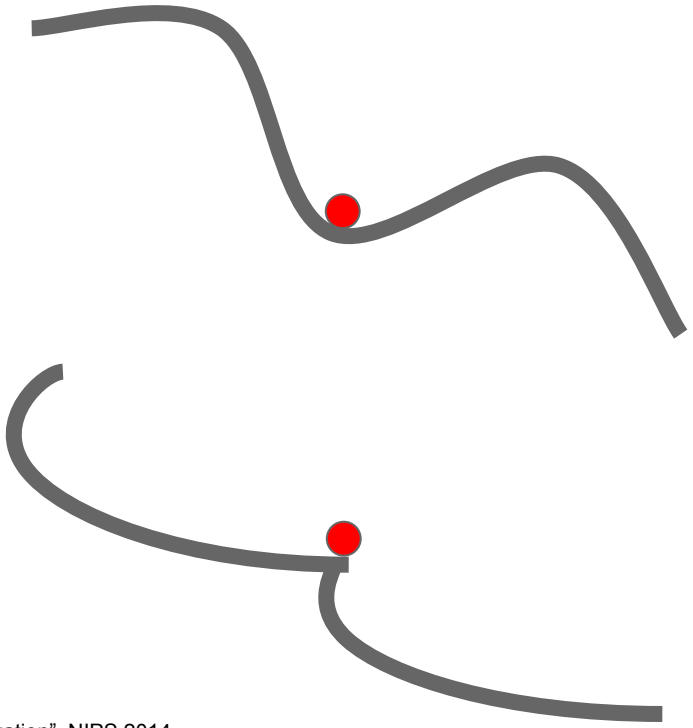
Zero gradient, gradient descent gets stuck



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



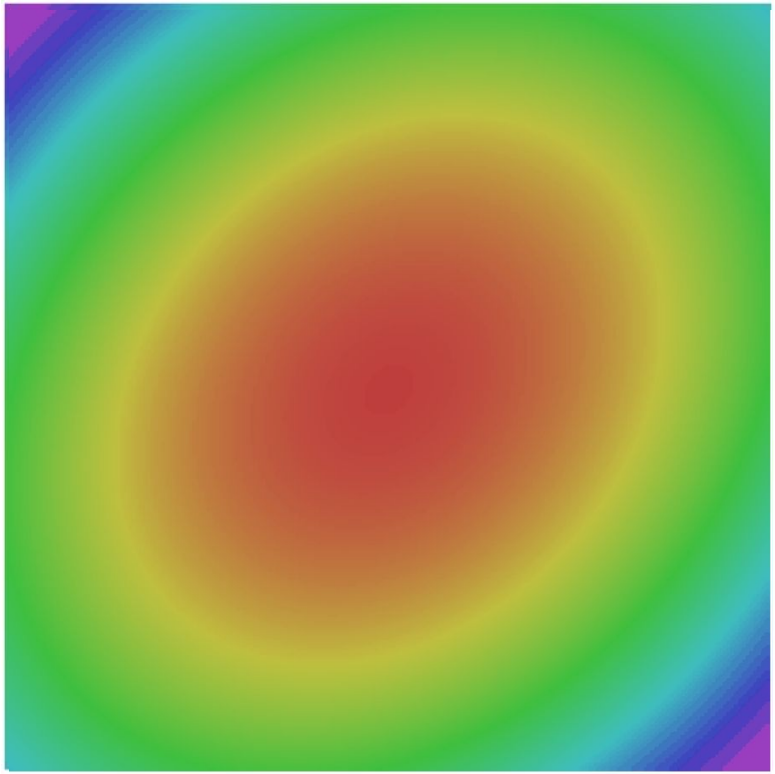
Dauphin et al, “Identifying and attacking the saddle point problem in high-dimensional non-convex optimization”, NIPS 2014

Optimization: Problem #3 with SGD

Our gradients come from minibatches so they can be noisy!

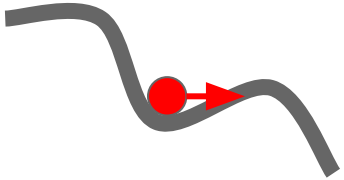
$$L(W) = \frac{1}{N} \sum_{i=1}^{N} L_i(x_i, y_i, W)$$

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

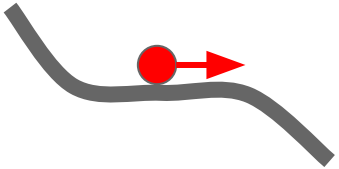


SGD + Momentum

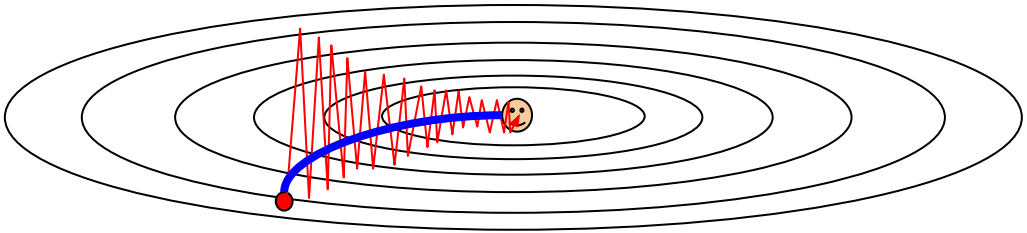
Local Minima



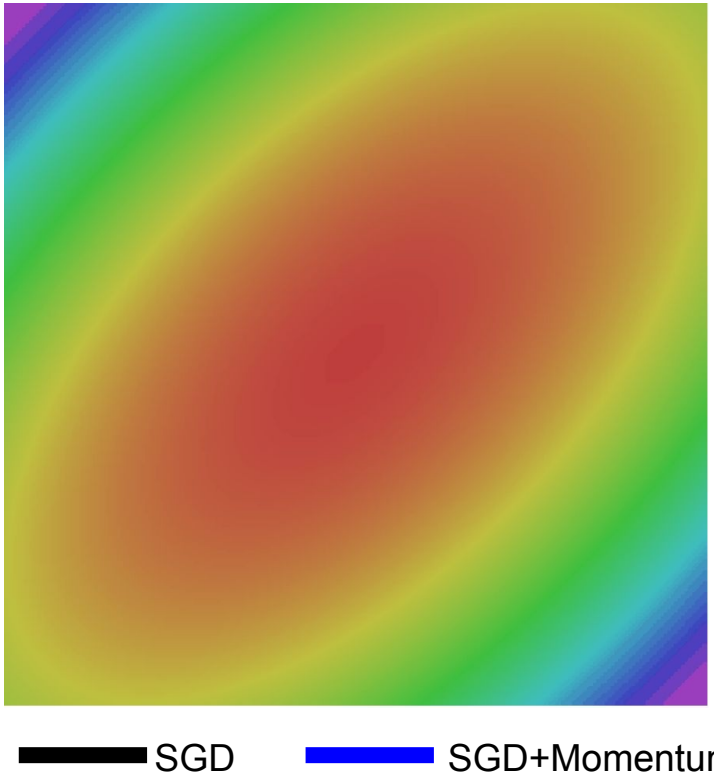
Saddle points



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:
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  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

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

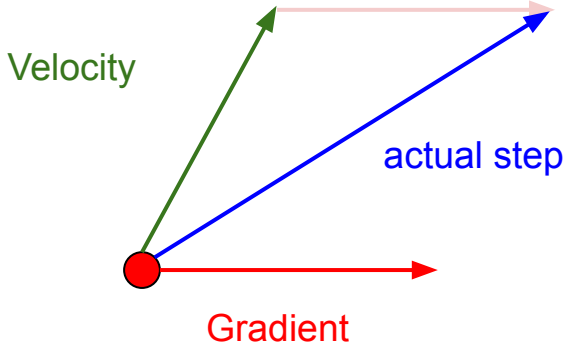
```
vx = 0
while True:
  dx = compute_gradient(x)
  vx = rho * vx + dx
  x -= learning_rate * vx
```

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:

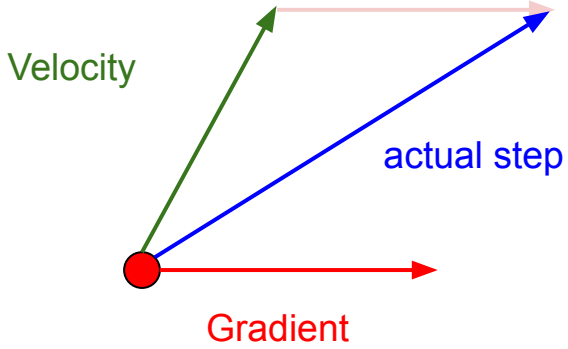


Combine gradient at current point with velocity to get step used to update weights

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

Nesterov Momentum

Momentum update:



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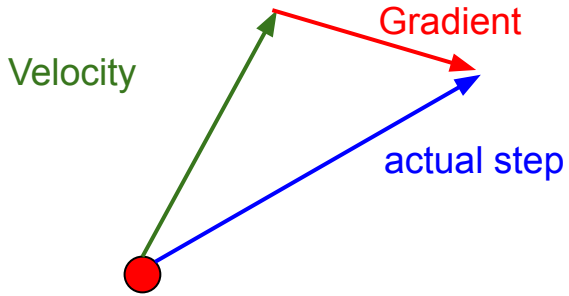
Nesterov Momentum



"Look ahead" to the point where updating using velocity would take us; compute gradient there and mix it with velocity to get actual update direction

Nesterov, "A method of solving a convex programming problem with convergence rate O(1/k^2)", 1983
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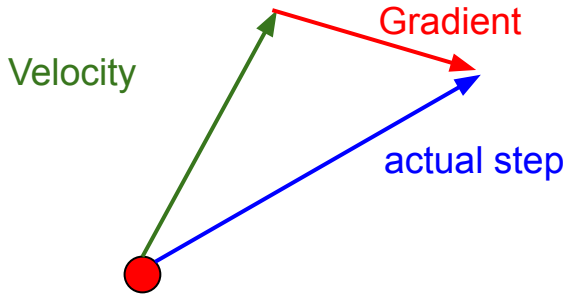
Nesterov Momentum

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



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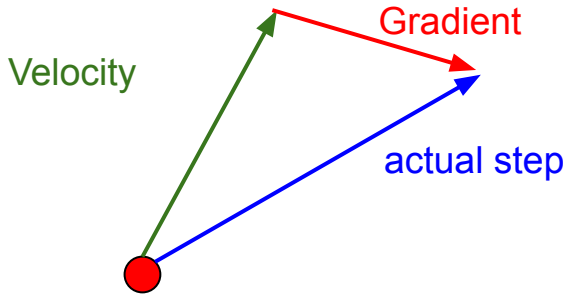
Nesterov Momentum

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

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



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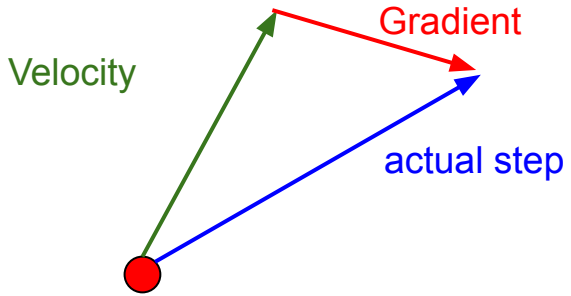
Change of variables $\tilde{x}_t = x_t + \rho v_t$ and rearrange:



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Nesterov Momentum

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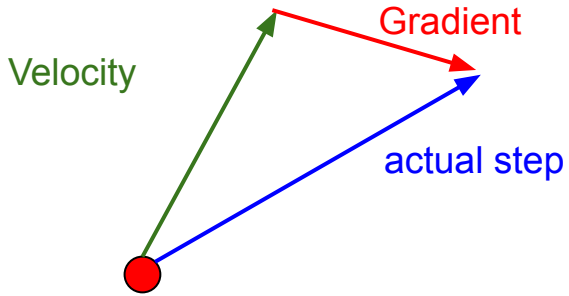


Change of variables $\tilde{x}_t = x_t + \rho v_t$ and rearrange:

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

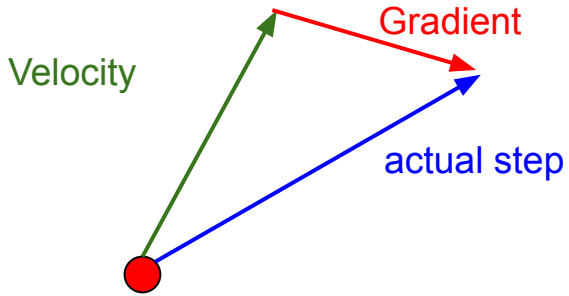
"Look ahead" to the point where updating using velocity would take us; compute gradient there and mix it with velocity to get actual update direction

Nesterov Momentum

That's it!

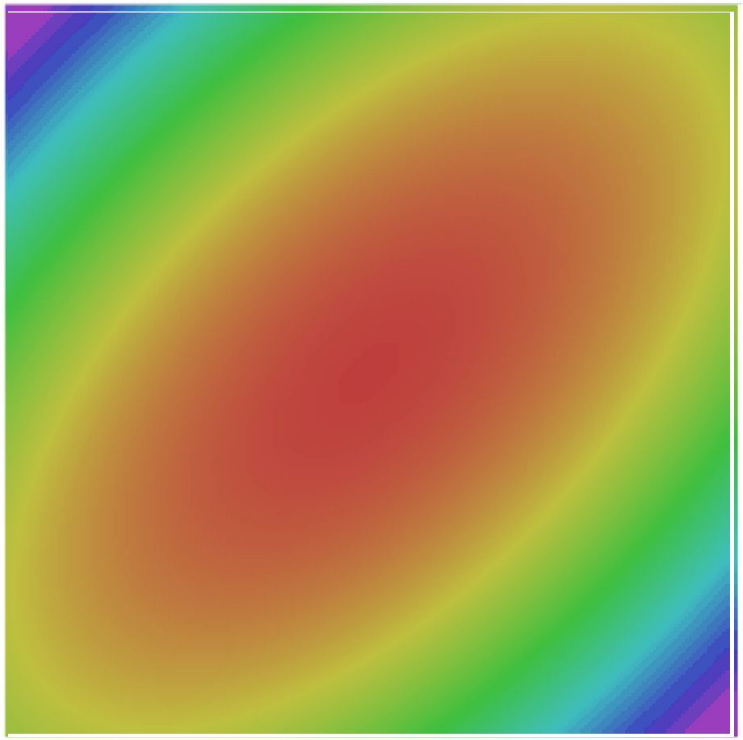
Step 1: Calculate the velocity at *t+1*
Step 2: Update the parameters using the velocities at *t+1* and *t*

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



"Look ahead" to the point where updating using velocity would take us; compute gradient there and mix it with velocity to get actual update direction

Nesterov Momentum



SGD

SGD+Momentum

Nesterov

AdaGrad

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

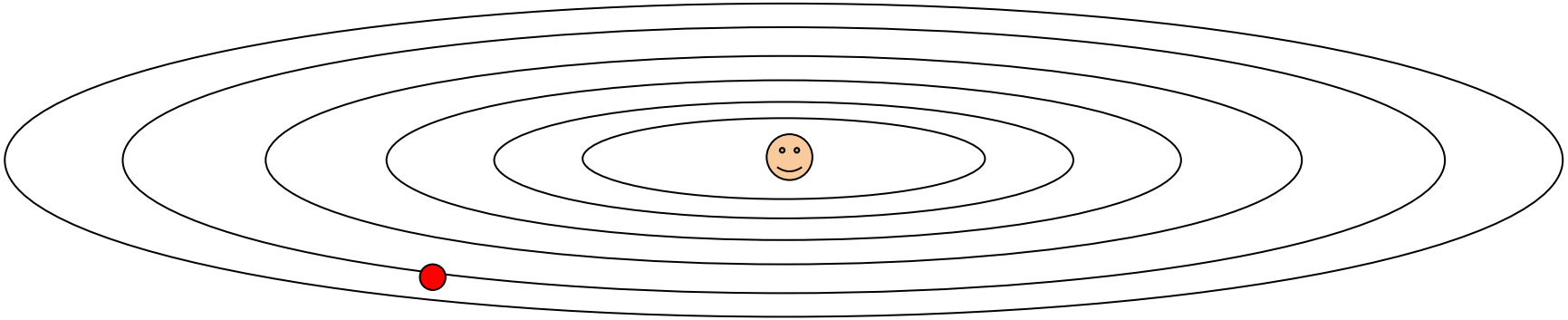
Added element-wise scaling of the gradient based on the historical sum of squares in each dimension

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

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

AdaGrad

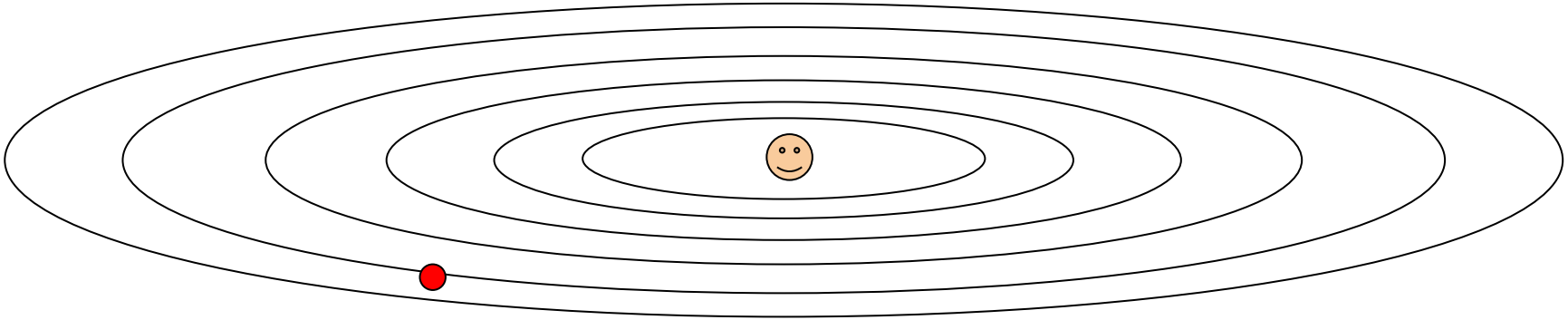
```
grad_squared = 0
while True:
  dx = compute_gradient(x)
  grad_squared += dx * dx
  x -= learning_rate * dx / (np.sqrt(grad_squared) + 1e-7)
```



Q: What happens with AdaGrad?

AdaGrad

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

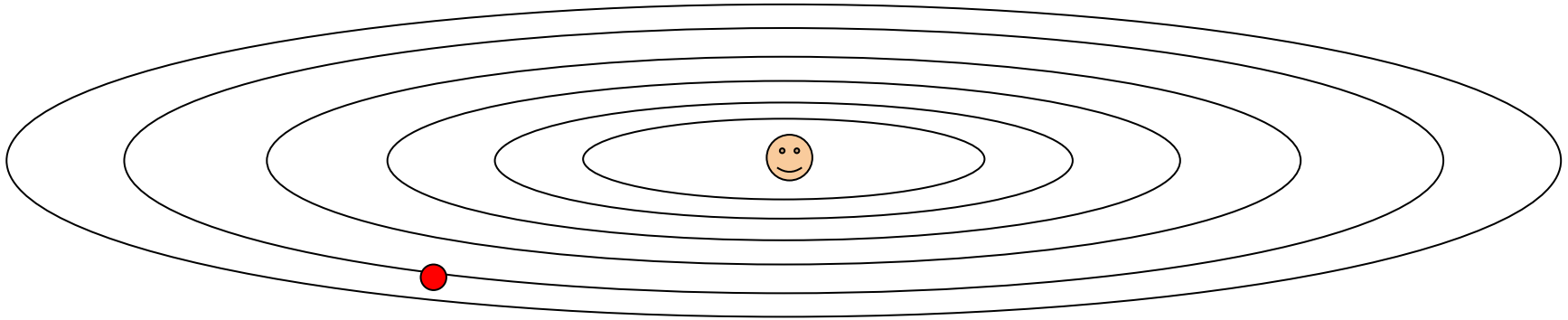


Q: What happens with AdaGrad?

Progress along “steep” directions is damped;
progress along “flat” directions is accelerated

AdaGrad

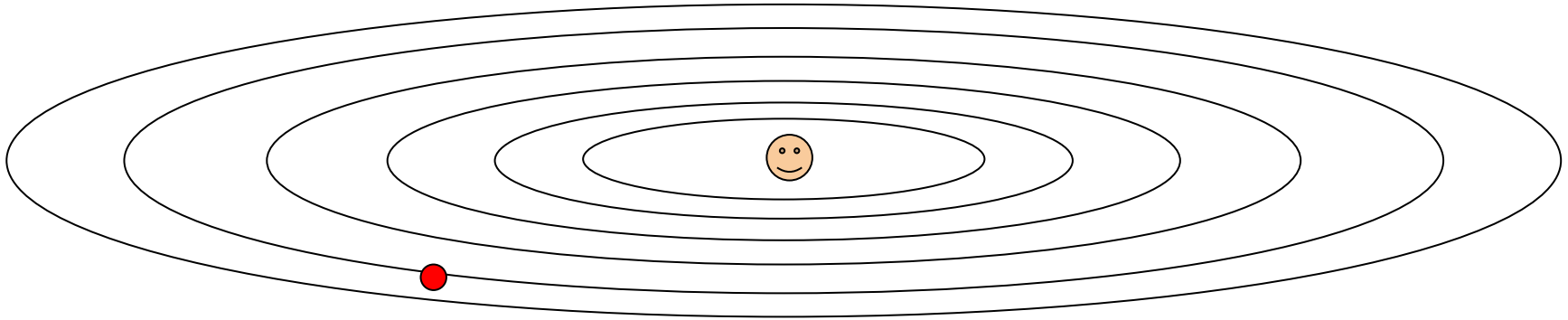
```
grad_squared = 0
while True:
  dx = compute_gradient(x)
  grad_squared += dx * dx
  x -= learning_rate * dx / (np.sqrt(grad_squared) + 1e-7)
```



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

AdaGrad

```
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

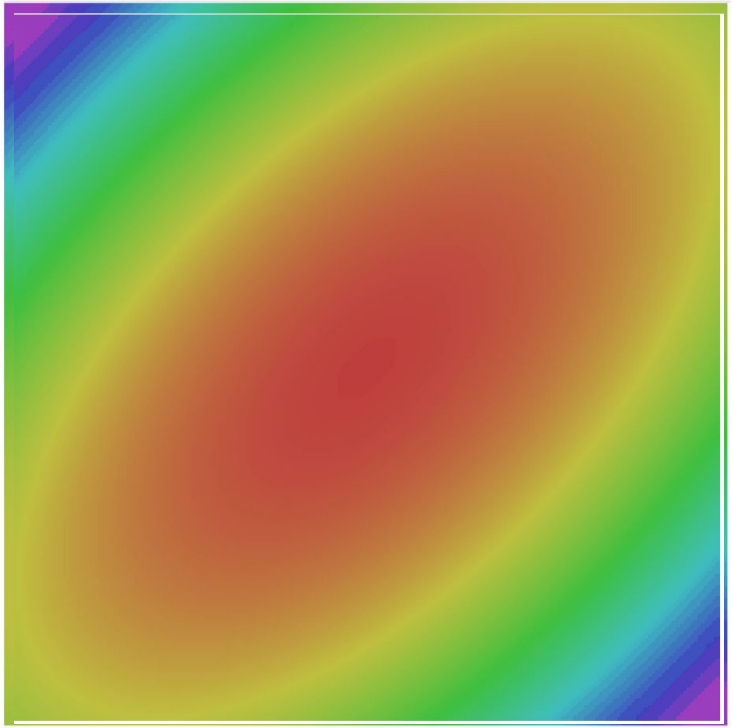
```
grad_squared = 0
while True:
  dx = compute_gradient(x)
  grad_squared += dx * dx
  x -= learning_rate * dx / (np.sqrt(grad_squared) + 1e-7)
```

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



SGD

SGD+Momentum

RMSProp

AdaGrad

(stuck due to decaying lr)

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))
```

Kingma and Ba, “Adam: A method for stochastic optimization”, ICLR 2015

Adam (almost)

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first_moment = 0
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while True:
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  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?

Kingma and Ba, "Adam: A method for stochastic optimization", ICLR 2015

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

Kingma and Ba, "Adam: A method for stochastic optimization", ICLR 2015

Adam (full form)

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

Momentum

Bias correction

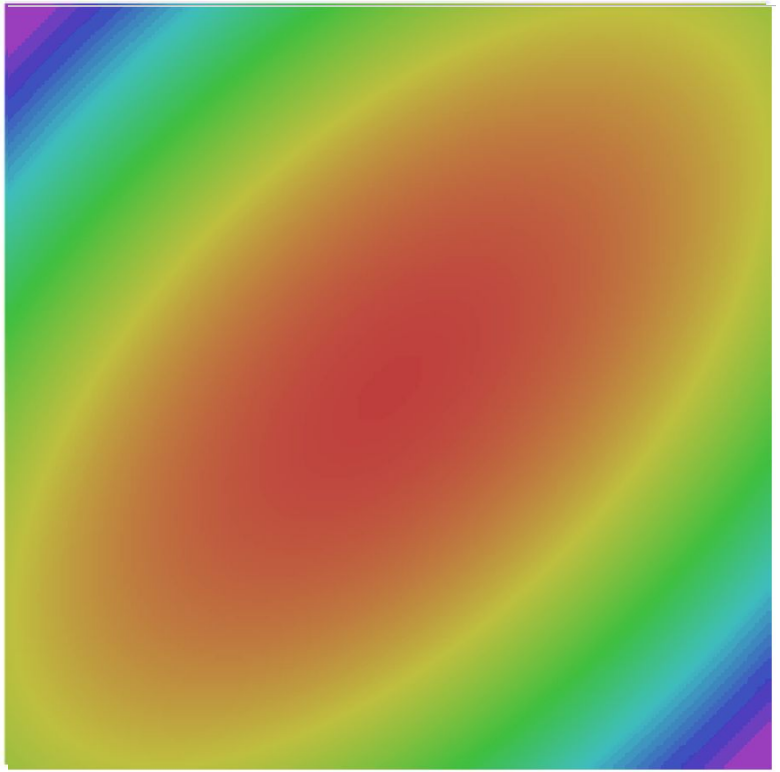
AdaGrad / RMSProp

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

Adam with beta1 = 0.9, beta2 = 0.999, and learning_rate = 1e-3 or 5e-4 is a great starting point for many models!

Kingma and Ba, "Adam: A method for stochastic optimization", ICLR 2015

Adam



SGD

SGD+Momentum

RMSProp

Adam

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

$$L(w) = L_{data}(w) + \boldsymbol{\lambda |w|^2}$$
$$g_t = \nabla L(w_t) = \nabla L_{data}(w_t) + \boldsymbol{2\lambda w_t}$$
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L2 Regularization and Weight Decay are equivalent for SGD, SGD+Momentum so people often use the terms interchangeably!

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Weight Decay

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L2 Regularization vs Weight Decay

Optimization Algorithm

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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

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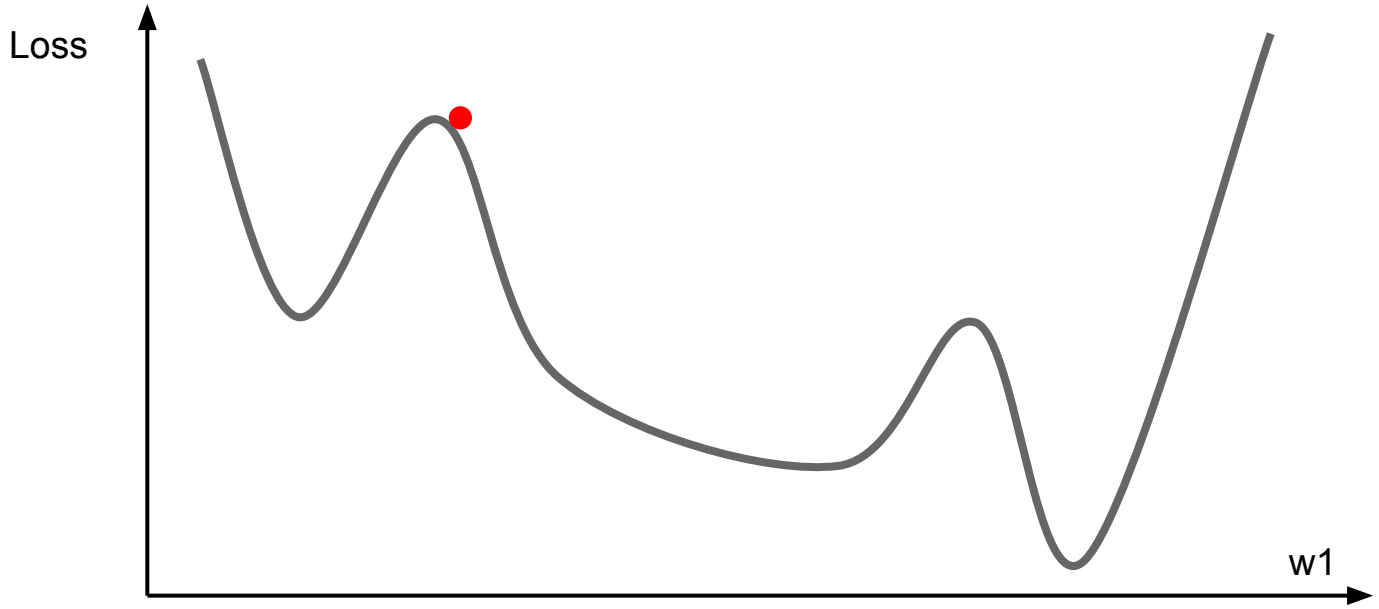
AdamW: Decoupled Weight Decay

Algorithm 2 Adam with L_2 regularization and Adam with decoupled weight decay (AdamW)

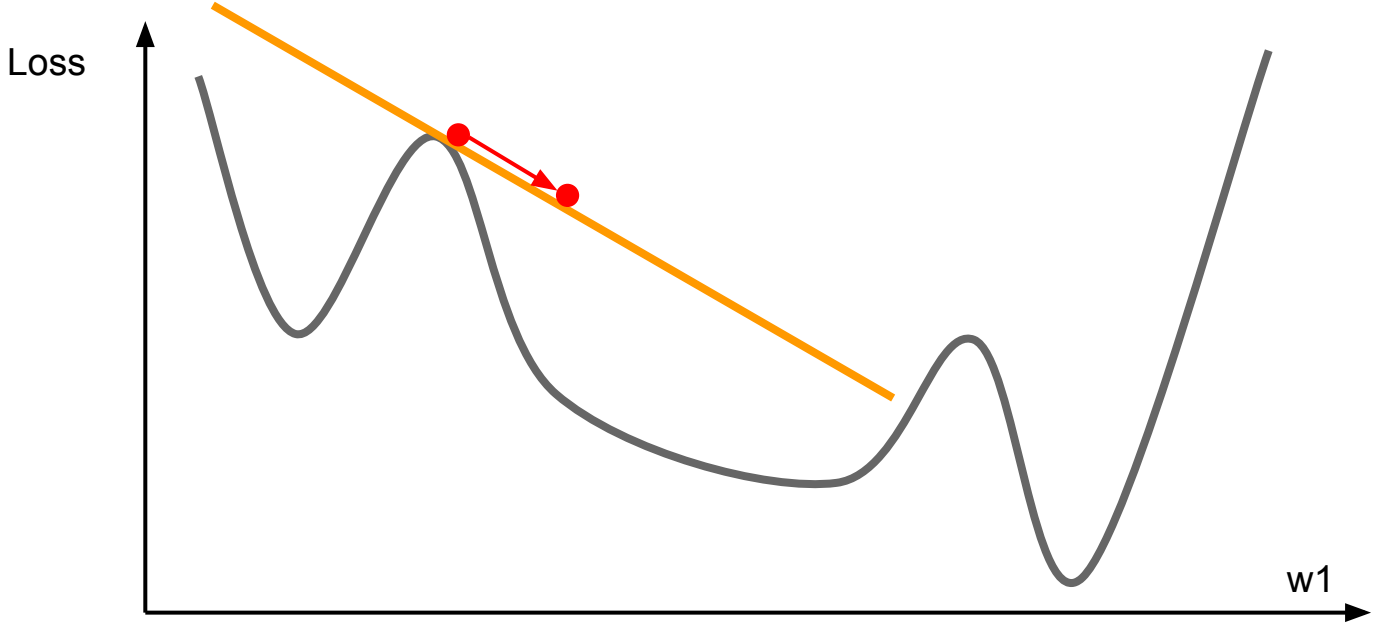
given $\alpha = 0.001, \beta_1 = 0.9, \beta_2 = 0.999, \epsilon = 10^{-8}, \lambda \in \mathbb{R}$
initialize time step $t \leftarrow 0$, parameter vector $\boldsymbol{\theta}_{t=0} \in \mathbb{R}^n$, first moment vector $\boldsymbol{m}_{t=0} \leftarrow \boldsymbol{0}$, second moment vector $\boldsymbol{v}_{t=0} \leftarrow \boldsymbol{0}$, schedule multiplier $\eta_{t=0} \in \mathbb{R}$
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
  $\boldsymbol{v}_t \leftarrow \beta_2 \boldsymbol{v}_{t-1} + (1 - \beta_2)\boldsymbol{g}_t^2$
  $\hat{\boldsymbol{m}}_t \leftarrow \boldsymbol{m}_t / (1 - \beta_1^t)$ ▷ β_1 is taken to the power of t
  $\hat{\boldsymbol{v}}_t \leftarrow \boldsymbol{v}_t / (1 - \beta_2^t)$ ▷ β_2 is taken to the power of t
  $\eta_t \leftarrow \text{SetScheduleMultiplier}(t)$ ▷ can be fixed, decay, or also be used for warm restarts
  $\boldsymbol{\theta}_t \leftarrow \boldsymbol{\theta}_{t-1} - \eta_t \left(\alpha \hat{\boldsymbol{m}}_t / (\sqrt{\hat{\boldsymbol{v}}_t} + \epsilon) + \lambda \boldsymbol{\theta}_{t-1} \right)$
until *stopping criterion is met*
return optimized parameters $\boldsymbol{\theta}_t$

First-Order Optimization



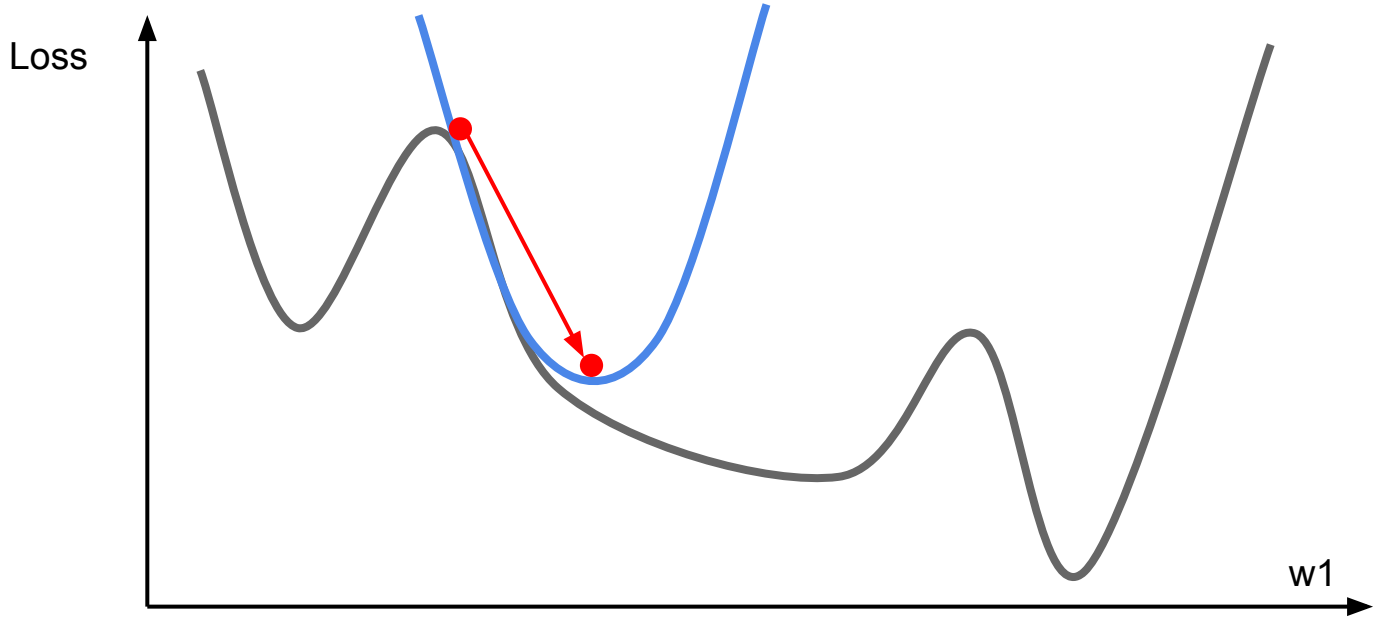
First-Order Optimization

(1) Use gradient form linear approximation
(2) Step to minimize the approximation



Second-Order Optimization

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



Second-Order Optimization

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 Optimization

second-order Taylor expansion:

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

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

Hessian has O(N^2) elements
Inverting takes O(N^3)
N = (Tens or Hundreds of) Millions

Q: Why is this bad for deep learning?

Second-Order Optimization

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

- 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.

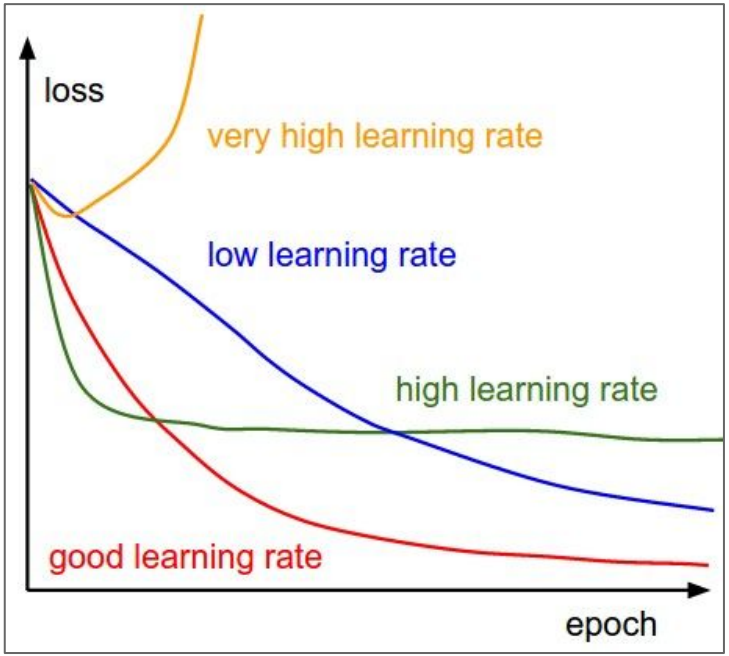
Le et al, “On optimization methods for deep learning, ICML 2011”
Ba et al, “Distributed second-order optimization using Kronecker-factored approximations”, ICLR 2017

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!

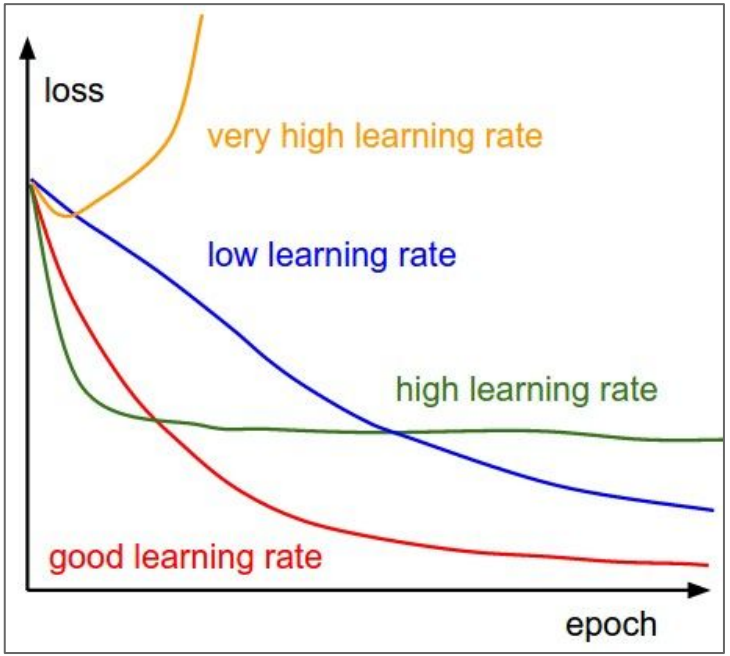
Learning rate schedules

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



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

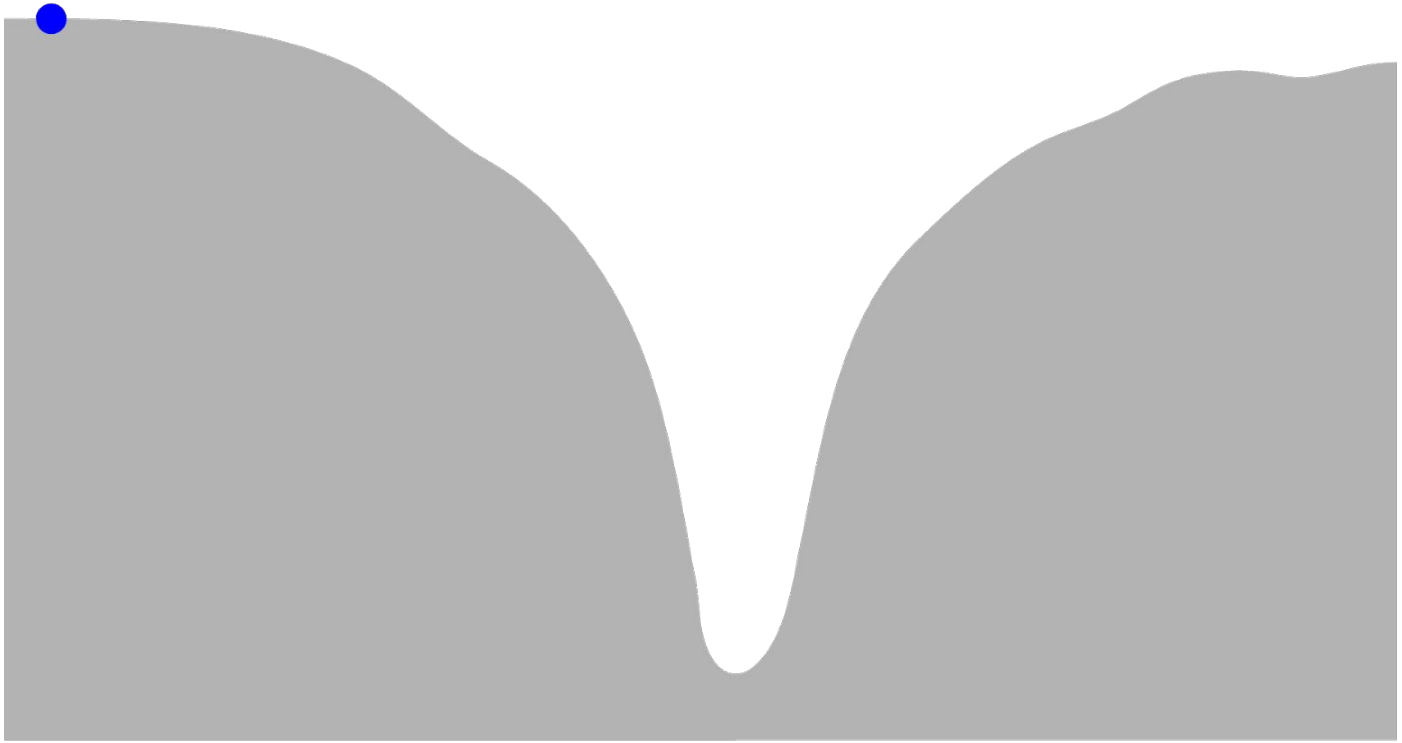
SGD, SGD+Momentum, Adagrad, RMSProp, Adam all have **learning rate** as a hyperparameter.



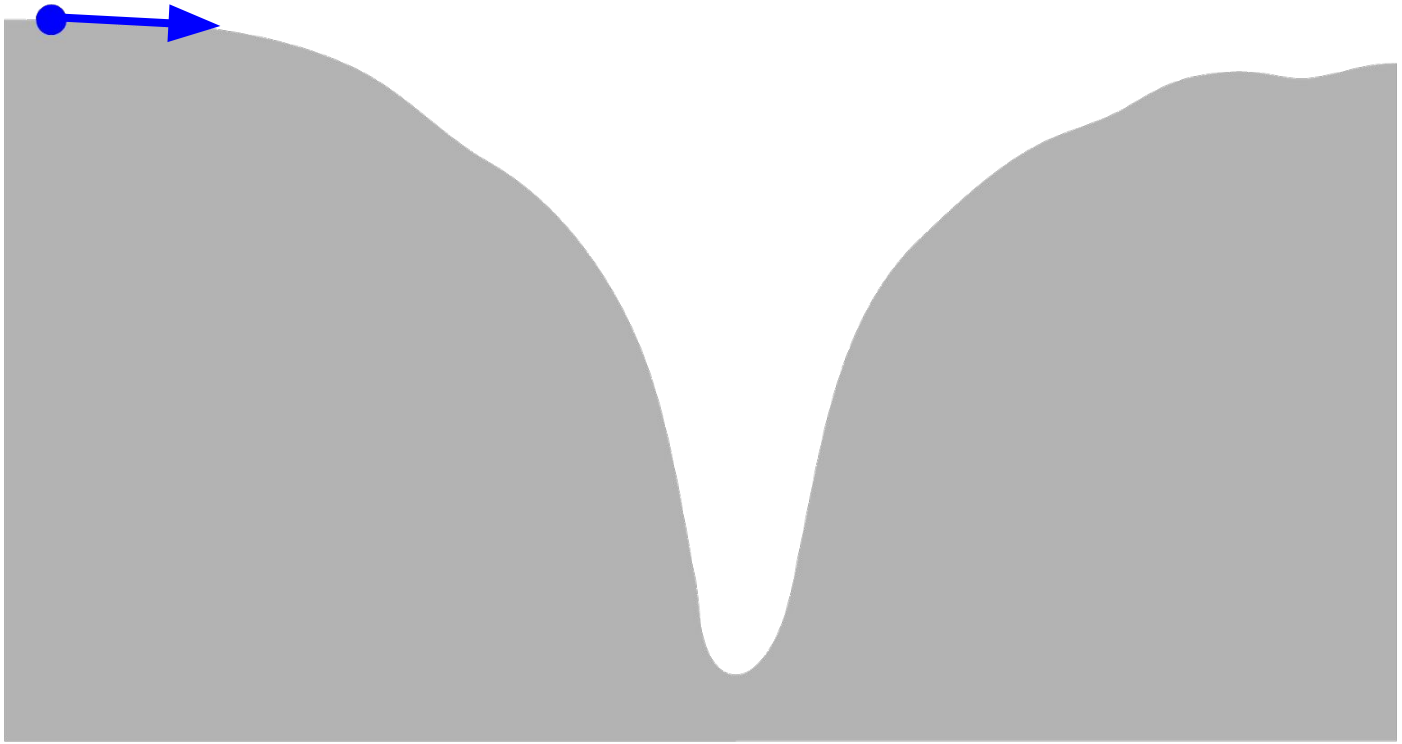
Q: Which one of these learning rates is best to use?

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

Phases of learning...



Phases of learning...



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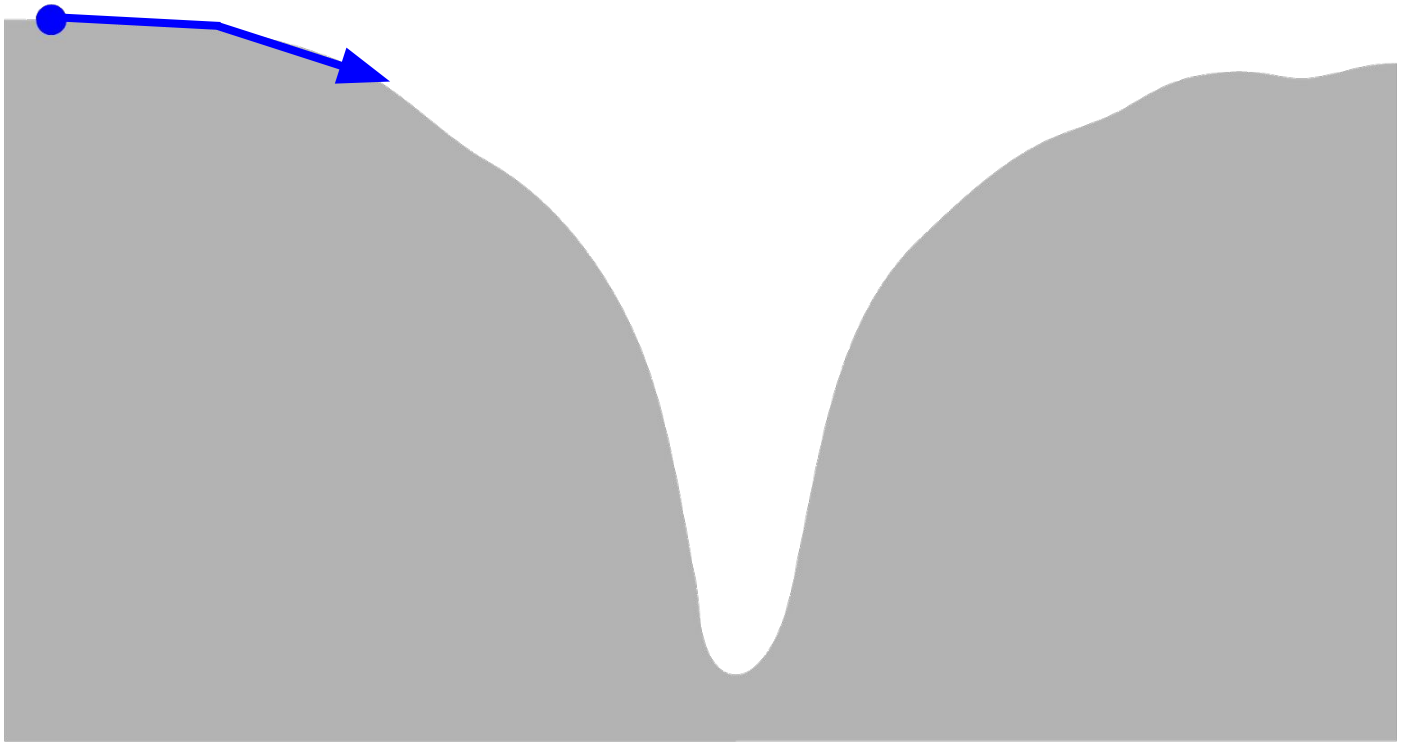

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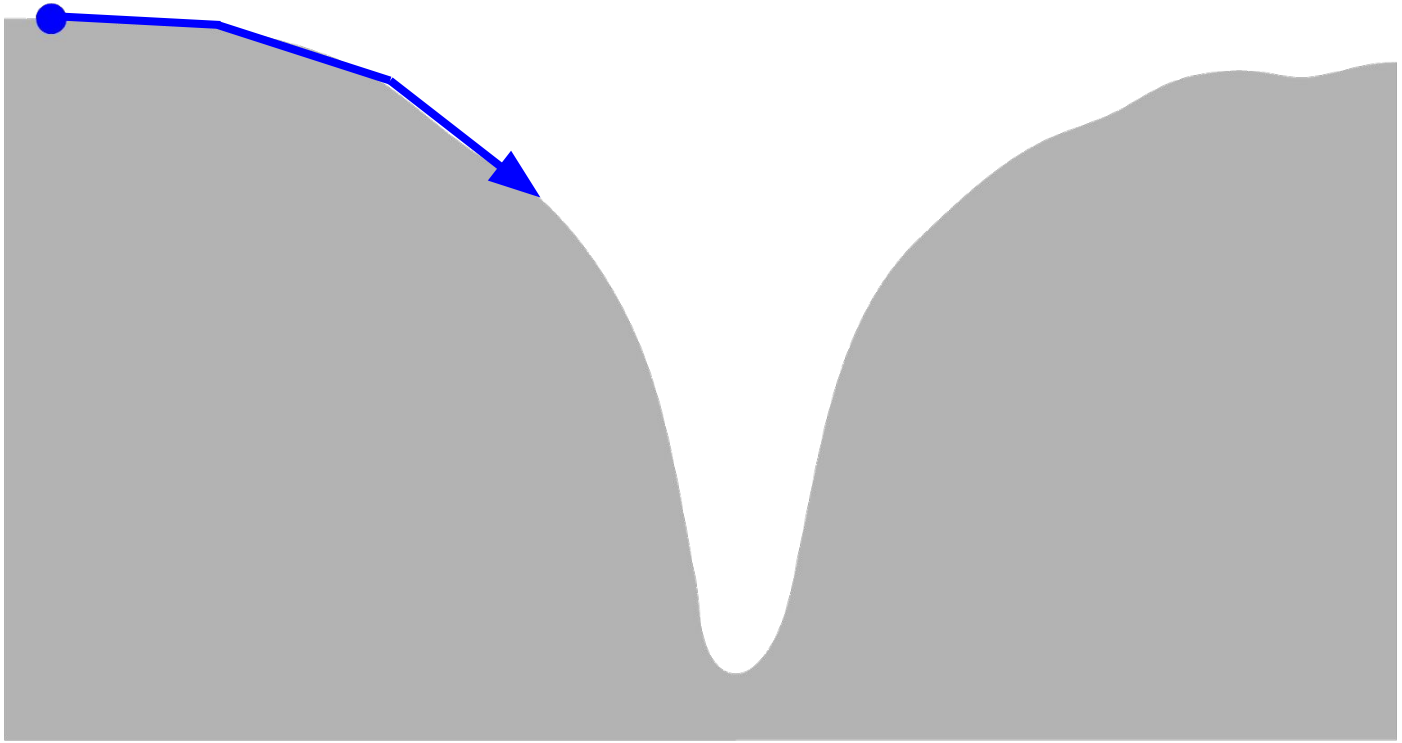

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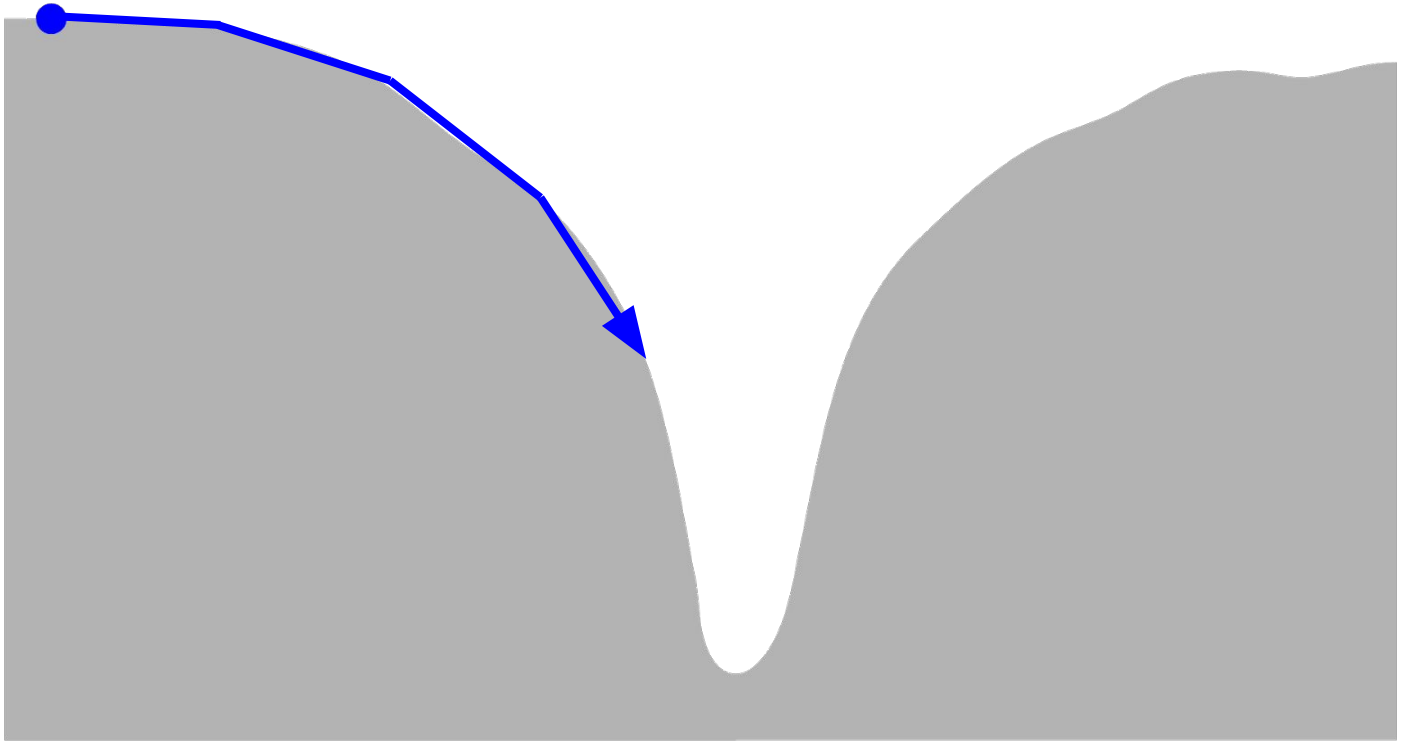

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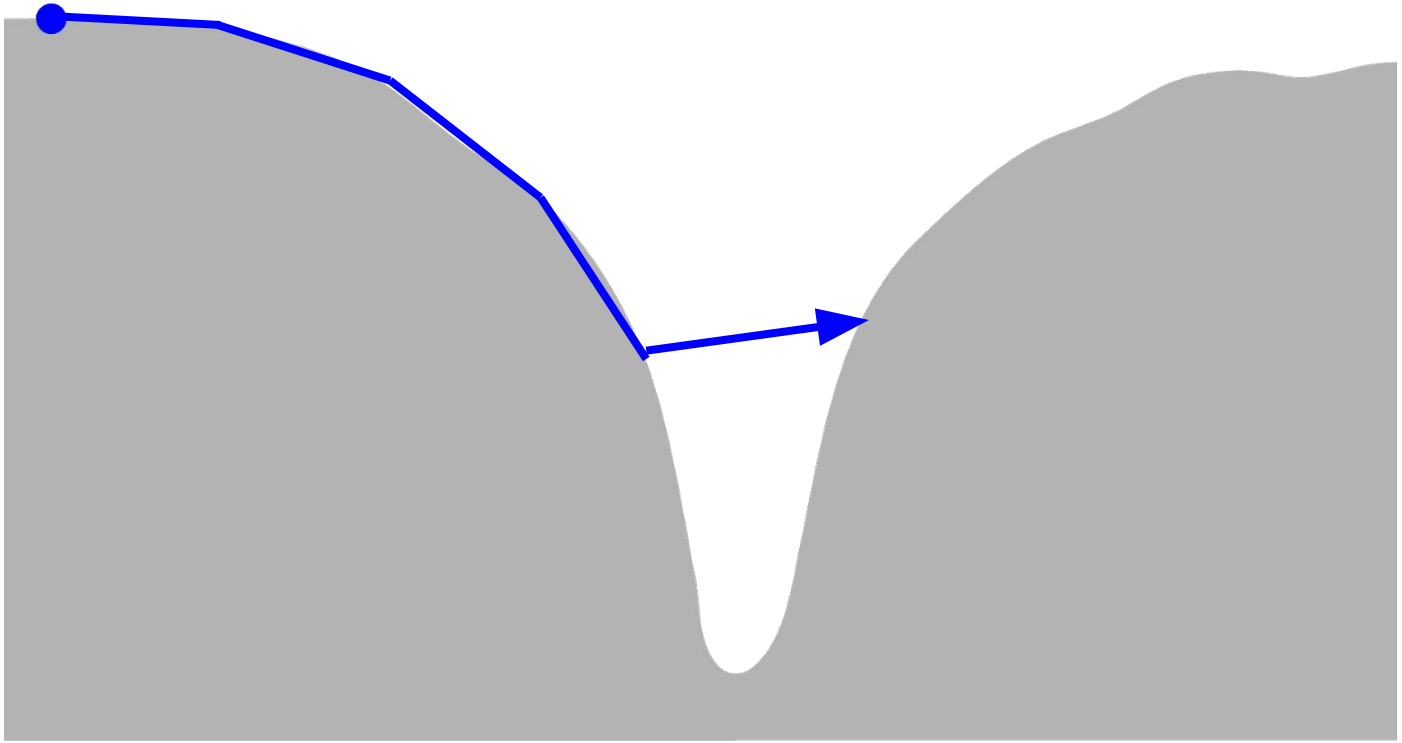

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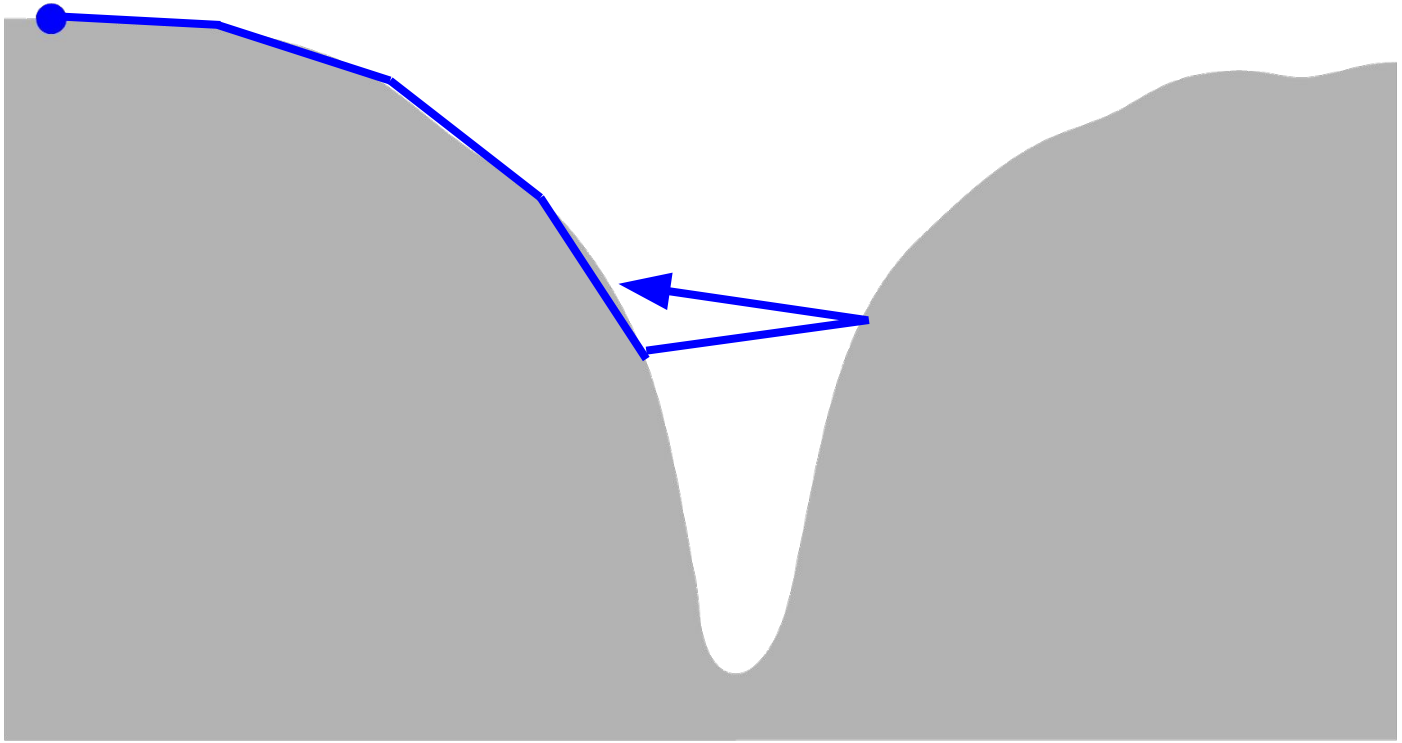

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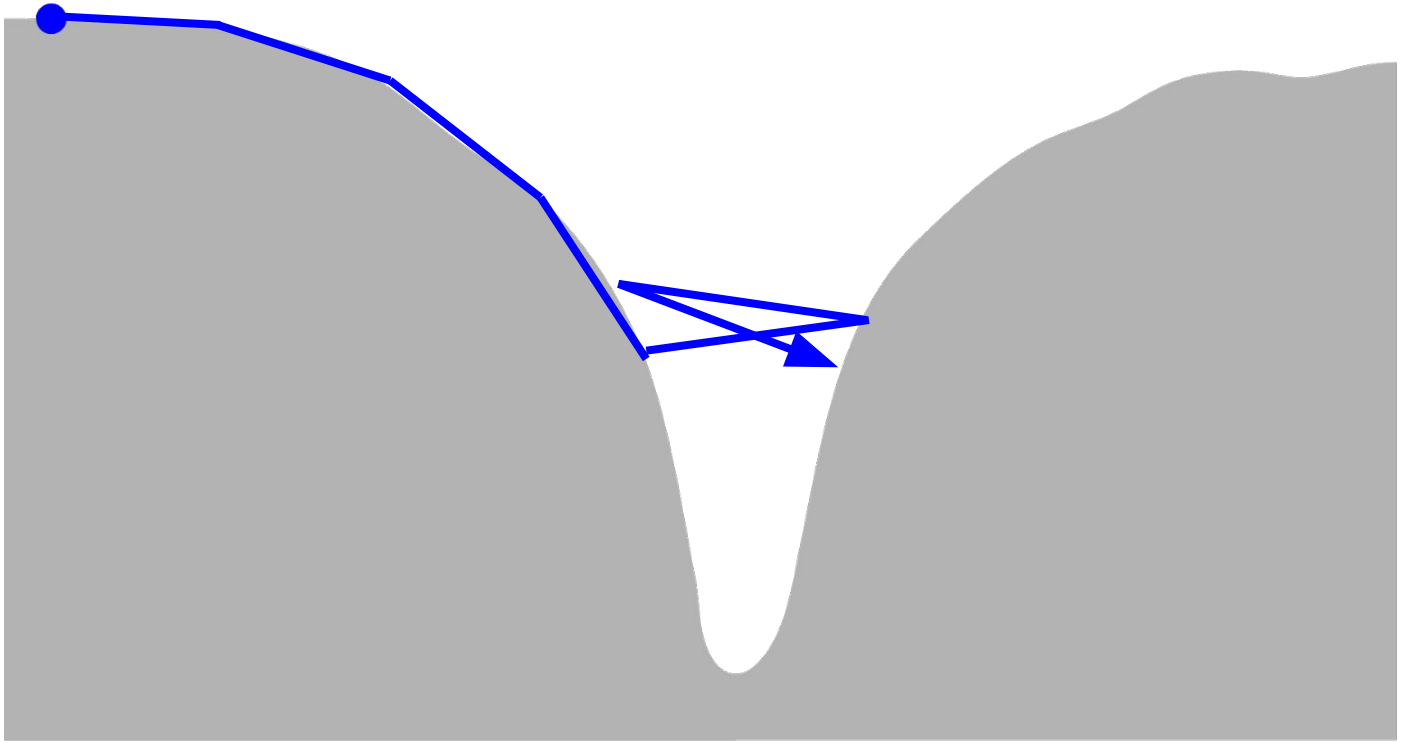

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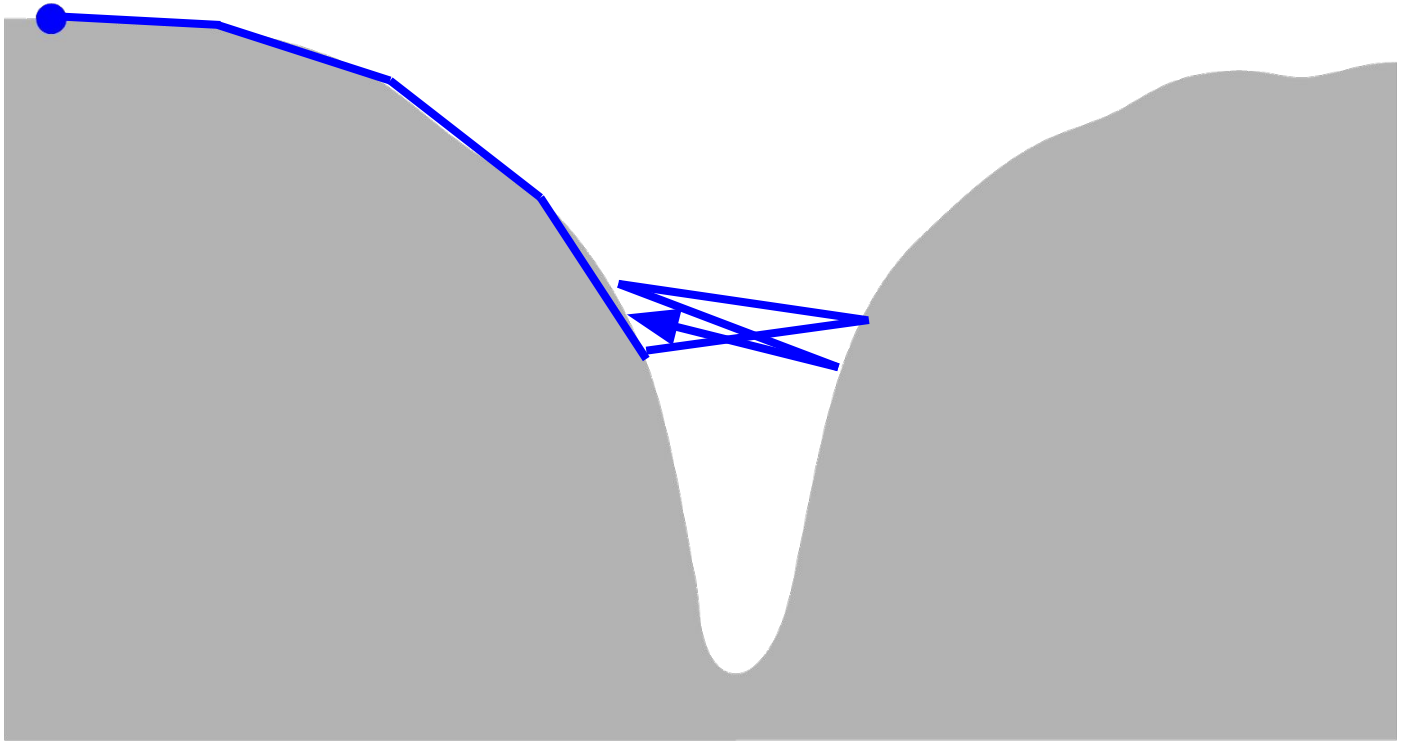
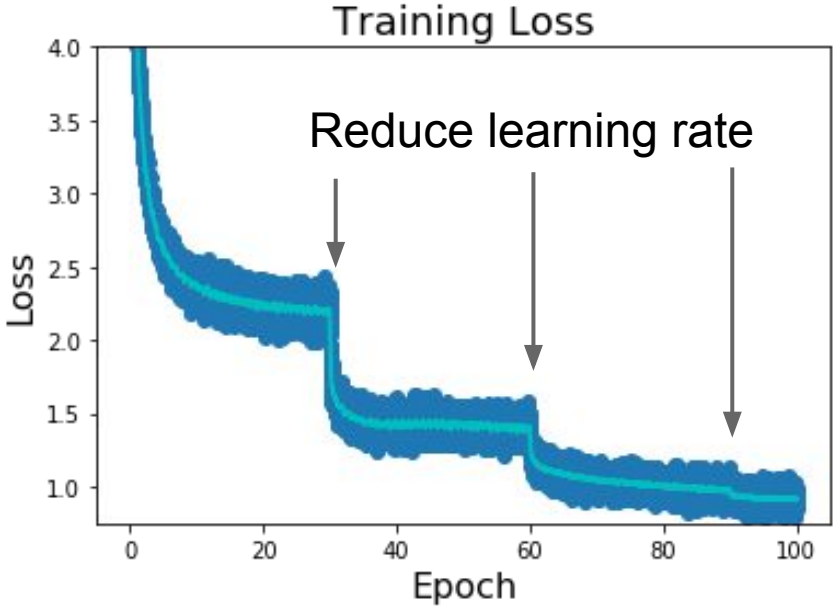
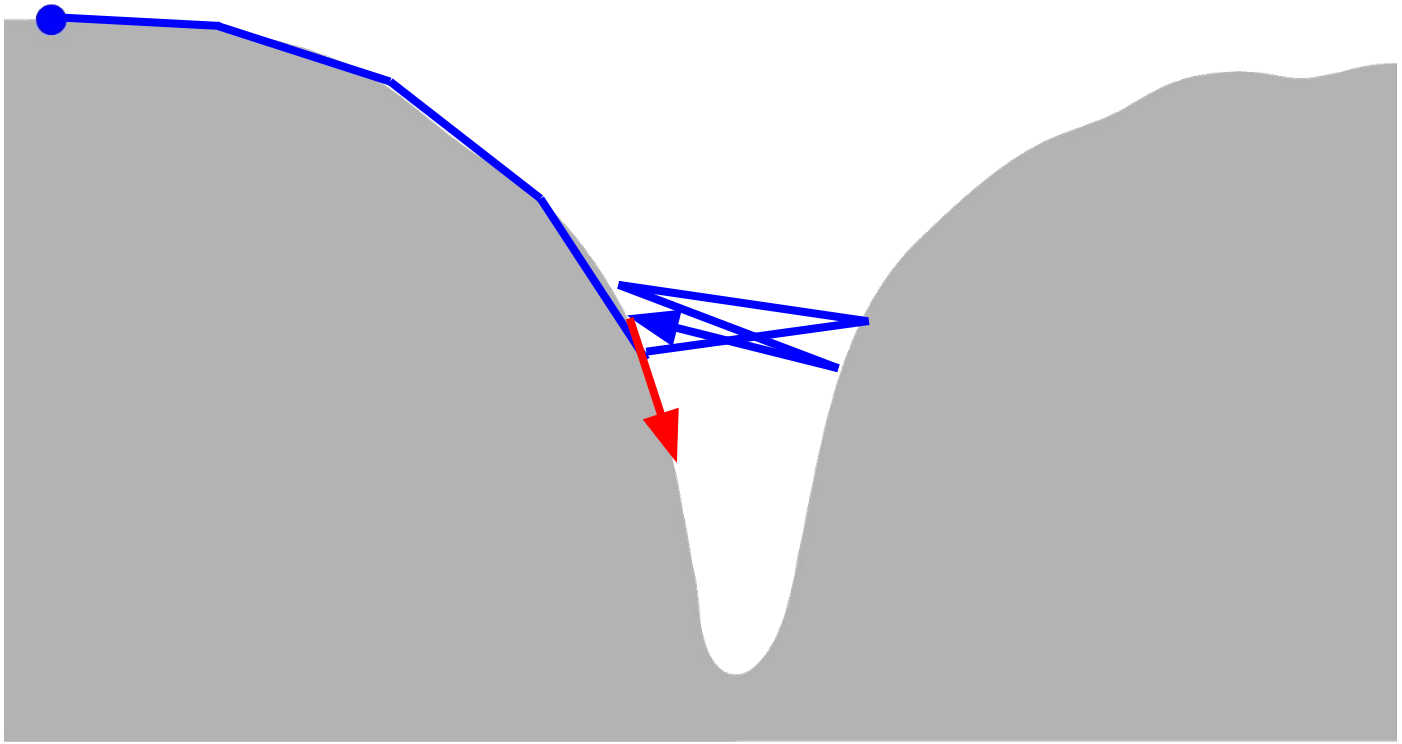


Learning rate decays over time



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...



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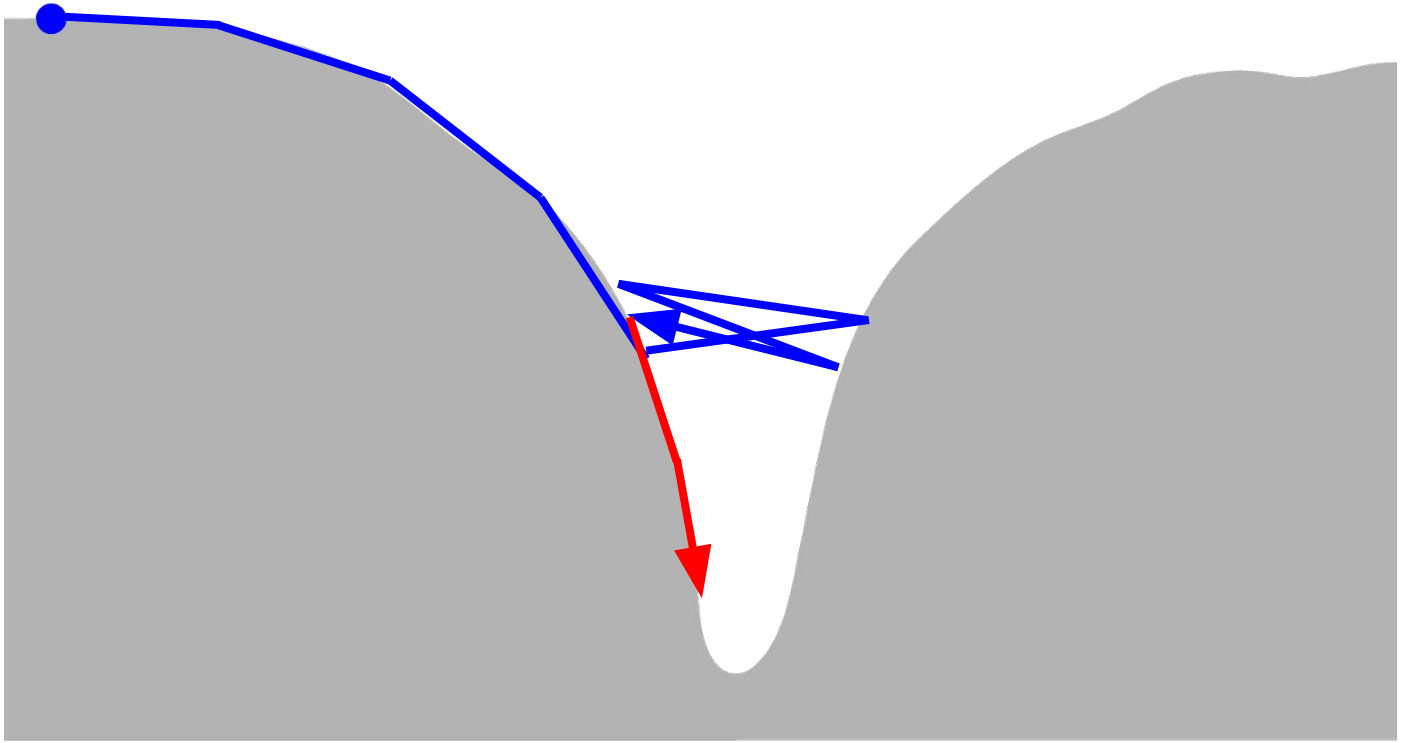
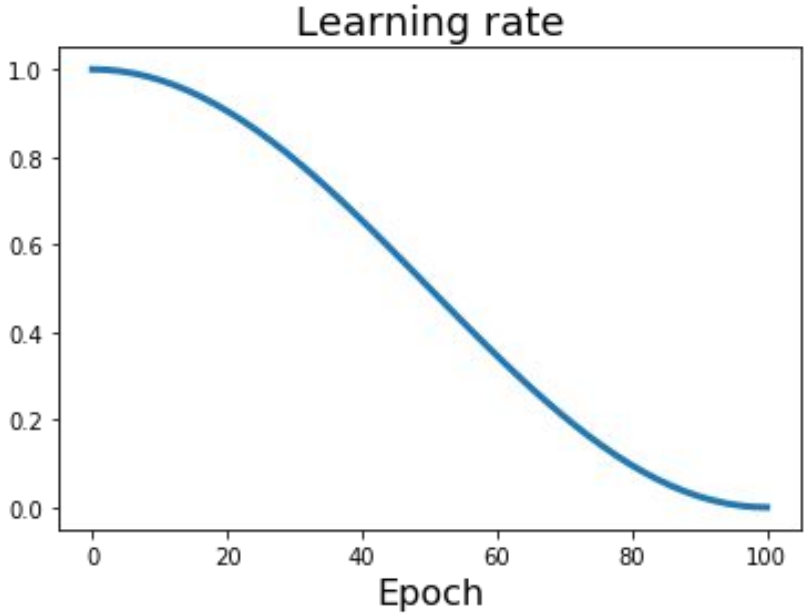


Learning Rate Decay



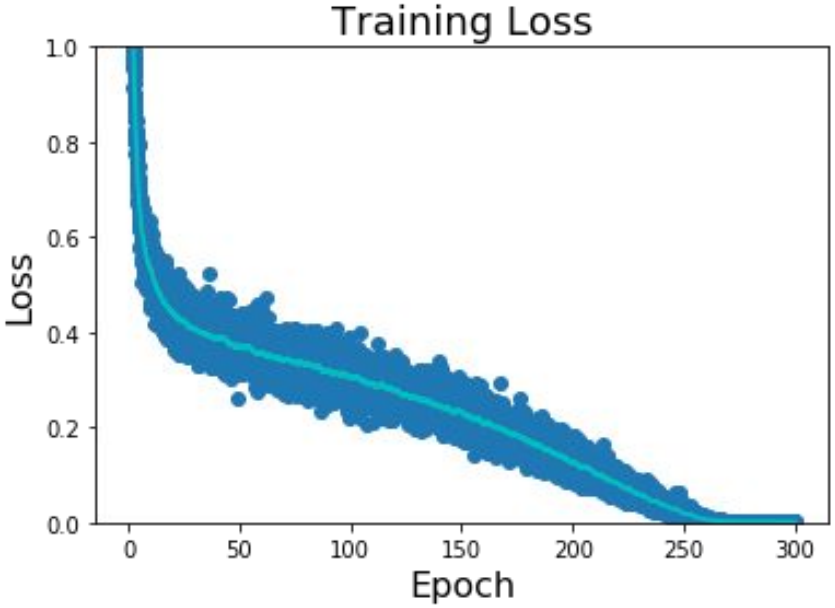
Step: Reduce learning rate at a few fixed points. E.g. for ResNets, multiply LR by 0.1 after epochs 30, 60, and 90.

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

α_0 : Initial learning rate
α_t : Learning rate at epoch t
T : Total number of epochs

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 Sequences with Sparse Transformers”, arXiv 2019

Learning Rate Decay



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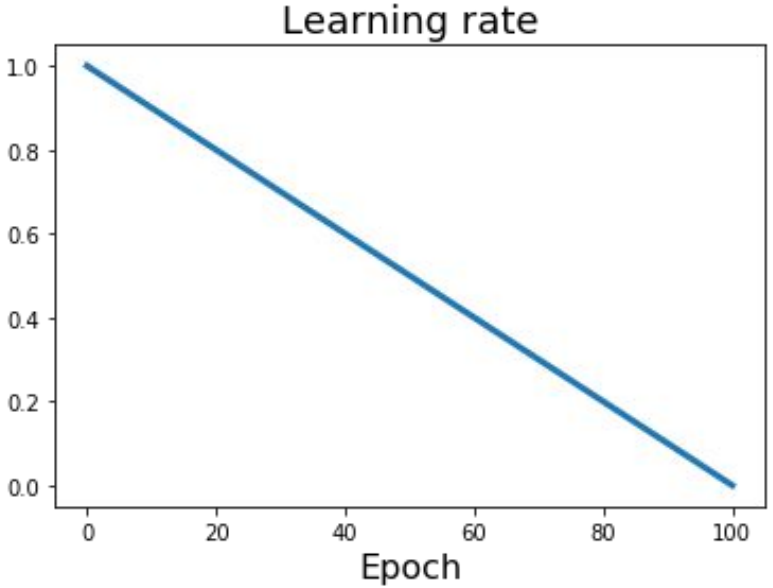

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Linear: $\alpha_t = \alpha_0(1 - t/T)$

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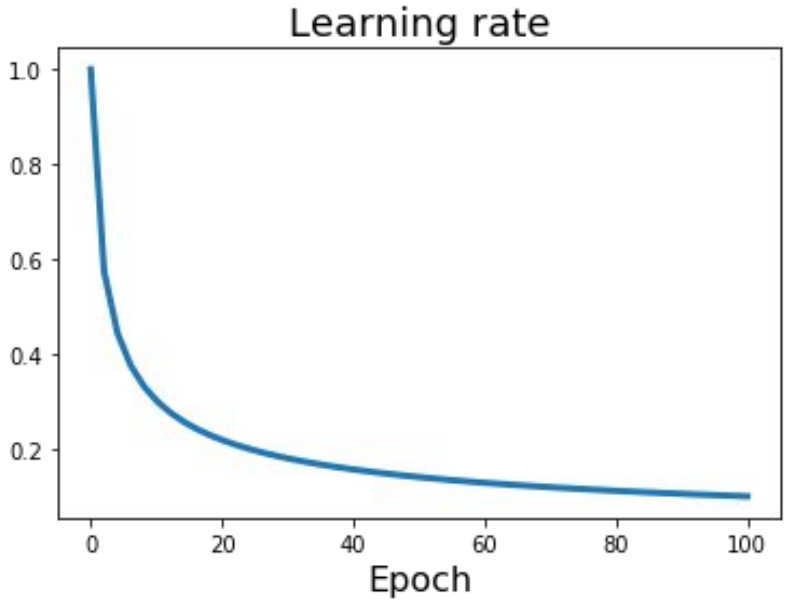
Devlin et al, “BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding”, 2018

Learning Rate Decay



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

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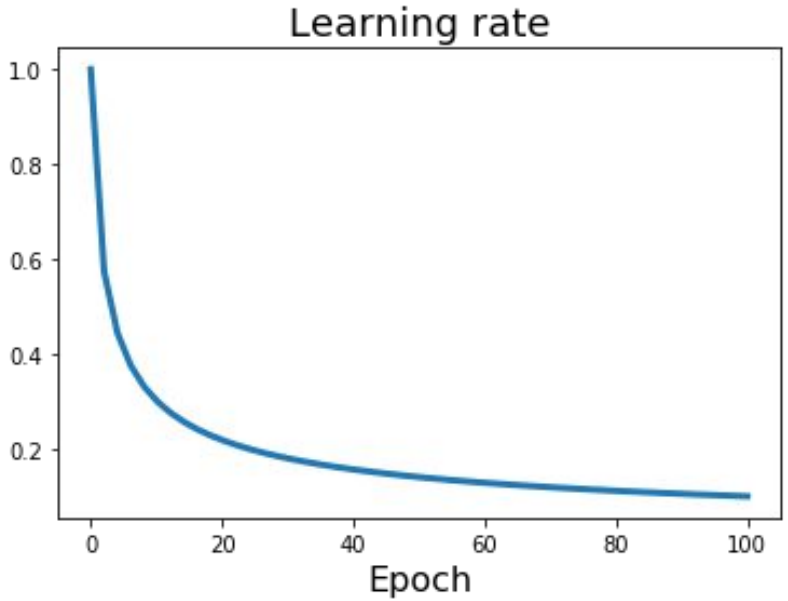
Vaswani et al, “Attention is all you need”, NIPS 2017

Learning Rate Decay



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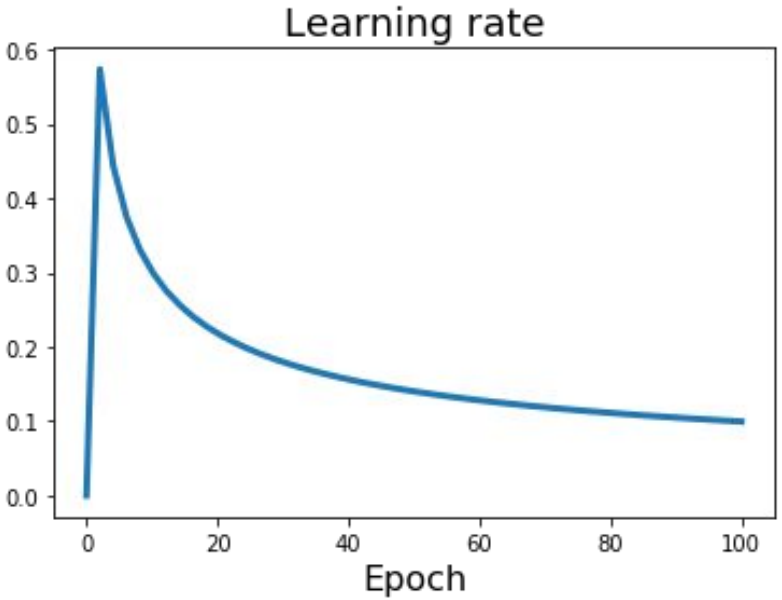
Inverse sqrt: $\alpha_t = \alpha_0/\sqrt{t}$

Constant: $\alpha_t = \alpha_0$

Vaswani et al, “Attention is all you need”, NIPS 2017

Learning Rate Decay: Linear Warmup

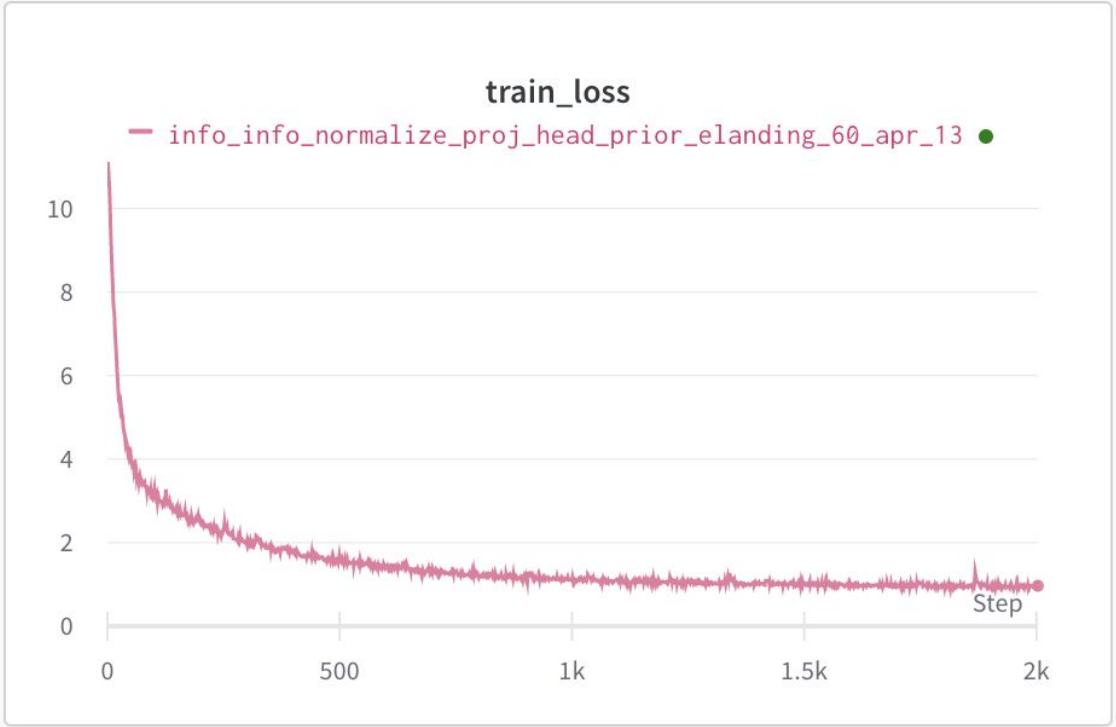


High initial learning rates can make loss explode; linearly increasing learning rate from 0 over the first ~5000 iterations can prevent this

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

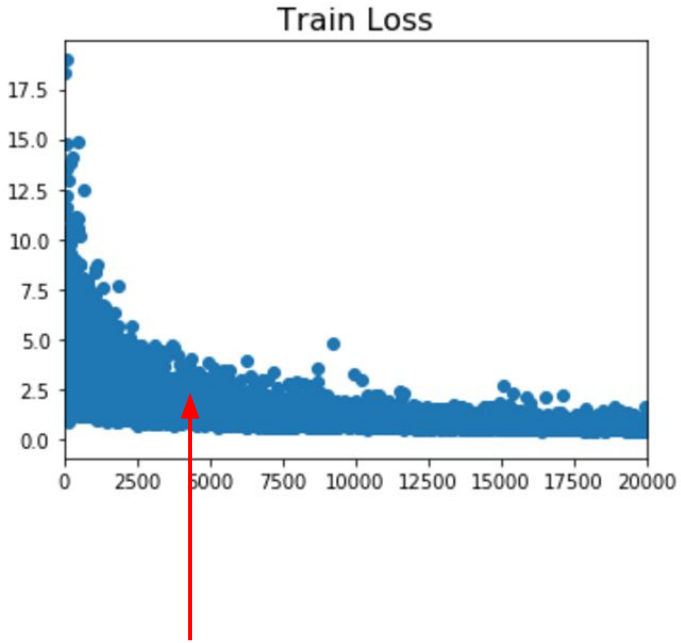
Goyal et al, “Accurate, Large Minibatch SGD: Training ImageNet in 1 Hour”, arXiv 2017

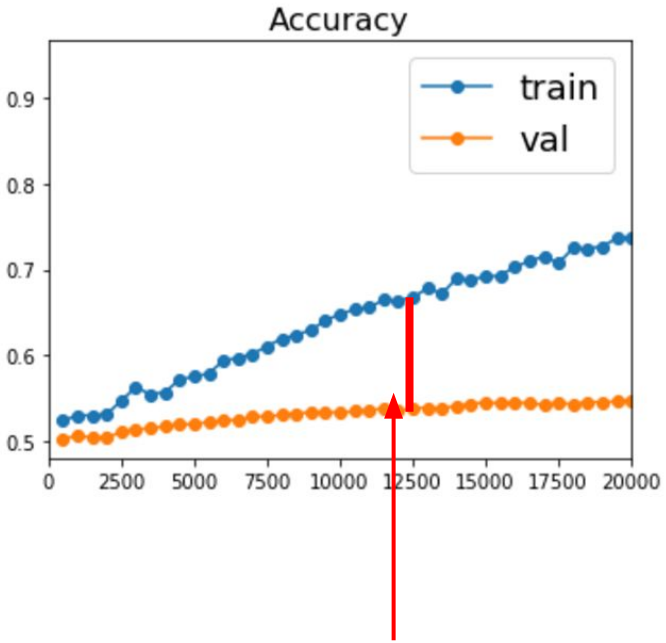
with cosine and warmup



Improve test error

Beyond Training Error

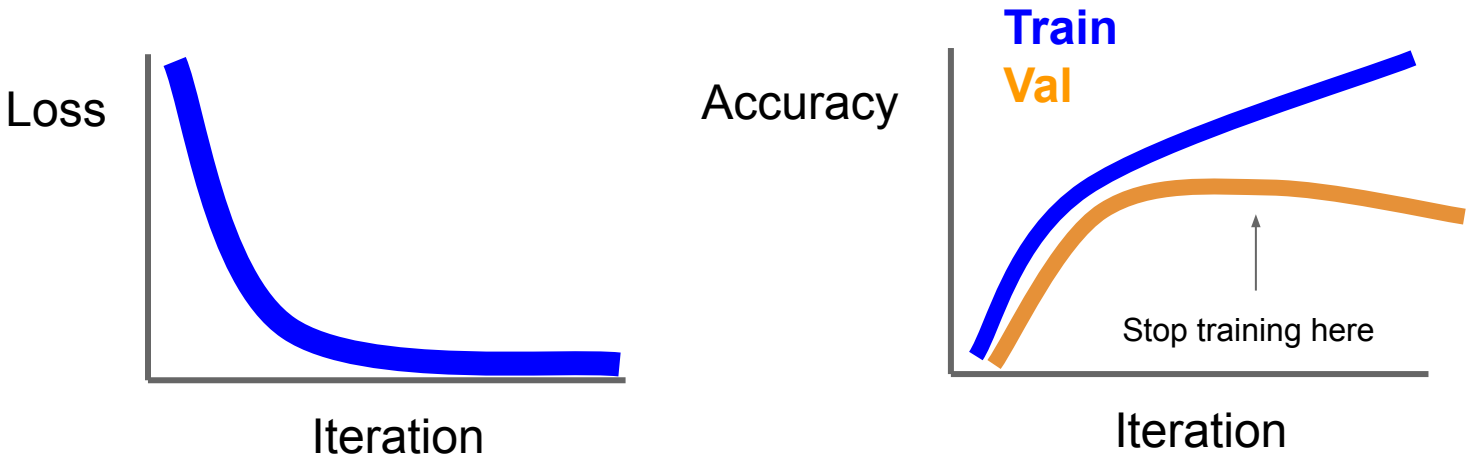




Better optimization algorithms help reduce training loss

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

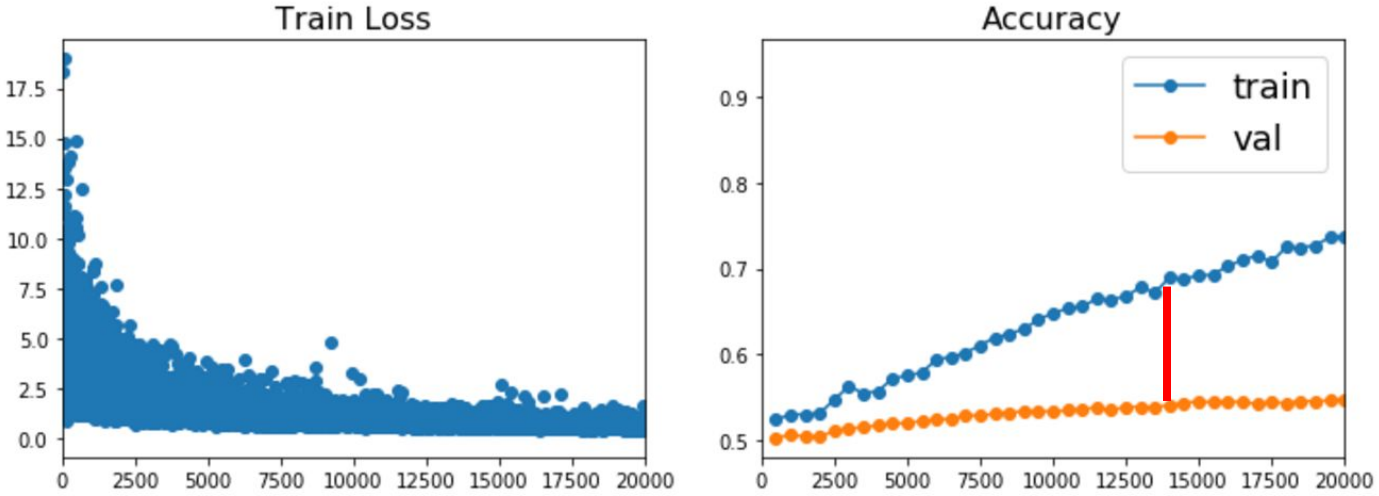
Model Ensembles

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

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

In common use:

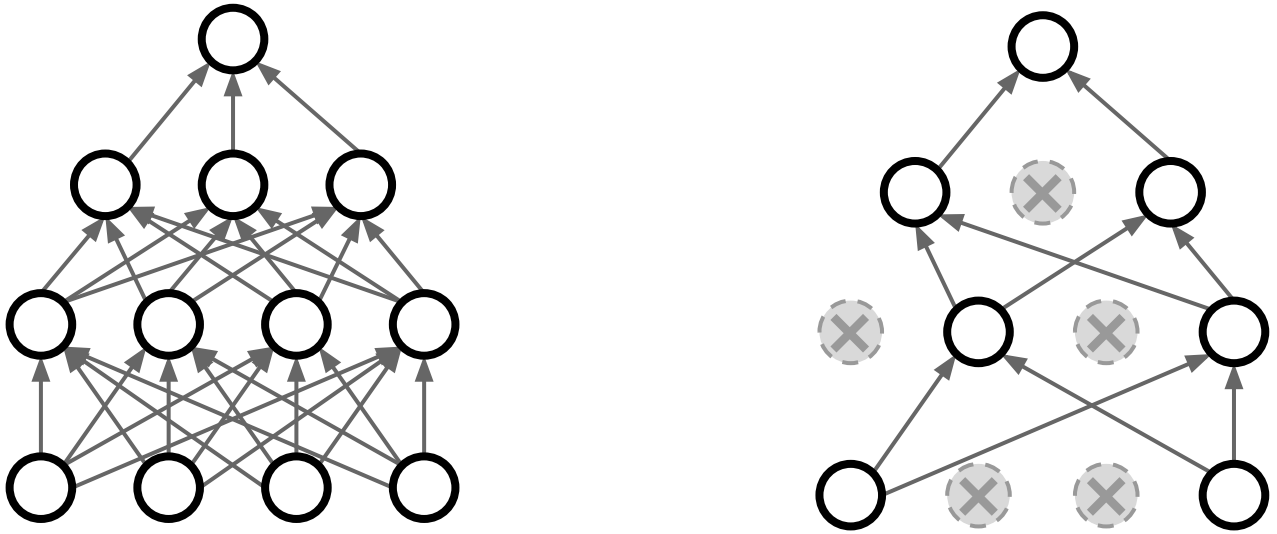
L2 regularization $R(W) = \sum_k \sum_l W_{k,l}^2$ (Weight decay)

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

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

Regularization: Dropout

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

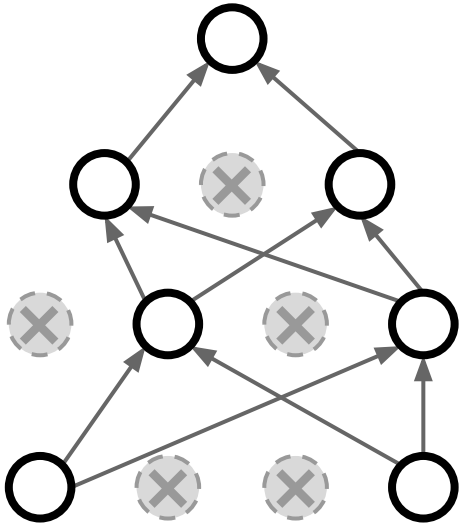


Srivastava et al, “Dropout: A simple way to prevent neural networks from overfitting”, JMLR 2014

Regularization: Dropout

```
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)
```

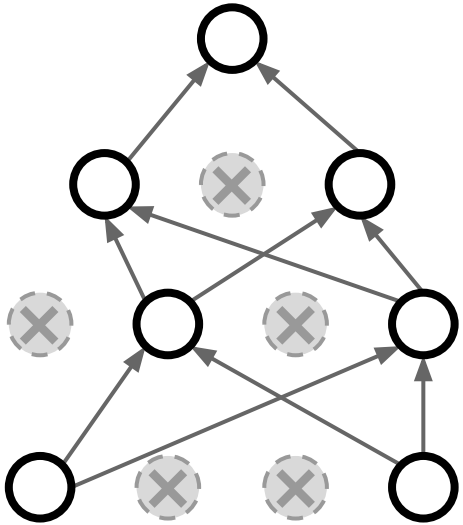
Example forward pass with a 3-layer network using dropout



Create a drop mask and multiply

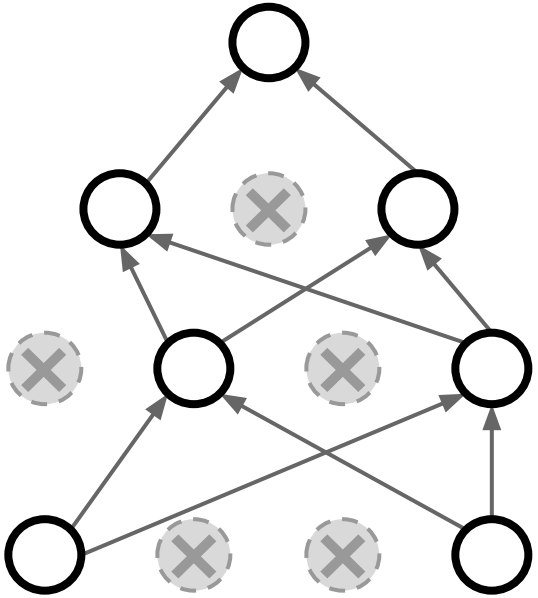
```
p = 0.5 # probability of keeping a unit active. higher = less dropout

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



Regularization: Dropout

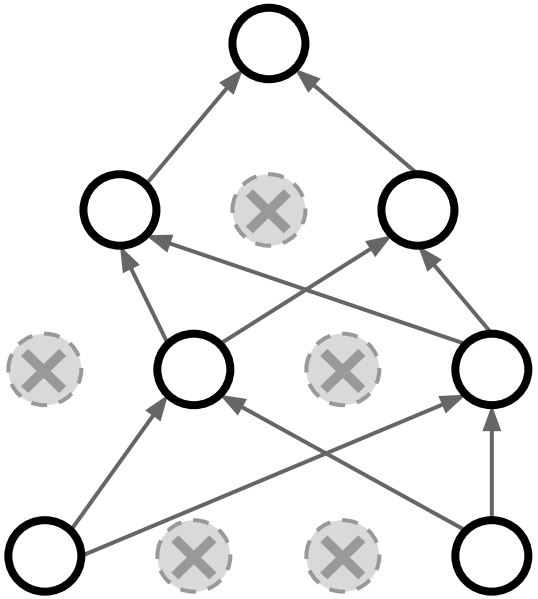
How can this possibly be a good idea?



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

Regularization: Dropout

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: Test time

Output (label)

Input (image)

Dropout makes our output random!

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

Random mask

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

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

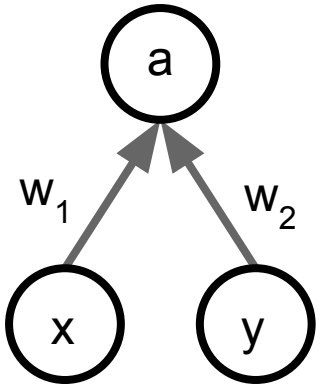
But this integral seems hard …

Dropout: Test time

Want to approximate the integral

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

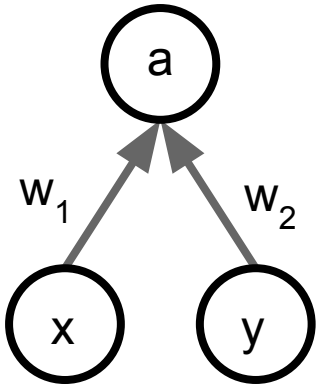
Consider a single neuron.



Dropout: Test time

Want to approximate the integral

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



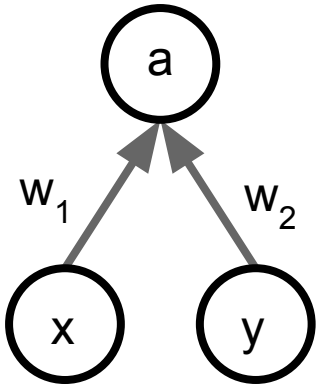
Consider a single neuron.

At test time we have: $E\big[a\big] = w_1 x + w_2 y$

Dropout: Test time

Want to approximate the integral

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



Consider a single neuron.

At test time we have: $E\big[a\big] = w_1 x + w_2 y$

During training we have:

$$E[a] = \tfrac{1}{4}(w_1 x + w_2 y) + \tfrac{1}{4}(w_1 x + w_2 0)$$

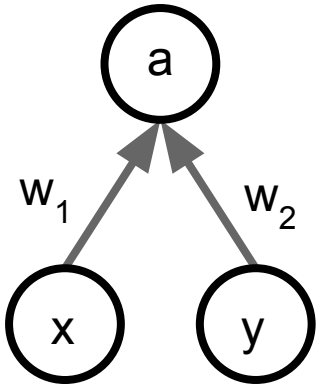
$$+ \tfrac{1}{4}(w_1 0 + w_2 0) + \tfrac{1}{4}(w_1 0 + w_2 y)$$

$$= \tfrac{1}{2}(w_1 x + w_2 y)$$

Dropout: Test time

Want to approximate the integral

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



Consider a single neuron.

At test time we have: $E\big[a\big] = w_1 x + w_2 y$

During training we have:

$$E[a] = \tfrac{1}{4}(w_1 x + w_2 y) + \tfrac{1}{4}(w_1 x + w_2 0)$$

$$+ \tfrac{1}{4}(w_1 0 + w_2 0) + \tfrac{1}{4}(w_1 0 + w_2 y)$$

$$= \tfrac{1}{2}(w_1 x + w_2 y)$$

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

Dropout: Test time

```
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

Dropout Summary

```
""" 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
```

drop in train time

scale at test time

More common: “Inverted dropout”

```python
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)

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
```

test time is unchanged!

Regularization: A common pattern

Training: Add some kind of randomness

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

Testing: Average out randomness (sometimes approximate)

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

Regularization: A common pattern

Training: Add some kind of randomness

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

Testing: Average out randomness (sometimes approximate)

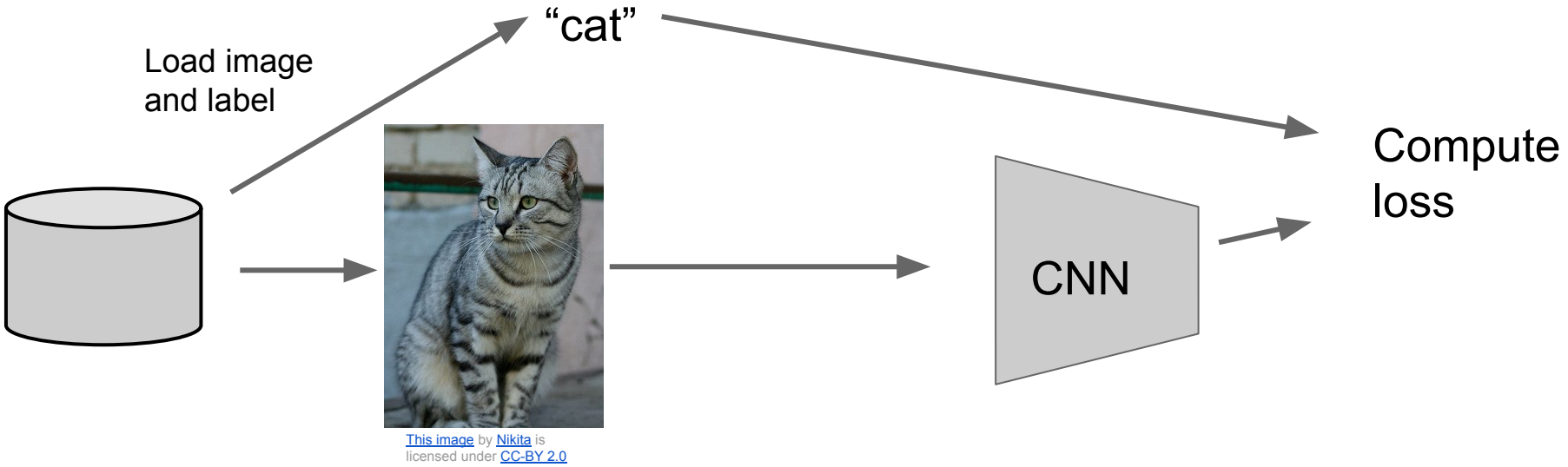
$$y = f(x) = E_z\big[f(x, z)\big] = \int p(z) f(x, z) dz$$

Example: Batch Normalization

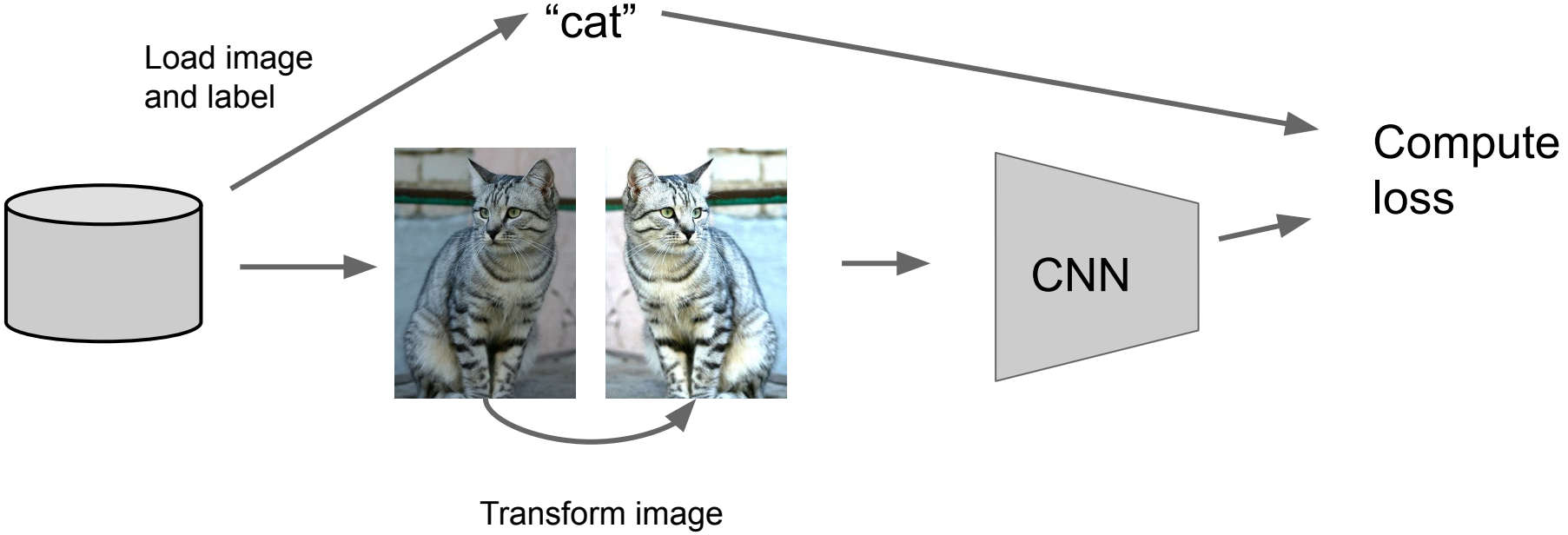
Training: Normalize using stats from random minibatches

Testing: Use fixed stats to normalize

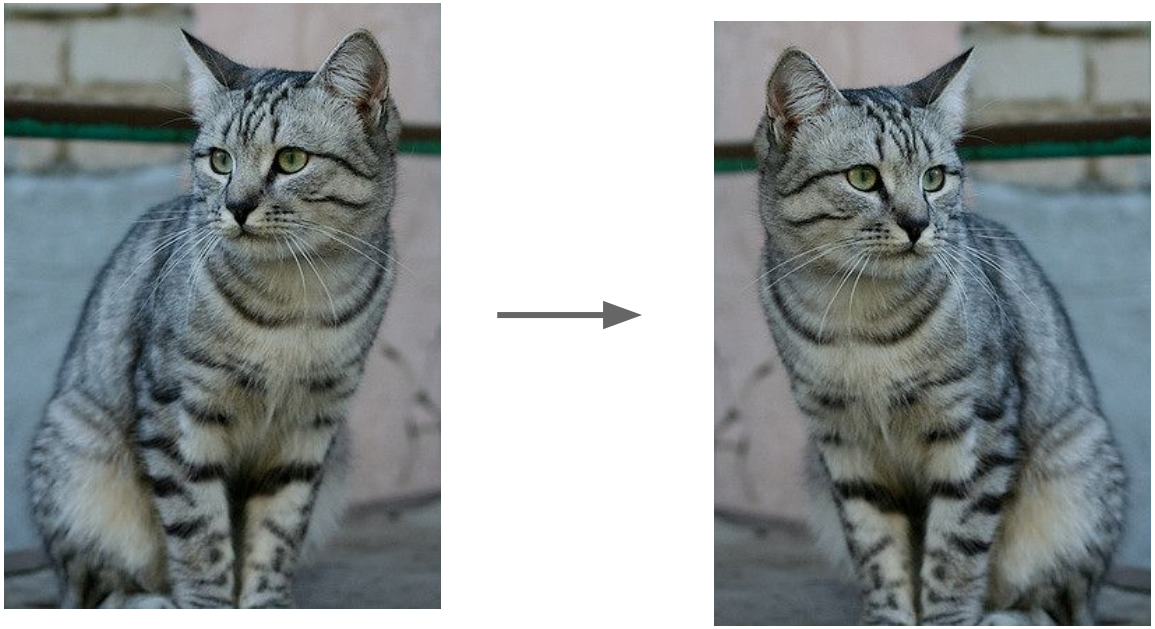
Regularization: Data Augmentation



Regularization: Data Augmentation



Data Augmentation
Horizontal Flips



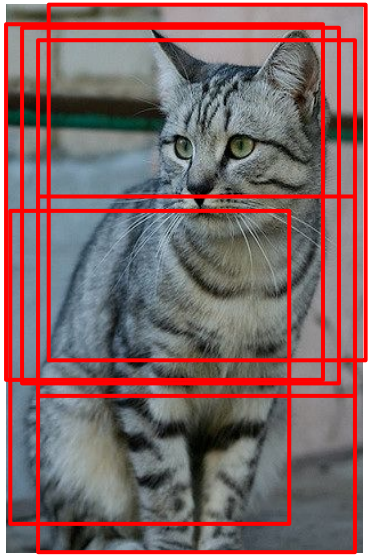
Data Augmentation

Random crops and scales

Training: sample random crops / scales

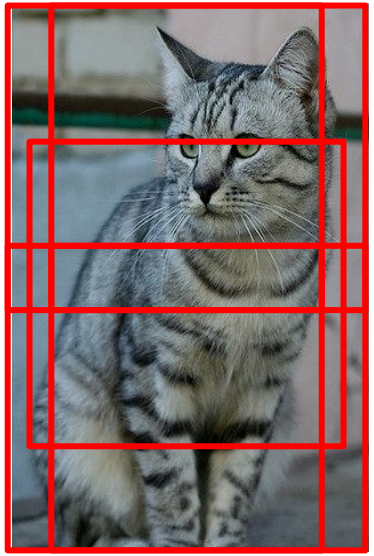
ResNet:

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

ResNet:

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

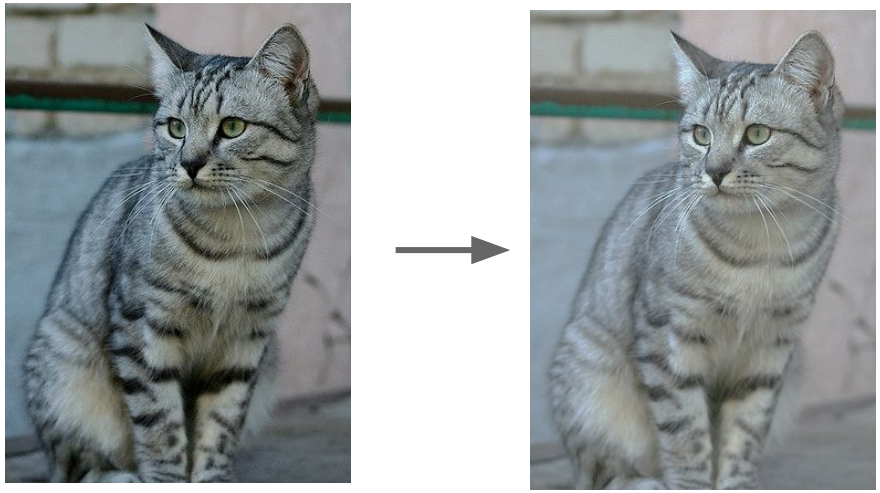
Testing: average a fixed set of crops

ResNet:

1. Resize image at 5 scales: {224, 256, 384, 480, 640}
2. For each size, use 10 224x224 crops: 4 corners + center, + flips

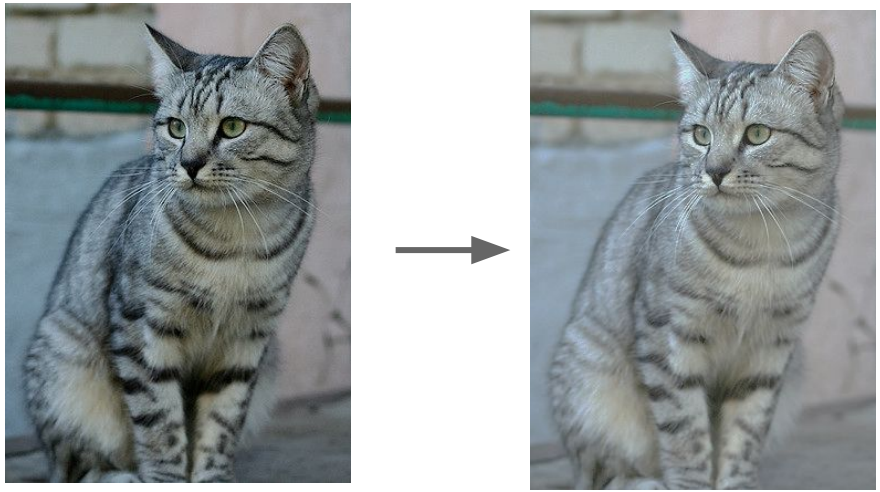
Data Augmentation
Color Jitter

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
1. Add offset to all pixels of a training image

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

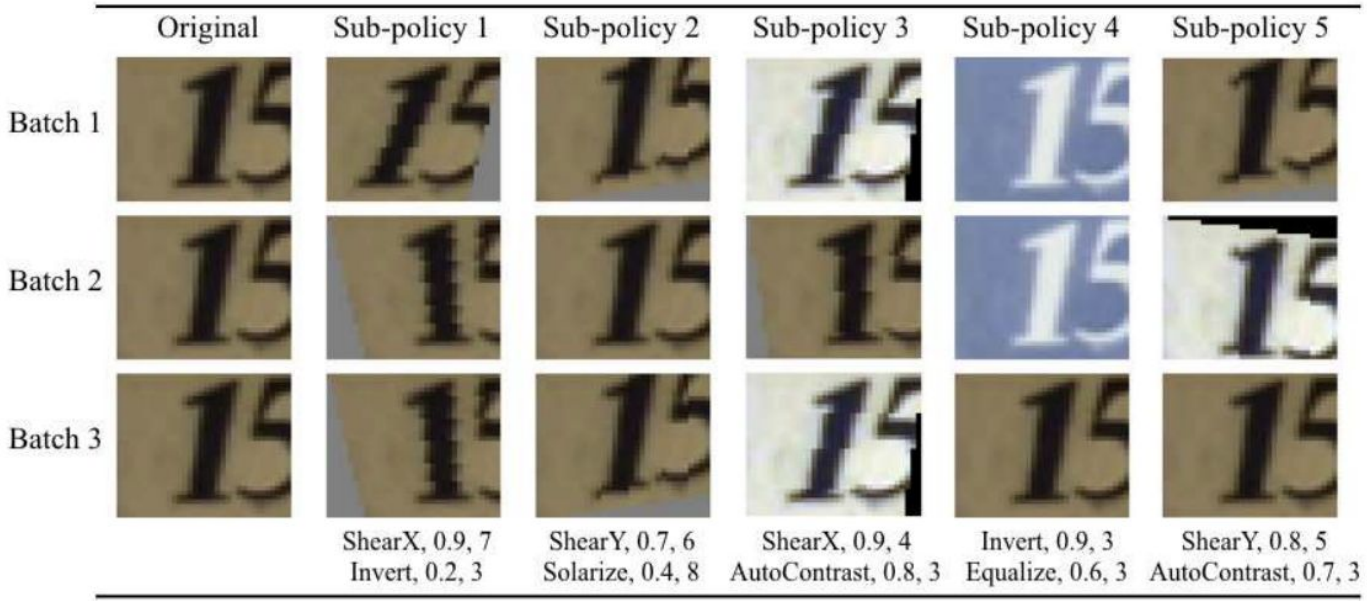
Data Augmentation

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

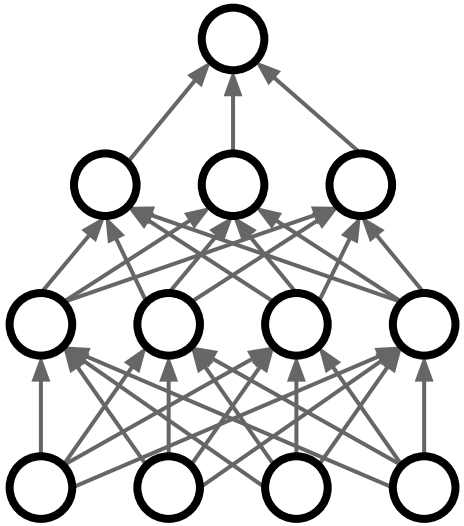
Examples:

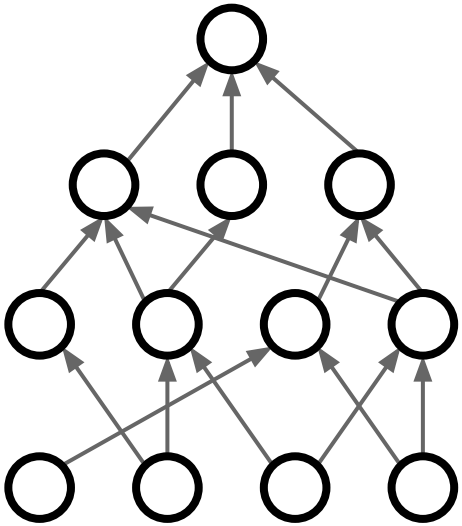
Dropout

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:

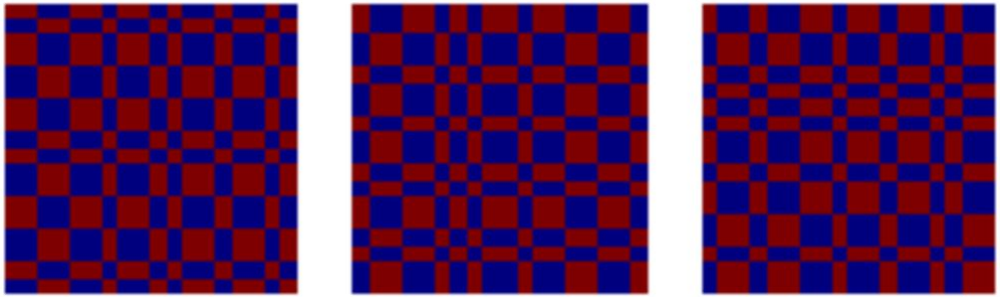
Dropout

Batch Normalization

Data Augmentation

DropConnect

Fractional Max Pooling

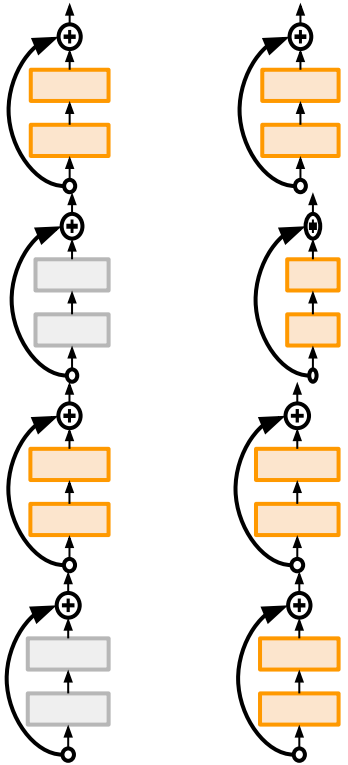


Graham, “Fractional Max Pooling”, arXiv 2014

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

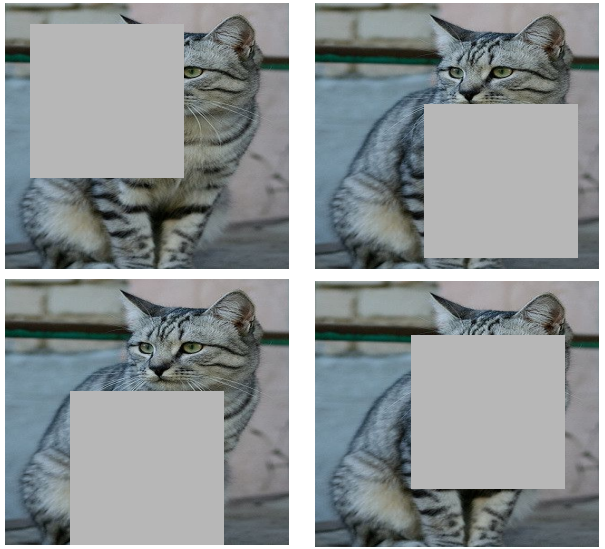
Regularization: Cutout

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



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

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

Regularization: Mixup

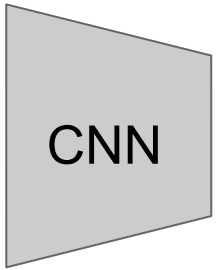
Training: Train on random blends of images

Testing: Use original images

Examples:

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

Randomly blend the pixels of pairs of training images, e.g. 40% cat, 60% dog



Target label:
cat: 0.4
dog: 0.6

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

Regularization: CutMix

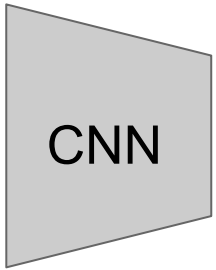
Training: Train on random blends of images

Testing: Use original images

Examples:

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

Replace random crops of one image with another: e.g. 60% of pixels from cat, 40% from dog



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

Standard Training:	Label Smoothing:
Cat: 100%	Cat: 90%
Dog: 0%	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

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

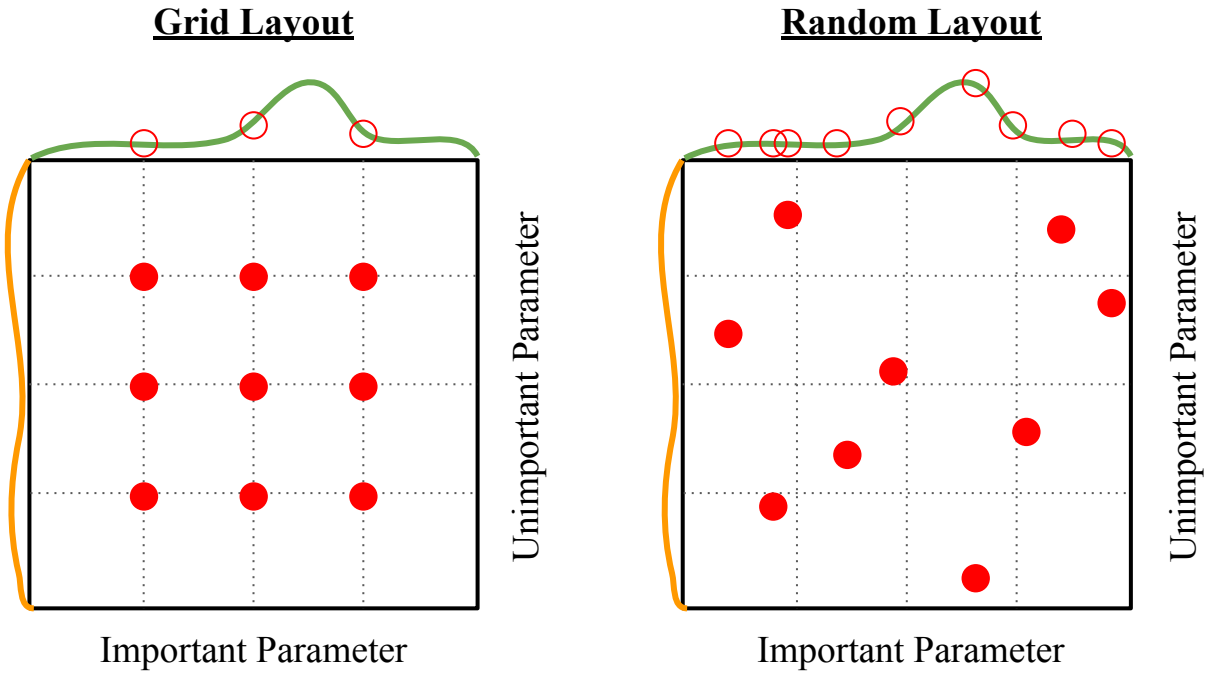


Illustration of Bergstra et al., 2012 by Shayne Longpre, copyright CS231n 2017

Choosing Hyperparameters

(without tons of GPUs)

Choosing Hyperparameters

Step 1: Check initial loss

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

Choosing Hyperparameters

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

Choosing Hyperparameters

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

Choosing Hyperparameters

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

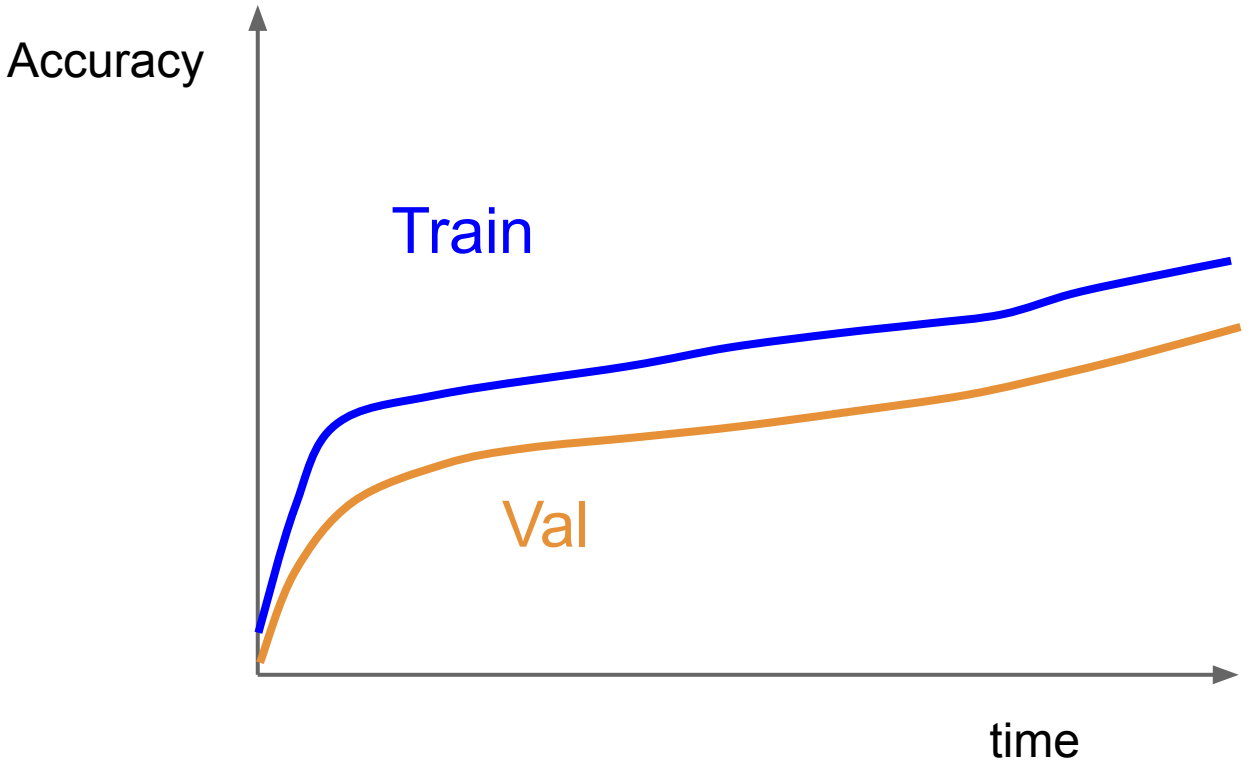
Choosing Hyperparameters

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

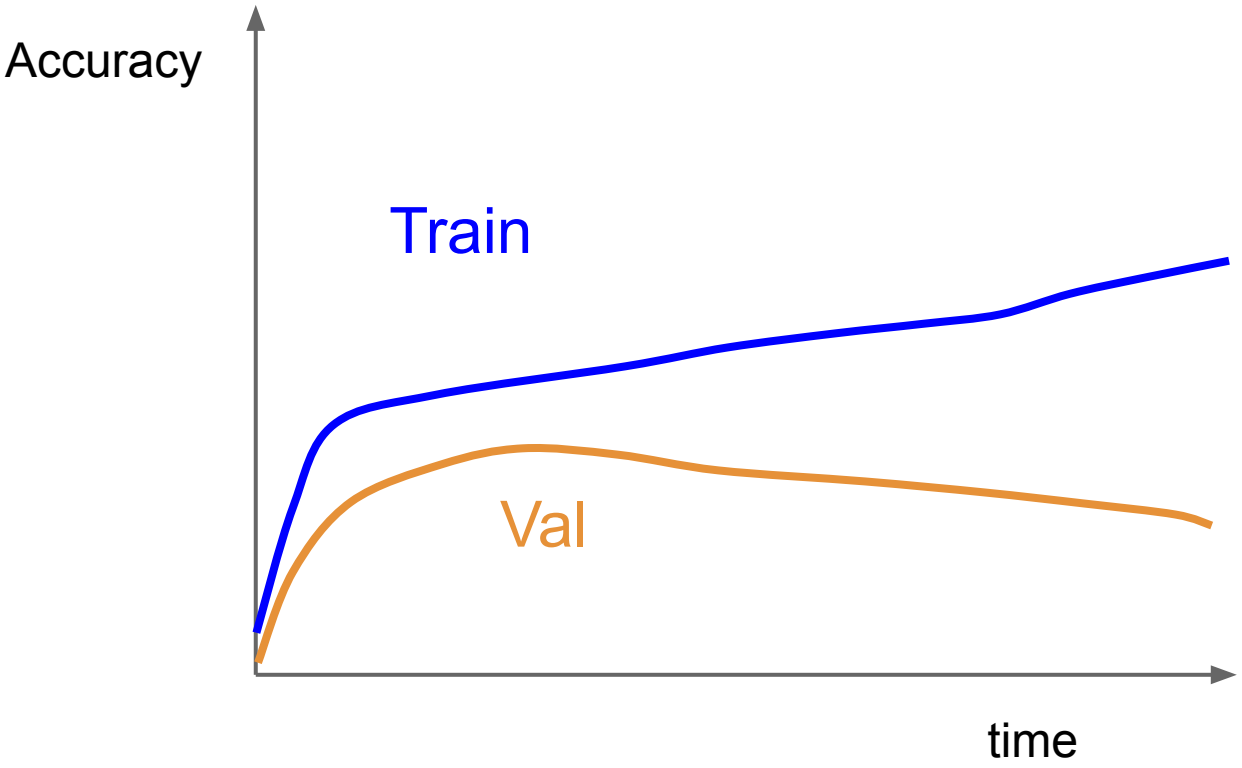
Pick best models from Step 4, train them for longer (~10-20 epochs) without learning rate decay

Choosing Hyperparameters

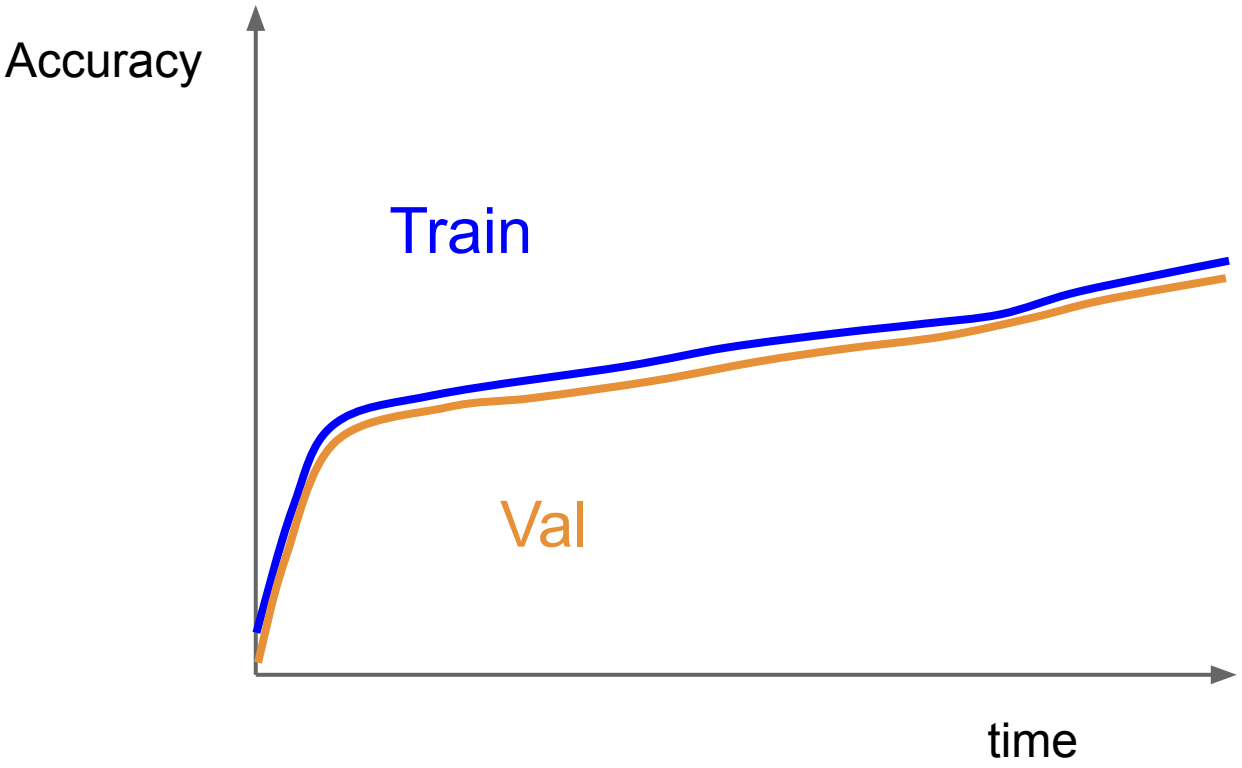
Step 1: Check initial loss
Step 2: Overfit a small sample
Step 3: Find LR that makes loss go down
Step 4: Coarse grid, train for ~1-5 epochs
Step 5: Refine grid, train longer
Step 6: Look at loss and accuracy curves



Q1. You see this. What should you do?



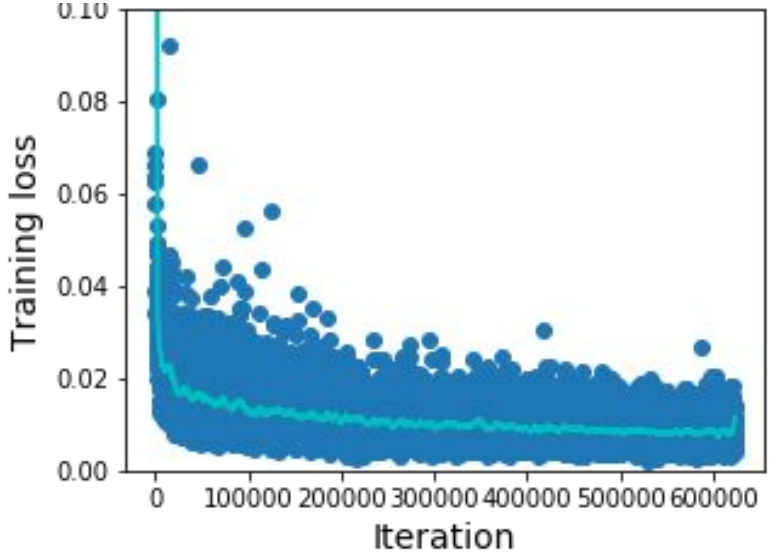
Q2. You see this. What should you do?



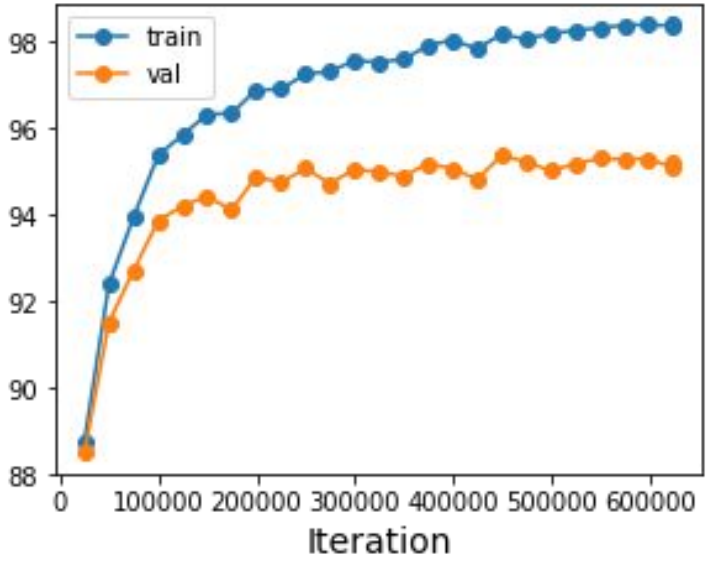
Q3. You see this. What should you do?

Look at learning curves!

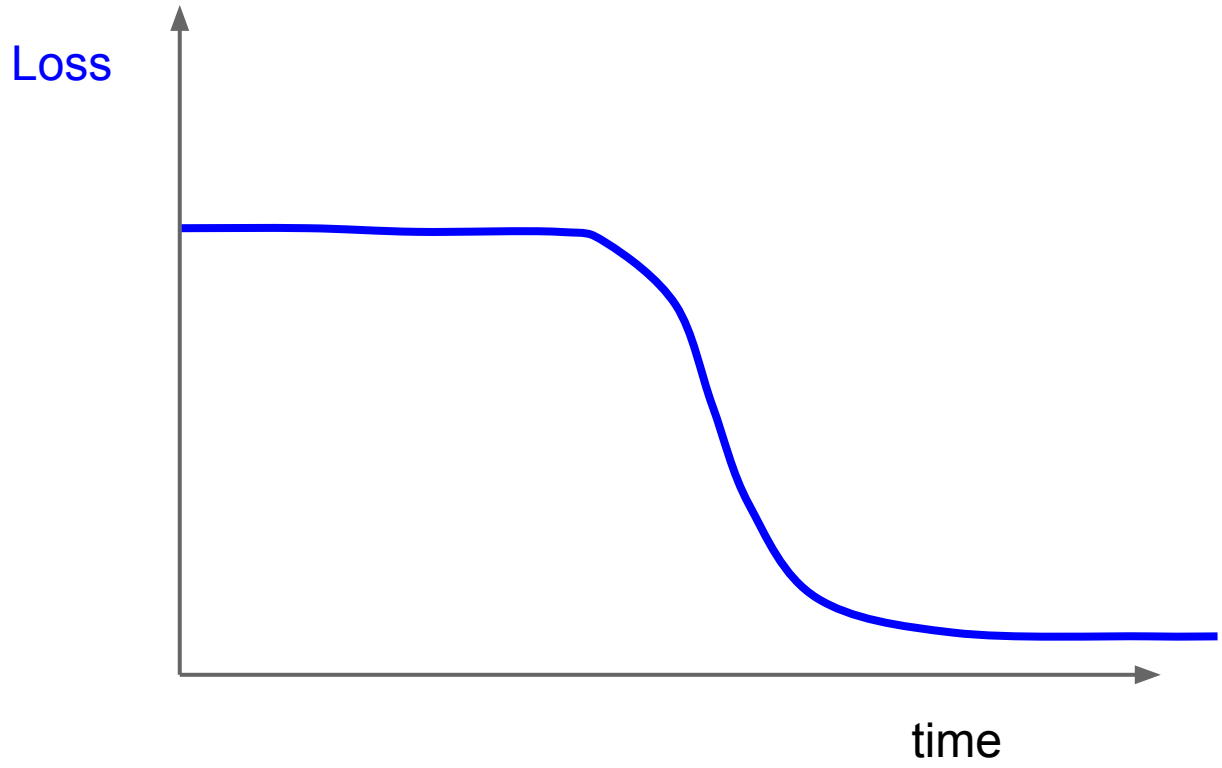
Training Loss



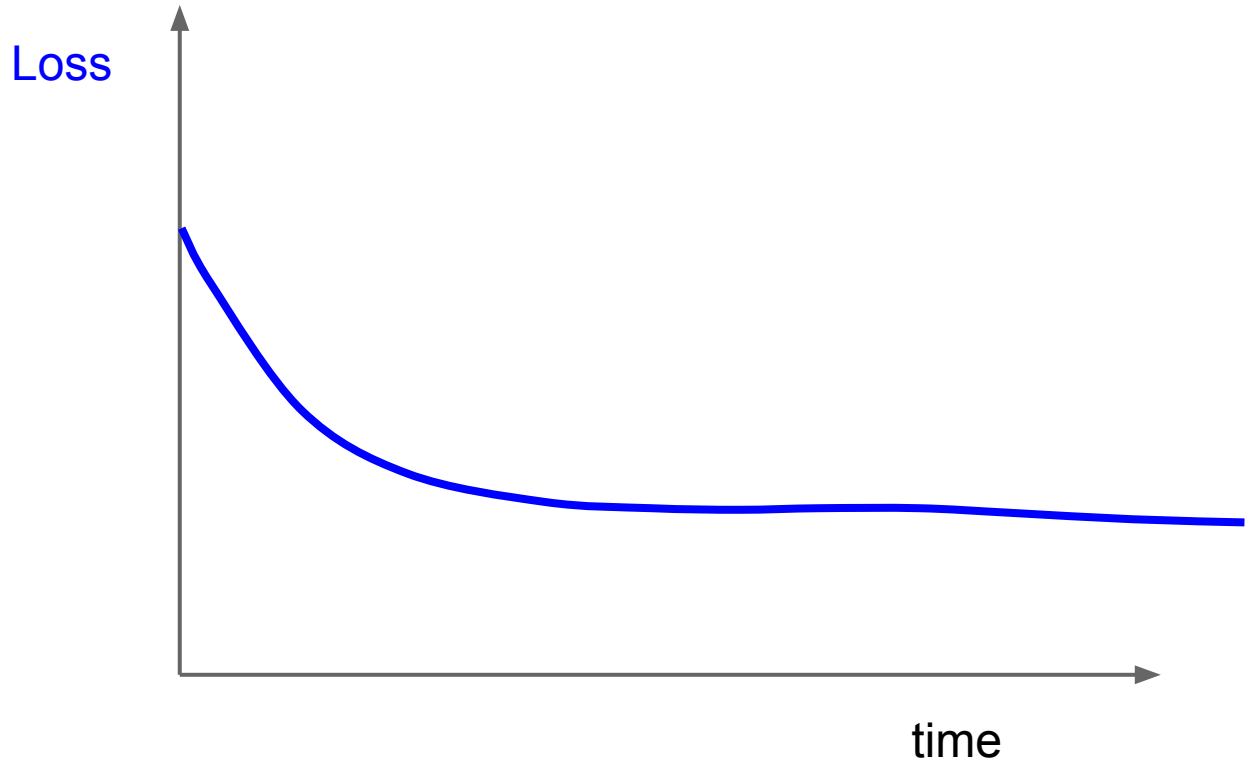
Train / Val Accuracy



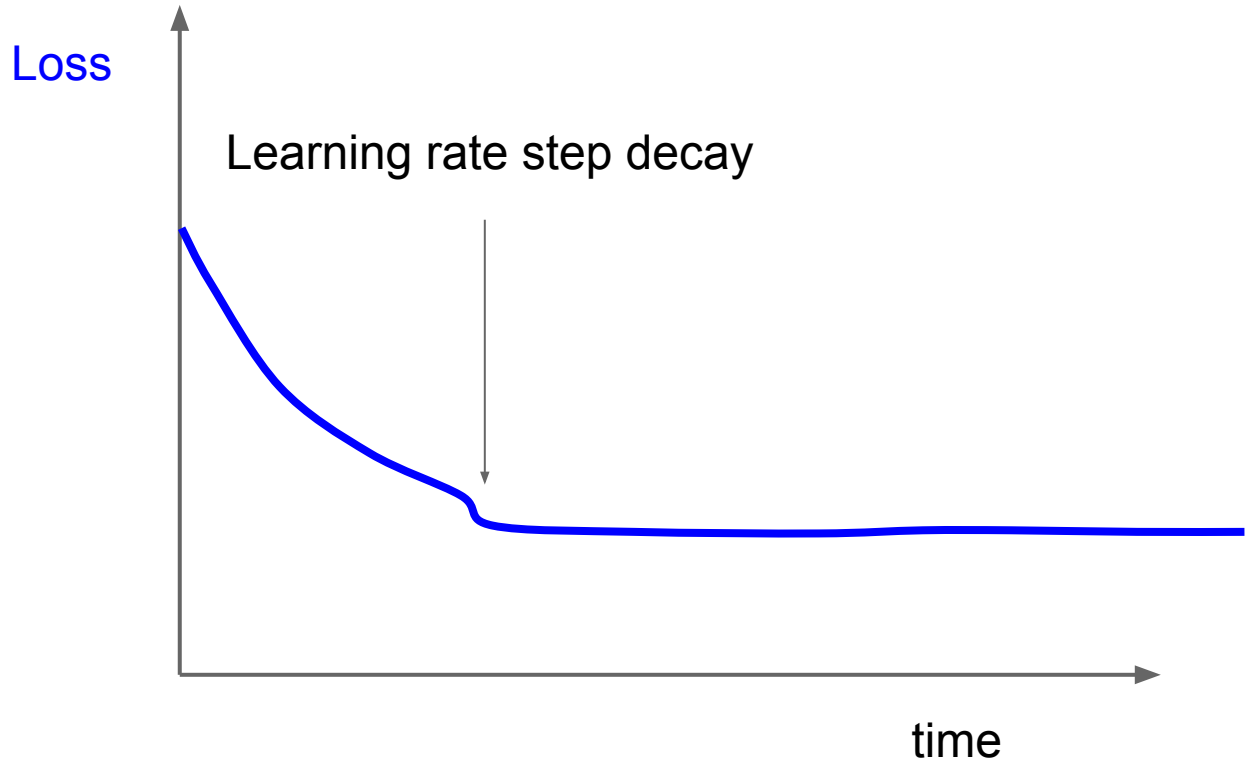
Losses may be noisy, use a scatter plot and also plot moving average to see trends better



Q4. You see this. What should you do?



Q5. You see this. What should you do?

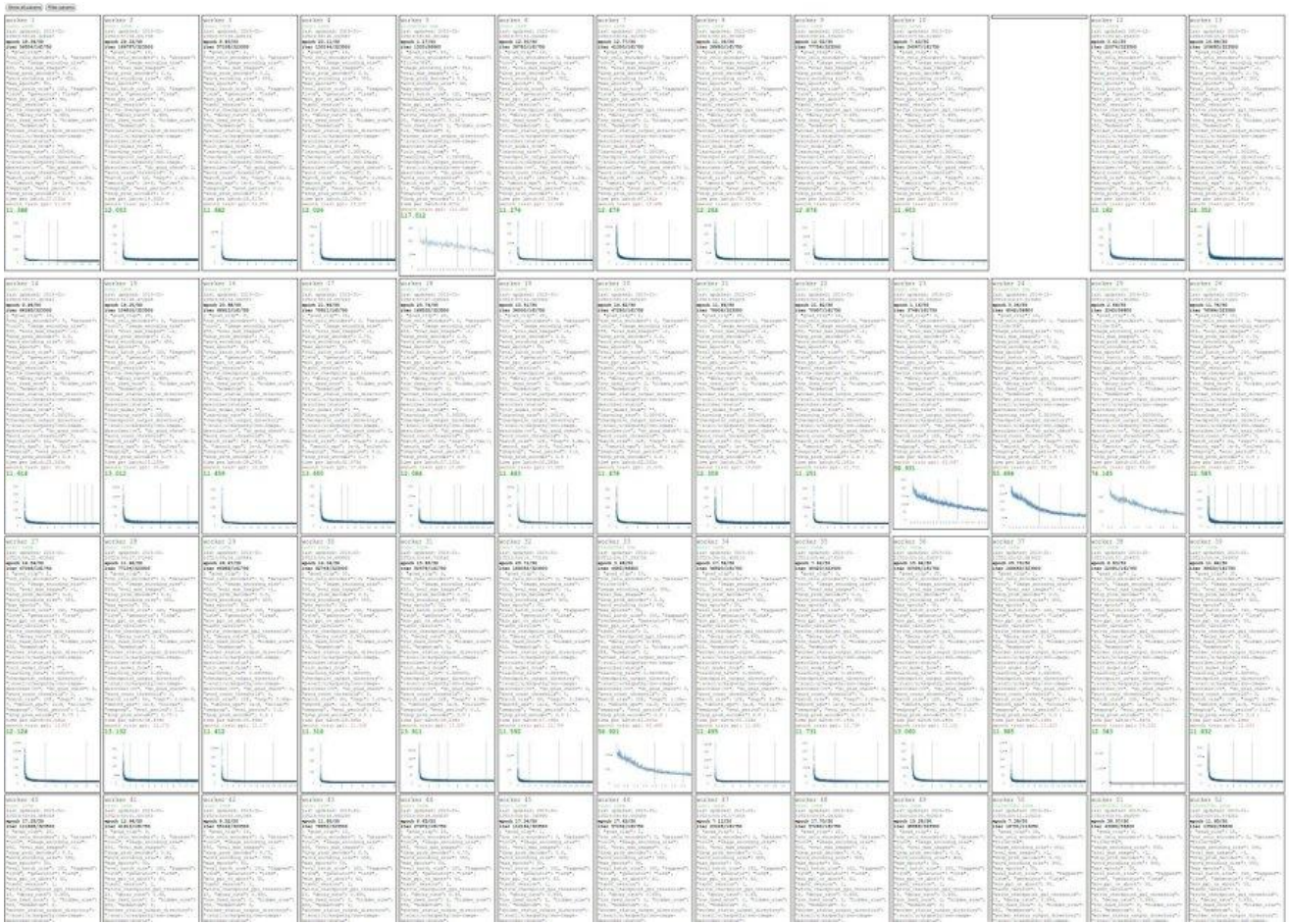


Q5. You see this. What should you do?

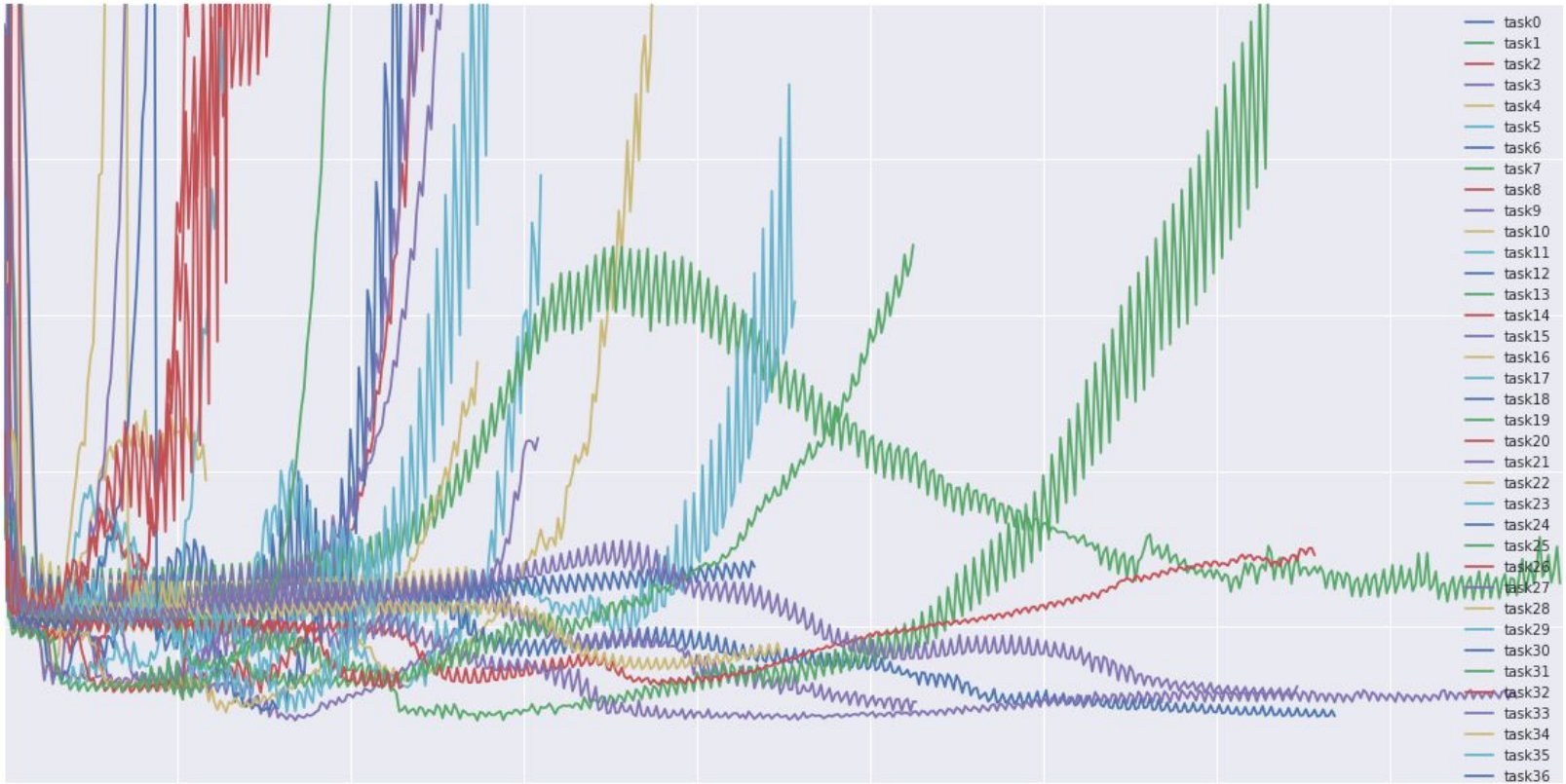
Cross-validation

We launch 100s of training runs all at once and visualize all our models training with different hyperparameters

check out [weights and biases]



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



Choosing Hyperparameters

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)

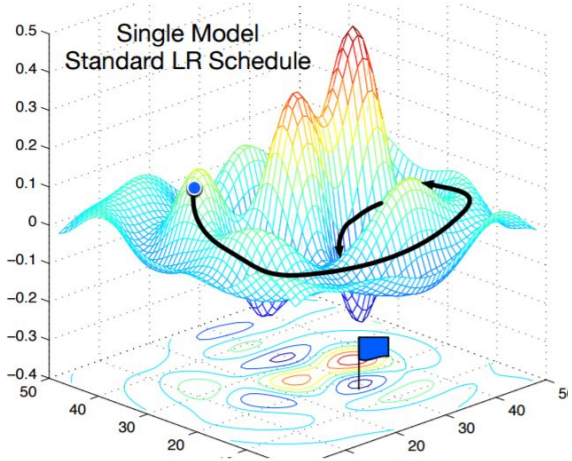
Summary

- 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
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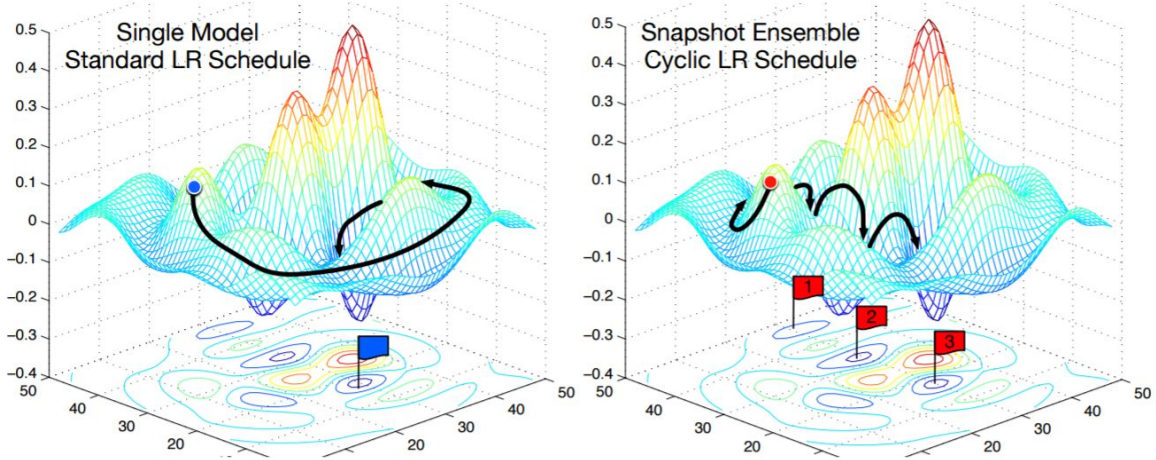
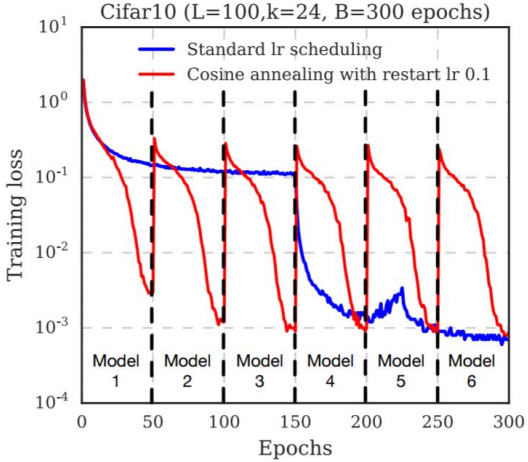
Model Ensembles: Tips and Tricks

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





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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