Neural Networks. Introduction to Deep Learning.

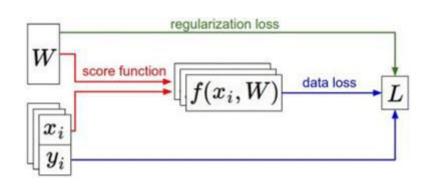
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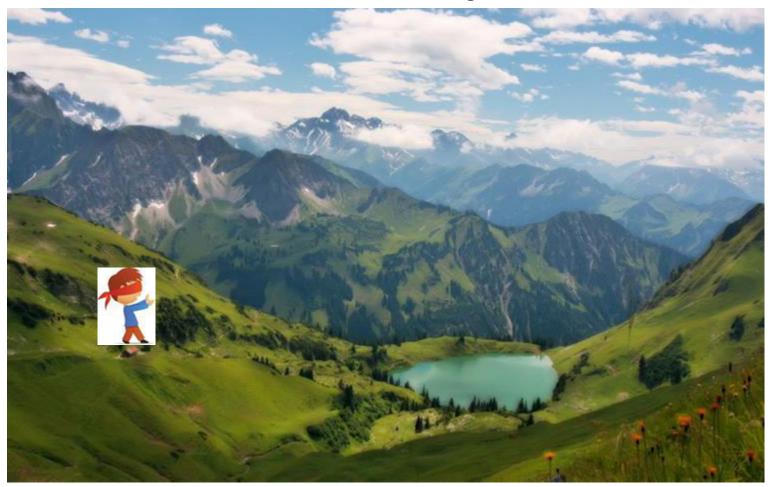
From previous lecture:

- We have some dataset of (x,y)
- We have a **score function**: $s = f(x; W) \stackrel{\text{e.g.}}{=} Wx$
- We have a **loss function**:

$$L_i = -\log(rac{e^{sy_i}}{\sum_j e^{s_j}})$$
 SVM $L_i = \sum_{j
eq y_i} \max(0, s_j - s_{y_i} + 1)$ $L = rac{1}{N} \sum_{i=1}^N L_i + R(W)$ Full loss



Gradient Descent Algorithm



Gradient Evaluation

1) Numerical approach

We choose a small positive h and apply the formula:

$$rac{df(x)}{dx} = \lim_{h o 0} rac{f(x+h) - f(x)}{h}$$

- We obtain an approximate value
- Very slow to compute

2) Analytic approach

We use calculus to determine the gradient's formula as a function of X and W

In summary:

=>

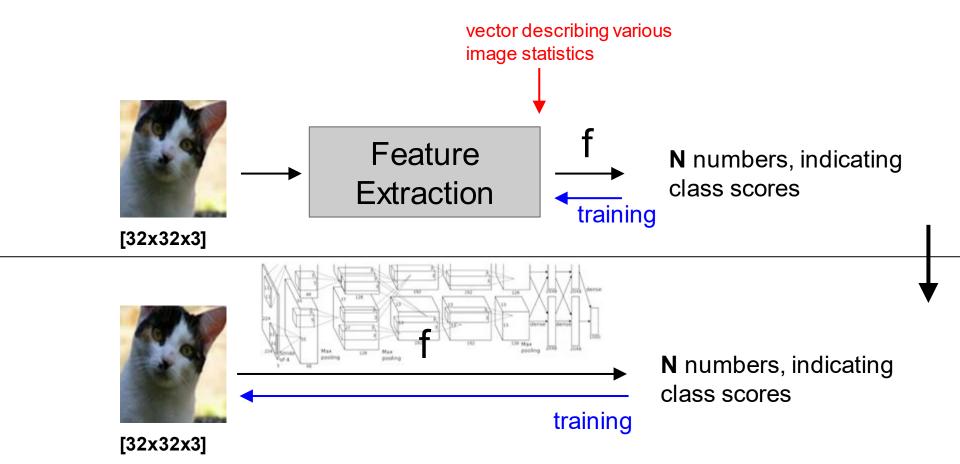
- Numerical gradient: approximate, slow, easy to write
- Analytic gradient: exact, fast, error-prone

<u>In practice:</u> Always use analytic gradient, but check implementation with numerical gradient. This is called a **gradient checking.**

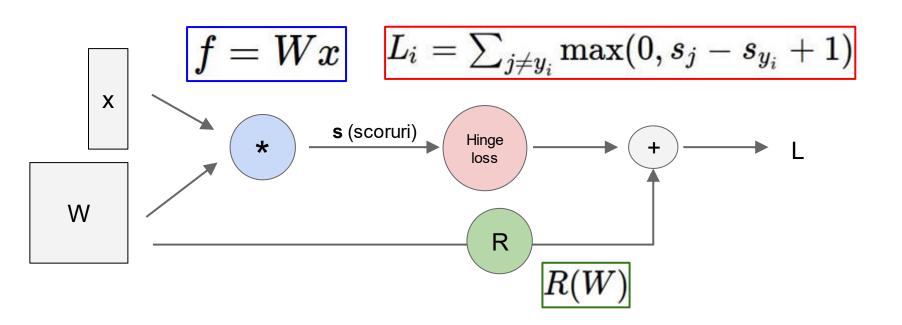
Gradient Descent (Python)

```
def GD(W0, X, goal, learningRate):
 perfGoalNotMet = true
 W = W0
 while perfGoalNotMet:
   gradient = eval gradient(X, W)
   W \text{ old} = W
   W = W – learningRate * gradient
   perfGoalNotMet = sum(abs(W - W old)) > goal
```

From feature extract to end-to-end learning



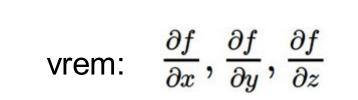
Computational Graph

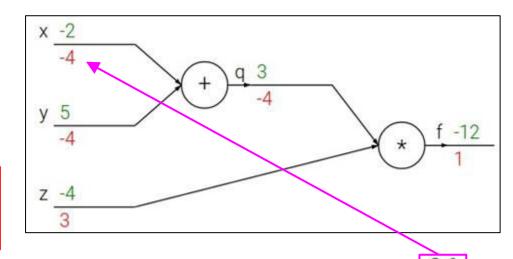


$$f(x, y, z) = (x + y)z$$

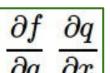
e.g. x = -2, y = 5, z = -4

$$q = x + y$$
 $\frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1$

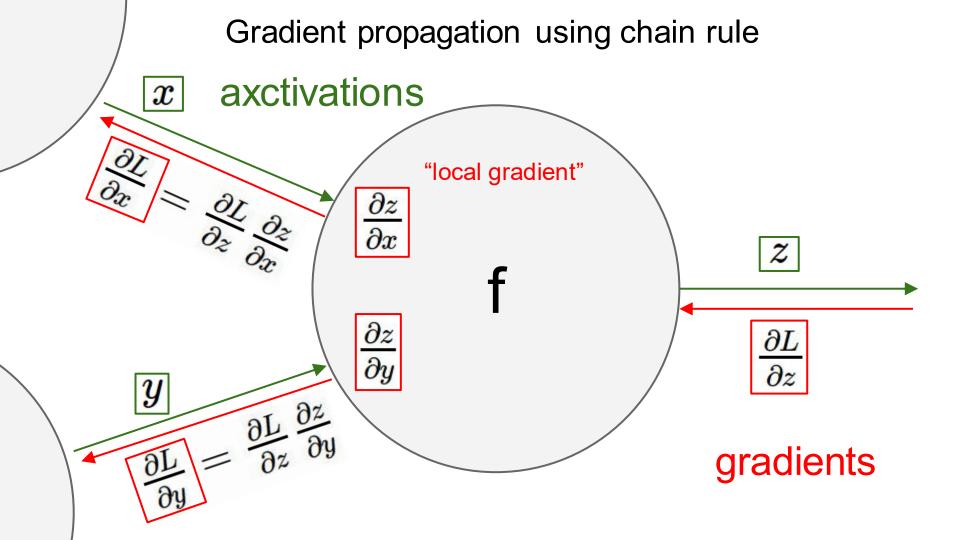




Chain rule:

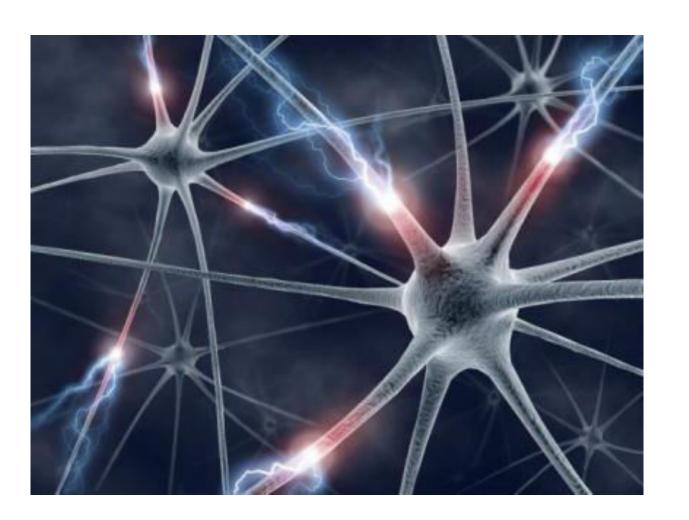


$$\frac{\partial f}{\partial q} \frac{\partial q}{\partial x}$$



From previous lecture...

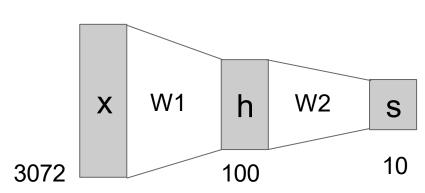
- Neural nets will be very large: no hope of writing down gradient formula by hand for all parameters
- Backpropagation = recursive application of the chain rule along a computational graph to compute the gradients of all inputs / parameters / intermediates
- Implementations maintain a graph structure, where the nodes implement the forward() / backward() API
- Forward: compute result of an operation and save any intermediates needed for gradient computation in memory
- Backward: apply the chain rule to compute the gradient of the loss function with respect to the inputs



Neural Network: without the brain stuff

f = Wx(**Before**) Linear score function: $f = W_2 \max(0, W_1 x)$

(Now) 2-layer Neural Network



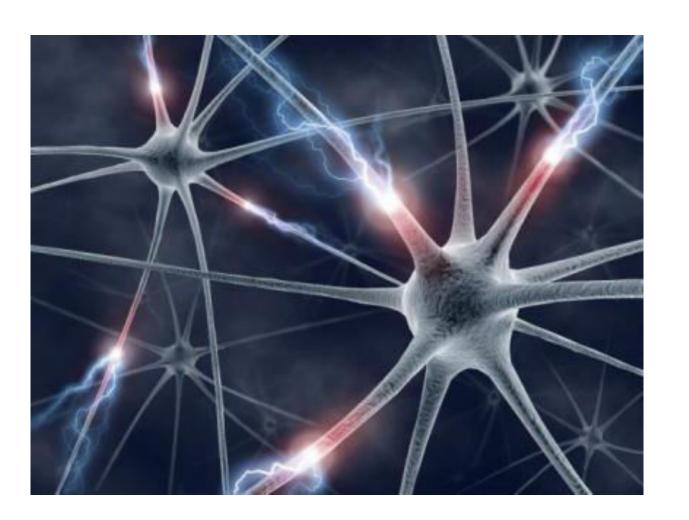
Neural Network: without the brain stuff

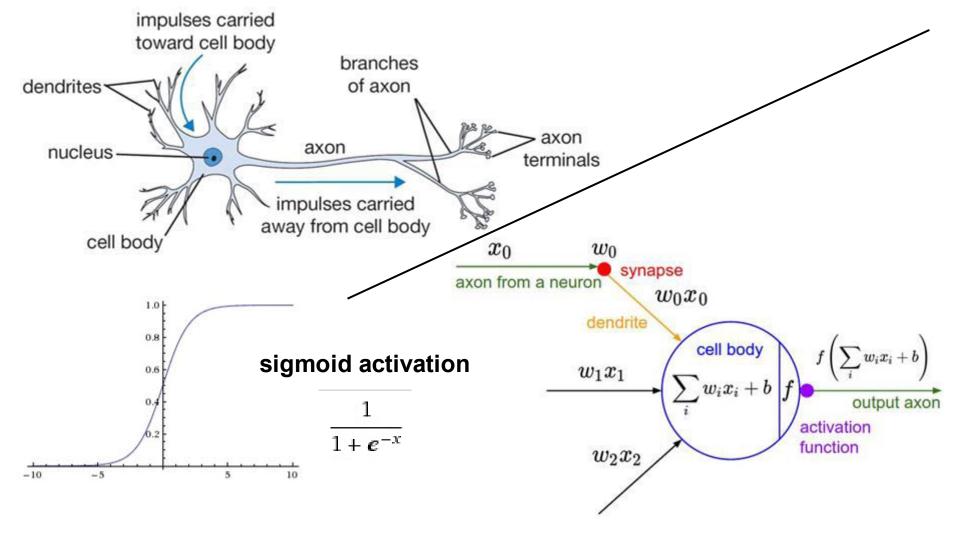
(**Before**) Linear score function: f = Wx

(Now) 2-layer Neural Network $f = W_2 \max(0, W_1 x)$

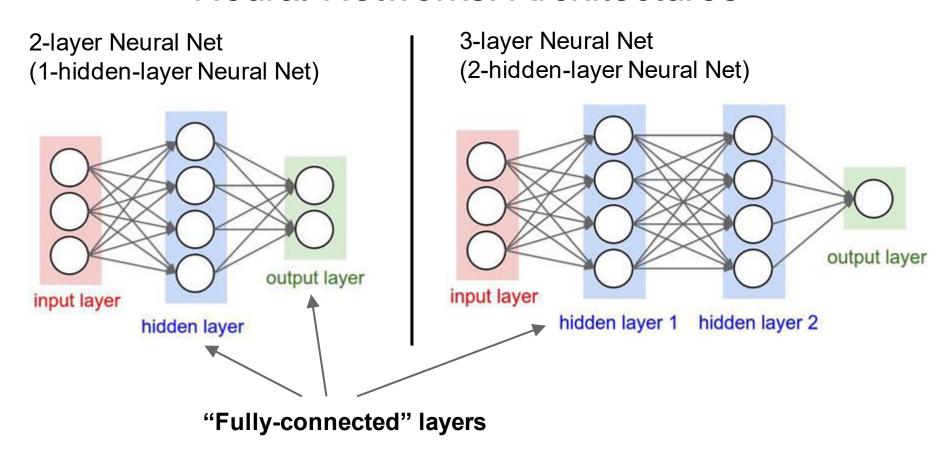
or 3-layer Neural Network

 $f=W_3\max(0,W_2\max(0,W_1x))$

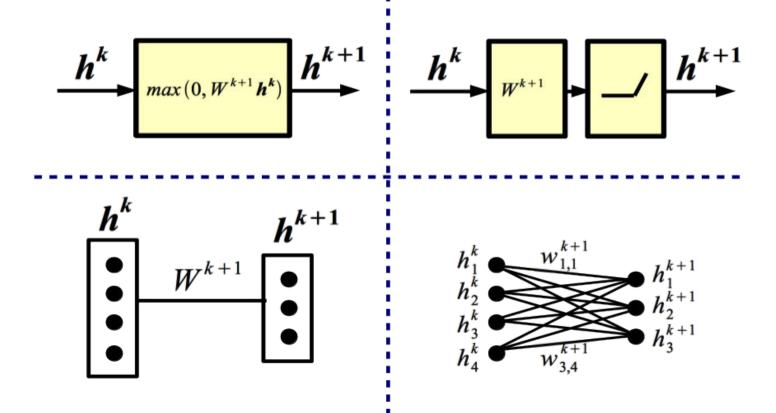




Neural Networks: Architectures



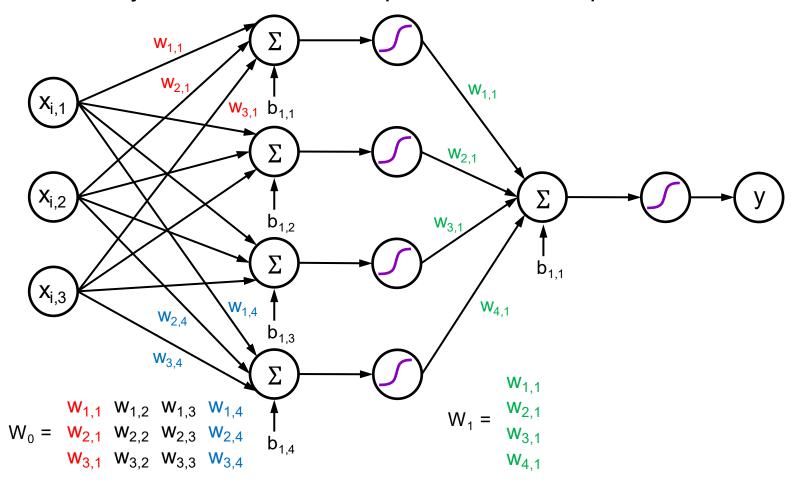
Equivalent Representations



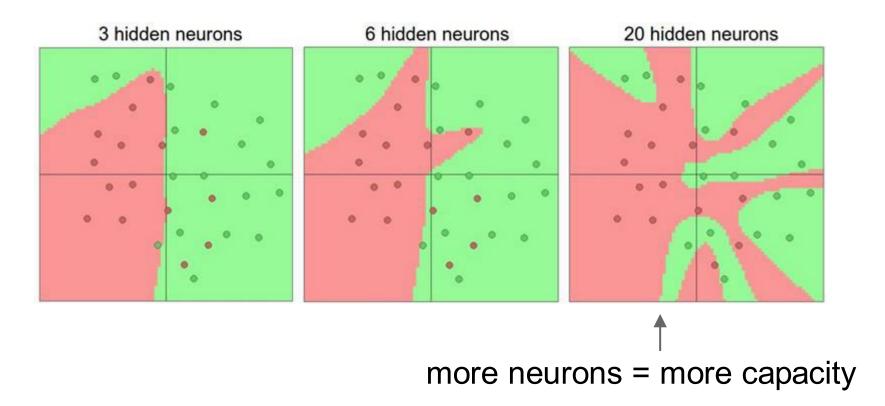
Training a 2-layer Neural Network needs ~11 lines (Python)

```
X = \text{np.array}([[0,0,1],[0,1,1],[1,0,1],[1,1,1]])
Y = np.array([[0,1,1,0]]).T
W0 = 2 * np.random.random((3,4)) - 1
W1 = 2 * np.random.random((4,1)) - 1
for i in range (5000):
  # forward pass
  11 = 1 / (1 + np.exp(-np.matmul(X, W0)))
  I2 = 1 / (1 + np.exp(-np.matmul(I1, W1)))
  # backward pass
  delta 12 = (Y - 12) * (12 * (1 - 12))
  delta 11 = \text{np.matmul}(\text{delta } 12, \text{W1.T})^* (11^* (1 - 11))
  # gradient descent
  W1 = W1 + np.matmul(I1.T, delta I2)
  W0 = W0 + np.matmul(X.T, delta 11)
```

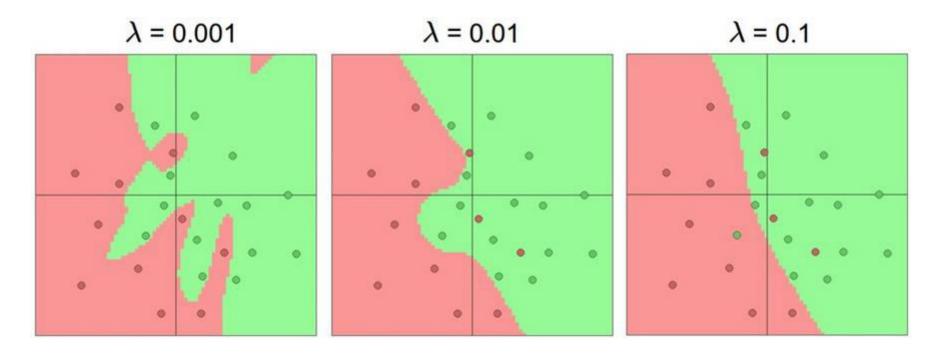
The 2-layer neural network implemented in the previous slide



Setting the number of layers and their sizes



Do not use size of neural network as a regularizer. Use stronger regularization instead:



Practical advice: In general, it is better to use stronger regularization than reducing the model's capacity

Choosing the right architecture

- We arrange neurons into fully-connected layers
- The abstraction of a **layer** has the nice property that it allows us to use efficient vectorized code (e.g. matrix multiplies)
- neural networks: bigger = better (but might have to regularize more strongly)

Training Neural Networks

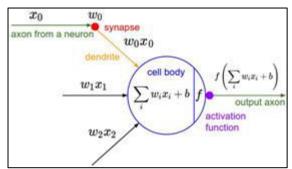
A bit of history

The **Mark I Perceptron** machine was the first implementation of the perceptron algorithm.

The machine was connected to a camera that used 20×20 cadmium sulfide photocells to produce a 400-pixel image.

Recognized letters of the alphabet.

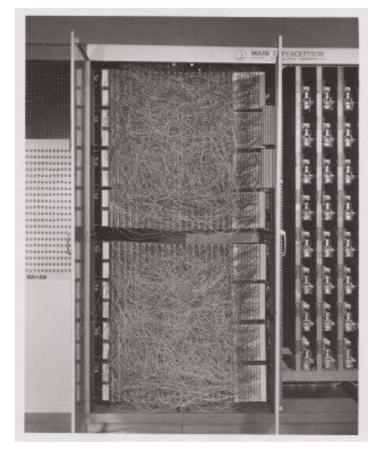
$$f(x) = \begin{cases} 1 & \text{if } w \cdot x + b > 0 \\ 0 & \text{otherwise} \end{cases}$$



Update rule:

$$w_i(t+1) = w_i(t) + \alpha(d_j - y_j(t))x_{j,i}$$

Frank Rosenblatt, ~1957: Perceptron



A bit of history

The **ADALINE** machine is based on memistors capable of executing logical operations and storing information.

Loss (sum squared error):

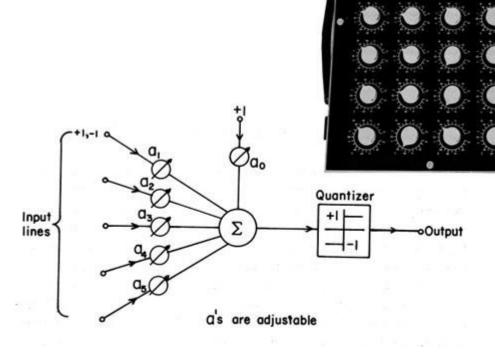
$$\frac{1}{2}\sum_{i}(d^{i}-y^{i})^{2}$$
, unde $y^{i}=(x^{i})^{T}w+b$

Update rule:

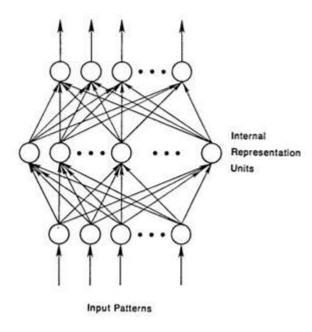
$$w^{k+1} = w^k + \mu \sum_{i=1}^m (d^i - y^i) x^i$$

$$b^{k+1} = b^k + \mu \sum_{i=1}^m (d^i - y^i)$$

Widrow and Hoff, ~1960: Adaline



A bit of history



To be more specific, then, let

$$E_{p} = \frac{1}{2} \sum_{j} (\epsilon_{pj} - o_{pj})^{2}$$
(2)

be our measure of the error on input/output pattern p and let $E = \sum E_p$ be our overall measure of the error. We wish to show that the delta rule implements a gradient descent in E when the units are linear. We will proceed by simply showing that

$$-\frac{\partial E_p}{\partial w_{ji}} = \delta_{pj} i_p$$

which is proportional to $\Delta_p w_{ji}$ as prescribed by the delta rule. When there are no hidden units it is straightforward to compute the relevant derivative. For this purpose we use the chair rule to write the derivative as the product of two parts: the derivative of the error with respect to the output of the unit times the derivative of the output with respect to the weight.

$$\frac{\partial E_p}{\partial w_{ji}} = \frac{\partial E_p}{\partial o_{pj}} \frac{\partial o_{pj}}{\partial w_{ji}}$$
. (3)

The first part tells how the error changes with the output of the jth unit and the second part tells how much changing w_{ji} changes that output. Now, the derivatives are easy to compute. First, from Equation 2

$$\frac{\partial E_g}{\partial \sigma_{gj}} = -(t_{gj} - \sigma_{gj}) = -\delta_{gj}. \tag{4}$$

Not surprisingly, the contribution of unit u_j to the error is simply proportional to δ_{gj} . Moreover, since we have linear units.

$$o_{pj} = \sum_{i} w_{ji} l_{pj}, \qquad (5)$$

from which we conclude that

$$\frac{\partial o_{pj}}{\partial w_n} = I_{pj}$$

Thus, substituting back into Equation 3, we see that

$$-\frac{\partial E_p}{\partial w_{ji}} = \delta_{pj} I_i \tag{6}$$

recognizable maths

Hinton et al. 1986: First time back-propagation became popular

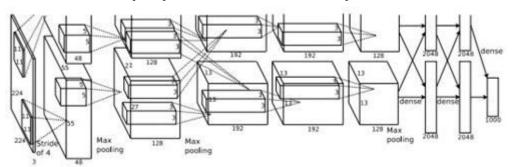
First strong results with deep learning

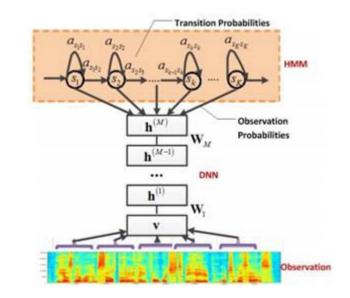
Context-Dependent Pre-trained Deep Neural Networks for Large Vocabulary Speech Recognition

George Dahl, Dong Yu, Li Deng, Alex Acero, 2010

Imagenet classification with deep convolutional neural networks

Alex Krizhevsky, Ilya Sutskever, Geoffrey E Hinton, 2012







Overview

1. One time setup

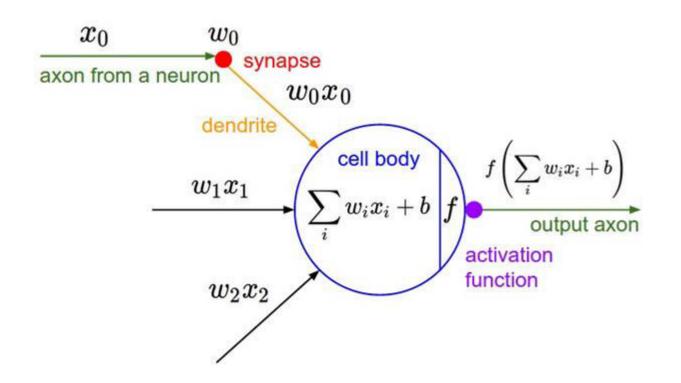
activation functions, preprocessing, weight initialization, regularization, gradient checking

2. Training dynamics

babysitting the learning process, parameter updates, hyperparameter optimization

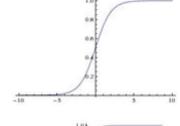
3. Evaluation

model ensembles

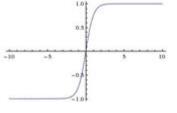


sigmoid

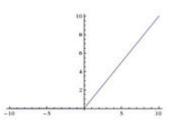
$$\sigma(x)=1/(1+e^{-x})$$



tanh tanh(x)

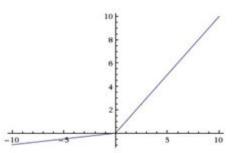


ReLU max(0,x)



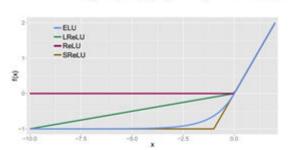
Leaky ReLU

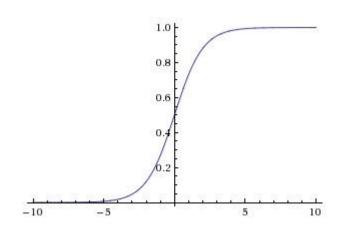
max(0.1x, x)



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

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





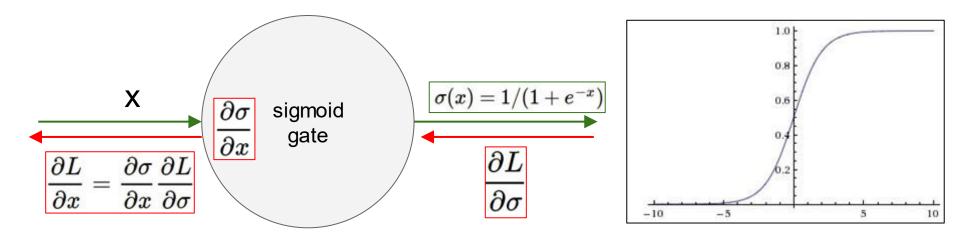
sigmoid

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

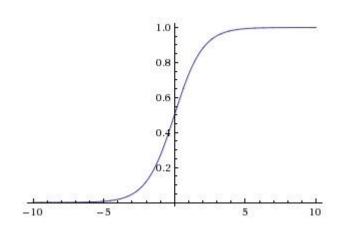
- Squashes numbers to range [0,1]
- Historically popular since they have nice interpretation as a saturating "firing rate" of a neuron

3 problems:

1. Saturated neurons "kill" the gradients



What happens when x = -10? What happens when x = 0? What happens when x = 10?



sigmoid

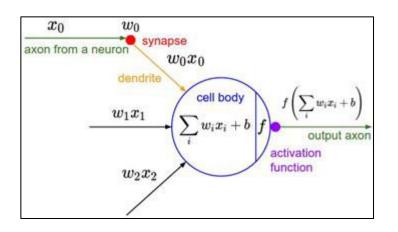
$$\sigma(x)=1/(1+e^{-x})$$

- Squashes numbers to range [0,1]
- Historically popular since they have nice interpretation as a saturating "firing rate" of a neuron

3 problems:

- 1. Saturated neurons "kill" the gradients
- 2. Sigmoid outputs are not zerocentered

Consider what happens when the input to a neuron (x) is always positive:



$$f\left(\sum_i w_i x_i + b
ight)$$

What can we say about the gradients on **w**?

Consider what happens when the input to a neuron is

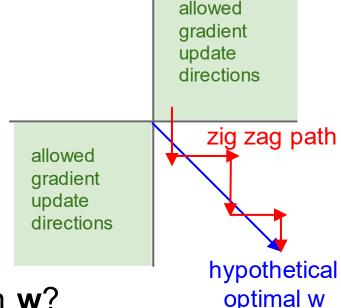
always positive...

$$f\left(\sum_i w_i x_i + b
ight)$$

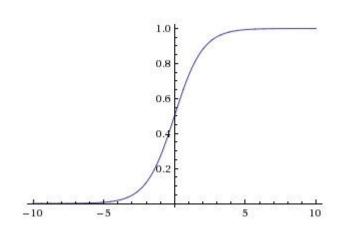
What can we say about the gradients on **w**?

Always all positive or all negative :(

Note: this is also why you want zero-mean data!



vector



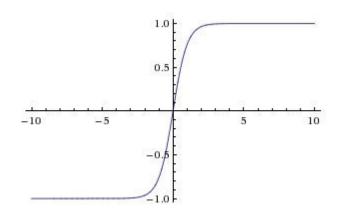
sigmoid

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

- Squashes numbers to range [0,1]
- Historically popular since they have nice interpretation as a saturating "firing rate" of a neuron

3 problems:

- 1. Saturated neurons "kill" the gradients
- 2. Sigmoid outputs are not zerocentered
- 3. exp() is a bit computationally expensive

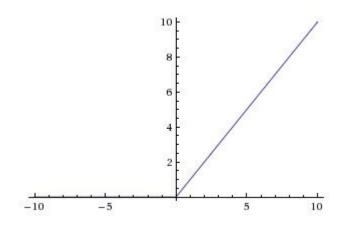


tanh(x)

$$rac{e^x-e^{-x}}{e^x+e^{-x}}$$

- Squashes numbers to range [-1,1]
- zero centered (nice)
- still kills gradients when saturated :(

[LeCun et al., 1991]

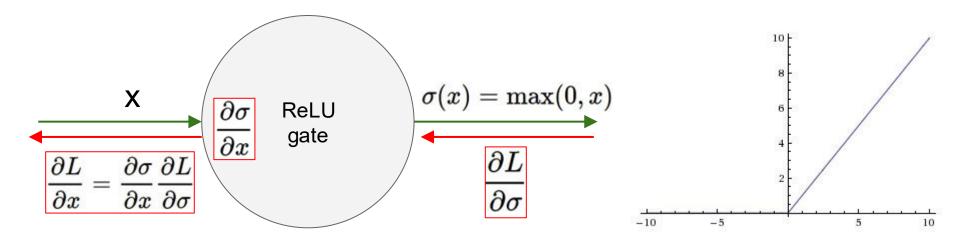


ReLU (Rectified Linear Unit)

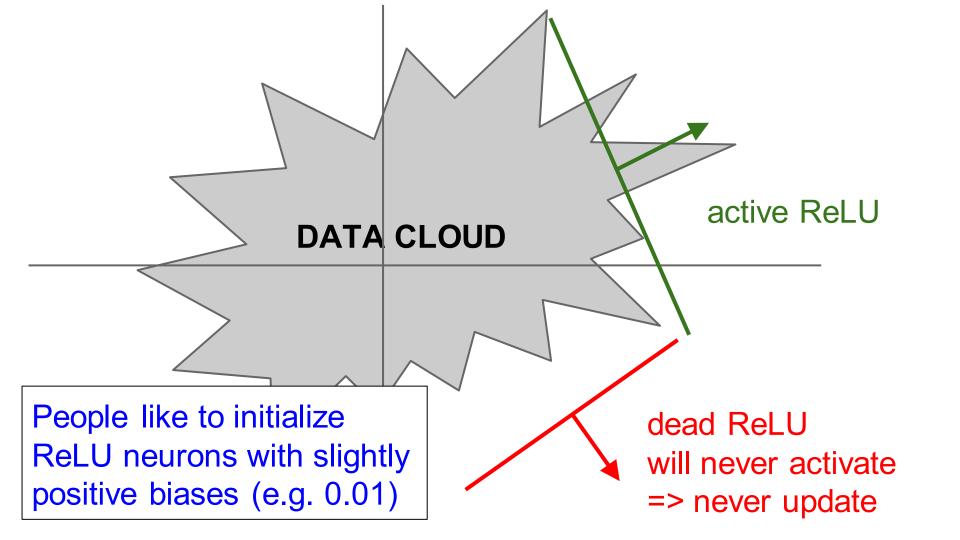
$$f(x) = \max(0,x)$$

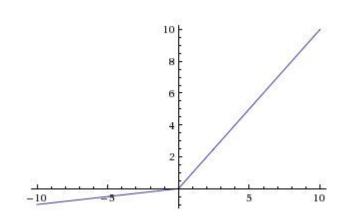
- Does not saturate (in +region)
- Very computationally efficient
- Converges much faster than sigmoid/tanh in practice (e.g. 6x)
- Not zero-centered output
- An annoyance: what is the gradient when x < 0?

[Krizhevsky et al., 2012]



What happens when x = -10? What happens when x = 0? What happens when x = 10?





Leaky ReLU

$$f(x) = \max(0.01x, x)$$

- Does not saturate
- Computationally efficient
- Converges much faster than sigmoid/tanh in practice! (e.g. 6x)
- will not "die"

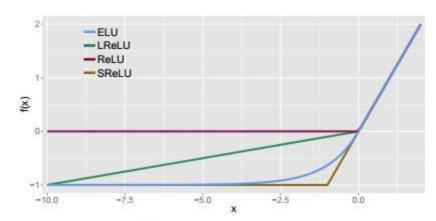
Parametric Rectifier (PReLU)

$$f(x) = \max(lpha x, x)$$
backprop into $lpha$
(parameter)

[Mass et al., 2013]

[He et al., 2015]

Exponential Linear Units (ELU)



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

- All benefits of ReLU
- Does not die
- Closer to zero mean outputs
- Computation requires exp()

Maxout "Neuron"

- Does not have the basic form of dot product -> nonlinearity
- Generalizes ReLU and Leaky ReLU
- Linear Regime! Does not saturate! Does not die!

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

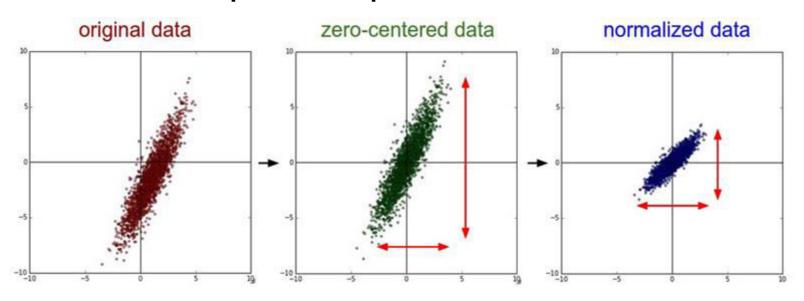
Problem: doubles the number of parameters/neurons:(

TLDR: In practice:

- Use ReLU. Be careful with your learning rates
- Try out Leaky ReLU / Maxout / ELU
- Try out tanh but don't expect much
- Avoid using sigmoid

Data Preprocessing

Step 1: Preprocess the data



(Assume X [NxD] is data matrix, each example in a row)

TLDR: In practice for images: center only

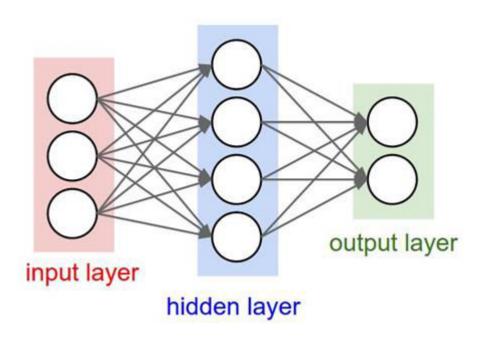
Consider CIFAR-10 example with [32,32,3] images:

- Subtract the mean image (e.g. AlexNet) (mean image = [32,32,3] array)
- Subtract per-channel mean (e.g. VGGNet) (mean along each channel = 3 numbers)

It is not mandatory to normalize data for deep networks

Weight Initialization

Q: what happens when W=0 init is used?



First idea: Small random numbers

W = np.random.normal(0, 0.01, (N,D)) (gaussian with zero mean and 0.01 standard deviation)

Works ~okay for small networks, but can lead to non-homogeneous distributions of activations across the layers of a network.

Second idea: Xavier Initialization

Problems with choosing the initial weights:

- If they are too small, the signal strength propagating in the network drops with each level until it becomes too small to be useful
- If they are too big, the signal strength propagating in the network grows with each level until it becomes too big to be useful
- Xavier initialization ensures that the weight have the right magnitude, keeping the signal strength in a reasonable interval.
- The initial weights come from a normal distribution of mean 0 and standard deviation given by the number of perceptrons in previous/next layer:

$$ext{Var}(W) = rac{2}{n_{ ext{in}} + n_{ ext{out}}}$$

Proper initialization is an active area of research...

Understanding the difficulty of training deep feedforward neural networks by Glorot and Bengio, 2010

Exact solutions to the nonlinear dynamics of learning in deep linear neural networks by Saxe et al, 2013

Random walk initialization for training very deep feedforward networks by Sussillo and Abbott, 2014

Delving deep into rectifiers: Surpassing human-level performance on ImageNet classification by He et al., 2015

Data-dependent Initializations of Convolutional Neural Networks by Krähenbühl et al., 2015

All you need is a good init by Mishkin and Matas, 2015

. . .

"you want unit gaussian activations? just make them so."

Consider a batch of activations at some layer. To make each dimension unit gaussian, apply:

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

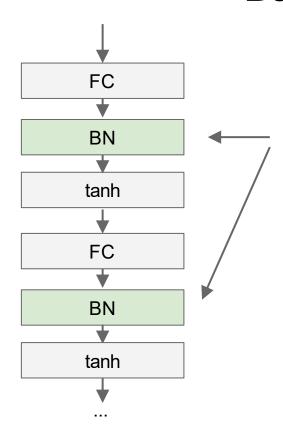
"you want unit gaussian activations? just make them so."

N X

1. Compute the empirical mean and variance independently for each dimension.

2. Normalize

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



Usually inserted after fully-connected or convolutional layers, and before nonlinearity.

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

Normalize:

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

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

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

Note, the network can learn:

$$\gamma^{(k)} = \sqrt{\operatorname{Var}[x^{(k)}]}$$

$$\beta^{(k)} = \mathrm{E}[x^{(k)}]$$

to recover the identity mapping.

Input: Values of x over a mini-batch: $\mathcal{B} = \{x_{1...m}\}$; Parameters to be learned: γ , β

Output: $\{y_i = BN_{\gamma,\beta}(x_i)\}$

$$u_{\mathcal{B}} \leftarrow \frac{1}{m} \sum_{i=1}^{m} x_{i}$$
 // mini-batch mean

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

$$\widehat{x}_i \leftarrow \frac{x_i - \mu_{\mathcal{B}}}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}}$$
 // normalize $y_i \leftarrow \gamma \widehat{x}_i + \beta \equiv \mathrm{BN}_{\gamma,\beta}(x_i)$ // scale and shift

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

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

Input: Values of x over a mini-batch: $\mathcal{B} = \{x_{1...m}\}$; Parameters to be learned: γ , β

Output: $\{y_i = BN_{\gamma,\beta}(x_i)\}$

$$u_{\mathcal{B}} \leftarrow \frac{1}{m} \sum_{i=1}^{m} x_{i}$$
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$$\widehat{x}_i \leftarrow \frac{x_i - \mu_{\mathcal{B}}}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}}$$
 // normalize
$$y_i \leftarrow \gamma \widehat{x}_i + \beta \equiv \text{BN}_{\gamma,\beta}(x_i)$$
 // scale and shift

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

Note: at test time BatchNorm layer functions differently:

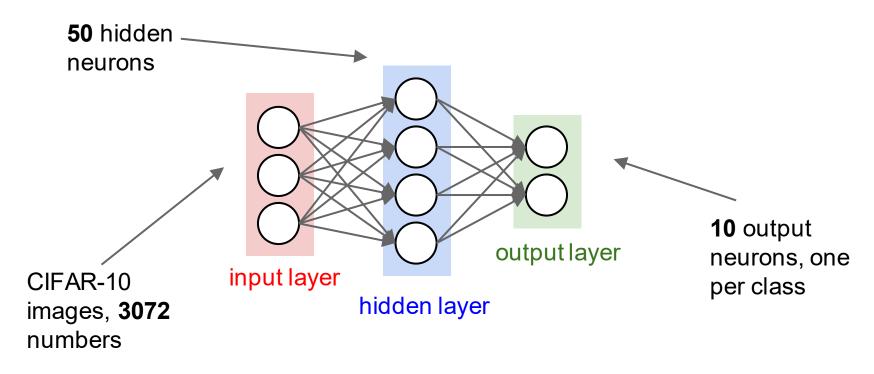
The mean/std are not computed based on the batch. Instead, a single fixed empirical mean of activations during training is used.

(e.g. can be estimated during training with running averages)

Babysitting the Learning Process

Step 2: Choose the architecture

Say we start with one hidden layer of 50 neurons, then we gradually add more layers

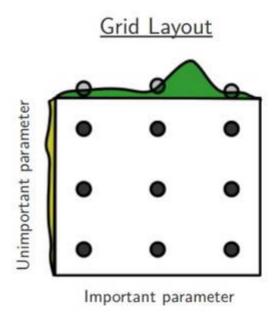


Practical Advice

- 1. Turn off regularization and check that the loss has a reasonable value (~2.5 for 10 classes is ok)
- 2. Turn on regularization and make sure that the value of the loss function grows, e.g. 3.2
- 3. Make sure that we can do overfitting on a small subset of the training data (e.g. 20 samples)
- 4. Start with small regularization and find learning rate that makes the loss go down

Hyperparameter Optimization

Random Search vs. Grid Search



Random Layout

Important parameter

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

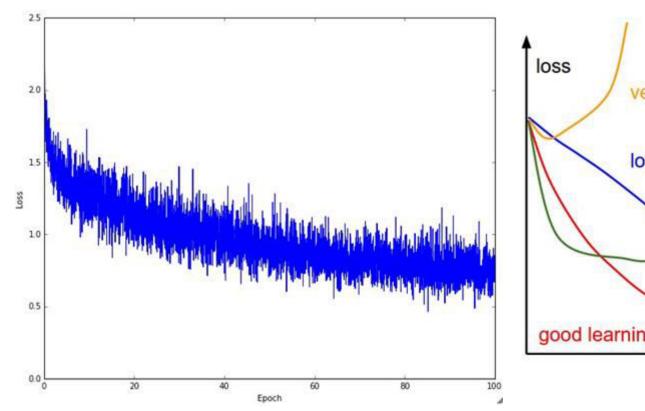
Hyperparameters to play with

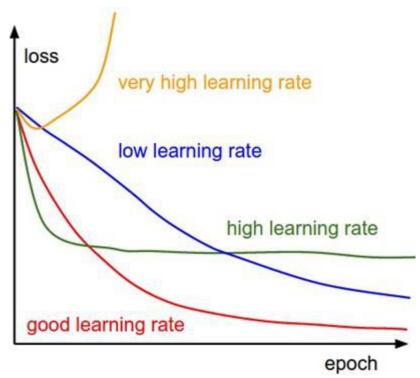
- Network architecture
- Learning rate, its decay schedule, update type
- Algorithm: SGD, SGD with momentum, Adam
- Regularization (L2 / Dropout strength)

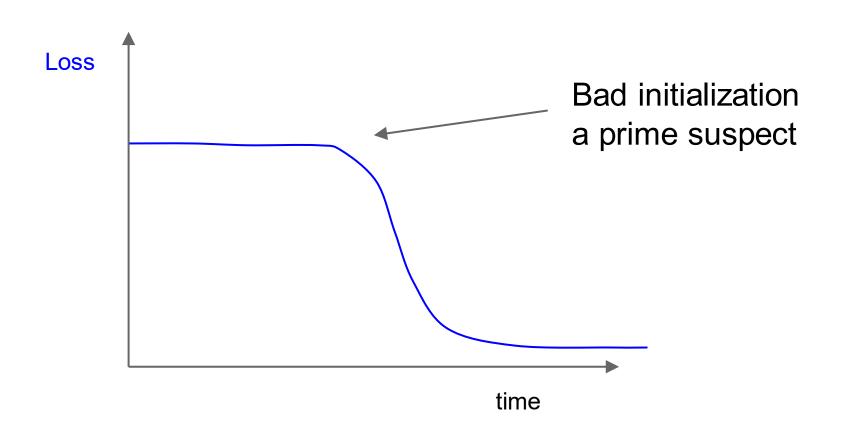
Neural networks practitioner music = loss function



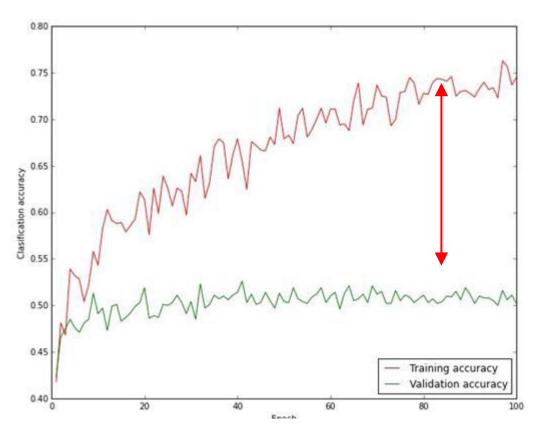
Monitor and visualize the loss curve







Monitor and visualize the accuracy



big gap = overfitting

=> increase regularization strength?

no gap

=> increase model capacity?

TLDRs

Summary

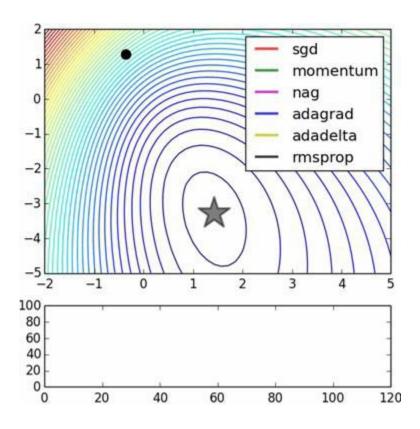
We looked in detail at:

- Activation Functions (use ReLU)
- Data Preprocessing (images: subtract mean)
- Weight Initialization (use Xavier init)
- Batch Normalization (use)
- Babysitting the Learning process
- Hyperparameter Optimization

(random sampling, in log space when appropriate)

Training Algorithm

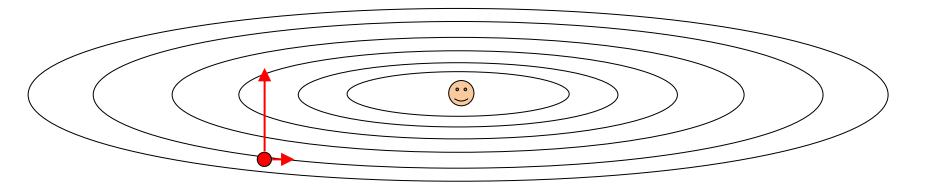
There are multiple training algorithms



Gradient Descent (Python)

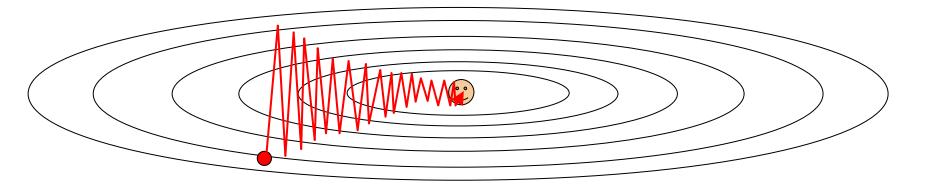
```
def GD(W0, X, goal, learningRate):
 perfGoalNotMet = true
 W = W0
 while perfGoalNotMet:
   gradient = eval gradient(X, W)
   W \text{ old} = W
   W = W – learningRate * gradient
   perfGoalNotMet = sum(abs(W - W old)) > goal
```

Suppose loss function is steep vertically but shallow horizontally:



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

Suppose loss function is steep vertically but shallow horizontally:



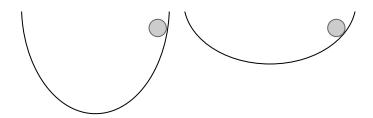
Q: What is the trajectory along which we converge towards the minimum with SGD? Very slow progress along flat direction, jitter along steep one

SGD with momentum (Python)

```
def GD(W0, X, goal, learningRate, mu):
 perfGoalNotMet = true
 W = W0
 V = 0
 while perfGoalNotMet:
   gradient = eval gradient(X, W)
   W \text{ old} = W
   V = mu * V – learningRate * gradient
   W = W + V
   perfGoalNotMet = sum(abs(W - W old)) > goal
```

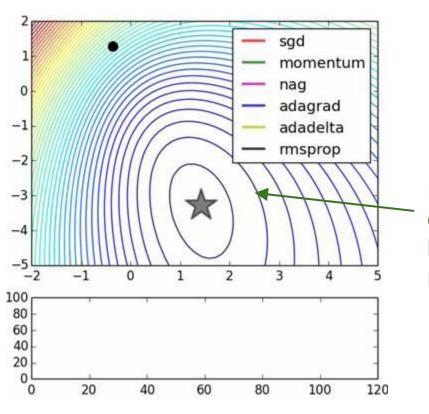
SGD with momentum

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



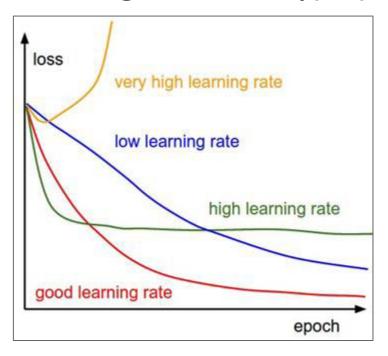
- Allows a velocity to "build up" along shallow directions
- Velocity becomes damped in steep direction due to quickly changing sign

SGD vs. SGD with momentum



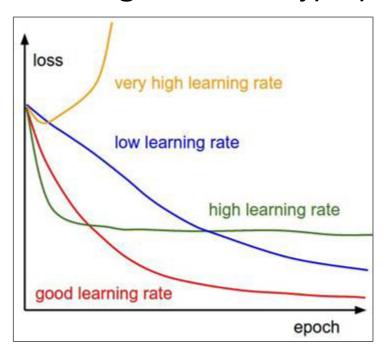
Notice momentum overshooting the target, but overall getting to the minimum much faster.

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



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

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



=> Learning rate decay over time!

step decay:

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

exponential decay:

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

1/t decay:

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

Evaluation:

Model Ensembles

Model Ensembles

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

Enjoy 2% extra performance

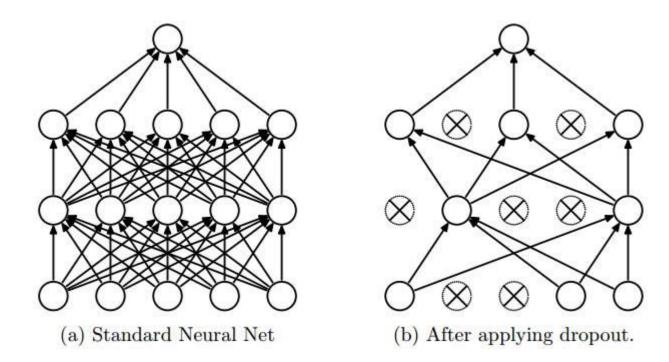
Tips & Tricks

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

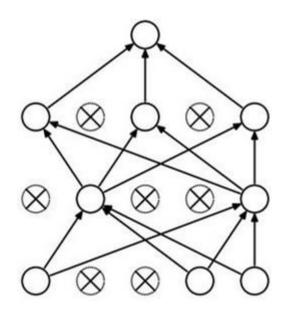
Regularization with **Dropout**

Regularization: **Dropout**

"randomly set some neurons to zero in the forward pass"



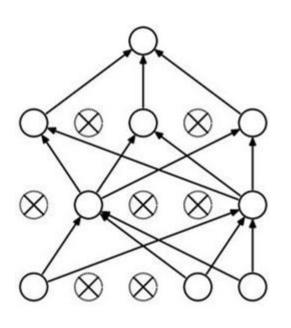
Waaaait a second... How could this possibly be a good idea?



Forces the network to have a redundant representation.



Waaaait a second... How could this possibly be a good idea?

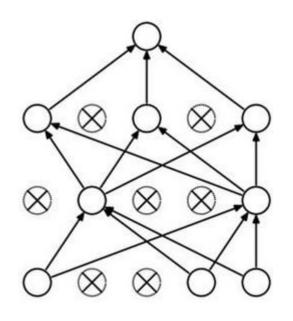


Another interpretation:

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

Each binary mask is one model, gets trained on only ~one datapoint.

At test time....



Ideally:

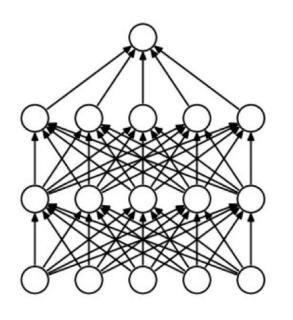
We want to integrate out all the noise

Monte Carlo approximation:

Do many forward passes with different dropout masks, average all predictions

At test time....

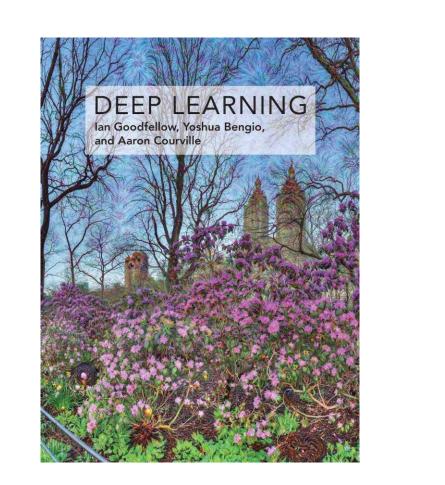
Can in fact do this with a single forward pass! (approximately)



Leave all input neurons turned on (no dropout).

(this can be shown to be an approximation to evaluating the whole ensemble)

Bibliography



O'REILLY"

