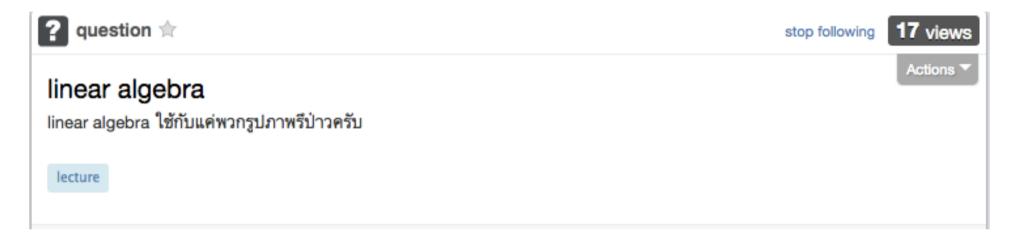
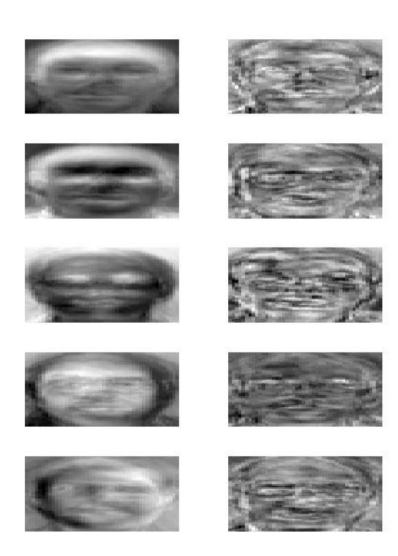
NEURAL NETWORKS

Loose ends from HW3

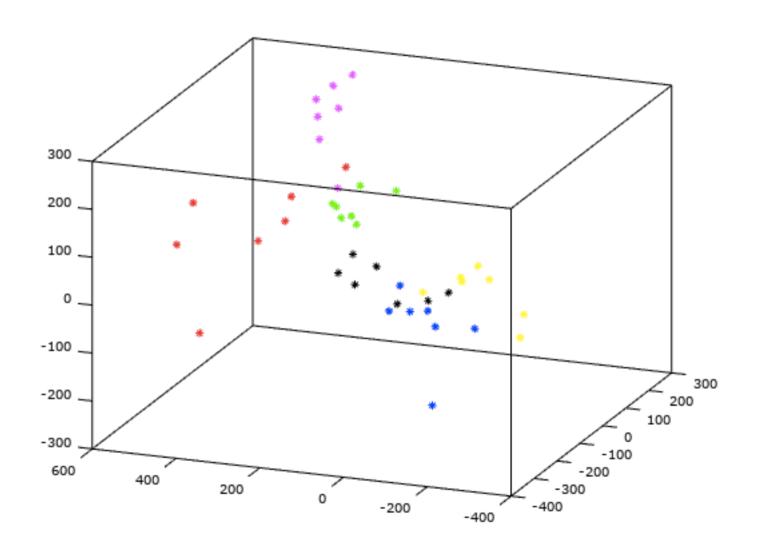


- PCA as a dimensionality reduction tool (compression)
- PCA/LDA as a feature analysis tool
- PCA/LDA as a visualization tool
- PCA as a feature normalization technique

PCA/LDA as a feature analysis tool



LDA as a visualization tool



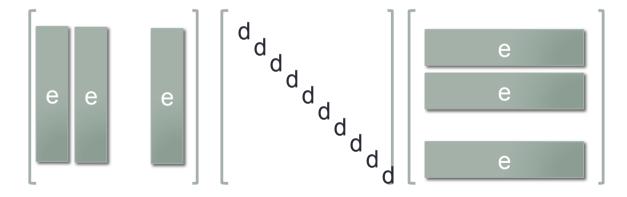
PCA as a feature normalization technique

- We said it's good to normalize features to [0,1],[-1,1], N(0,1).
 - Normalize each dimension independently
- Can we do better?

Whitening (PCA)

- Find the project along the dimensions that has the highest variance in the data
- Let \sumble be the covariance matrix. E is the matrix of eigen vectors, and D has eigen values along the diagonal. With eignenvalue decomposition:

$$\Sigma = EDE'$$

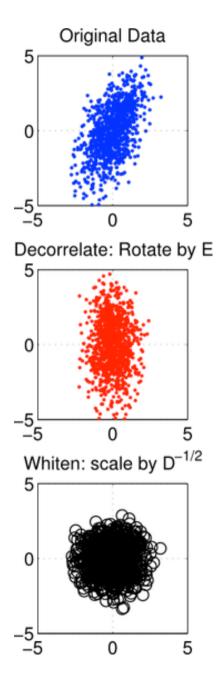


Whitening (PCA)

Whitening decorrelates and scale

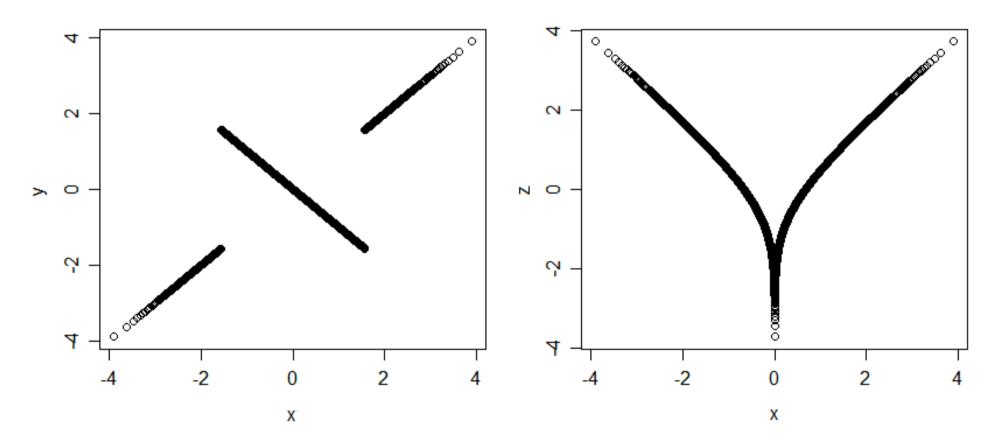
$$Y = D^{-1/2}E'X$$

- In homework we only use the decorrelates part (rotation)
- Some models prefer features to be of equal variance (SVMs, Neural networks)
- Scale according to the inverse of the variance.
- This decorrelates the featuers (on the global scale)
 - Correlations can still exist given class
 - Uncorrelated-ness does not imply independence
 - We usually assume so when working with real data though



Uncorrelated but dependence

 Below are example of variables with 0 correlation but definitely not independent



Whitening (PCA)

- What is the covariance matrix of data rotated by PCA?
- What is the covariance matrix of data whiten by PCA?

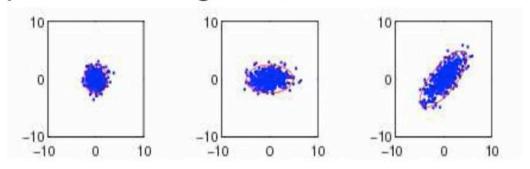
GMM/Gaussian fitting

- How many parameters are there in a 2x2 covariance matrix?
- How many data points do you need to estimate a 2v2 covariance matrix (at least)?

$$\begin{split} m_j &= \frac{1}{N} \Sigma_n w_{n,j} \\ \overrightarrow{\mu_j} &= \frac{\Sigma_n w_{n,j} \overrightarrow{x_n}}{\Sigma_n w_{n,j}} \\ \mathbf{\Sigma}_j &= \frac{\Sigma_n w_{n,j} (\overrightarrow{x_n} - \overrightarrow{\mu_j}) (\overrightarrow{x_n} - \overrightarrow{\mu_j})^T}{\Sigma_n w_{n,j}} \end{split}$$

Many forms of covariance matrix

Spherical, diagonal, full covariance



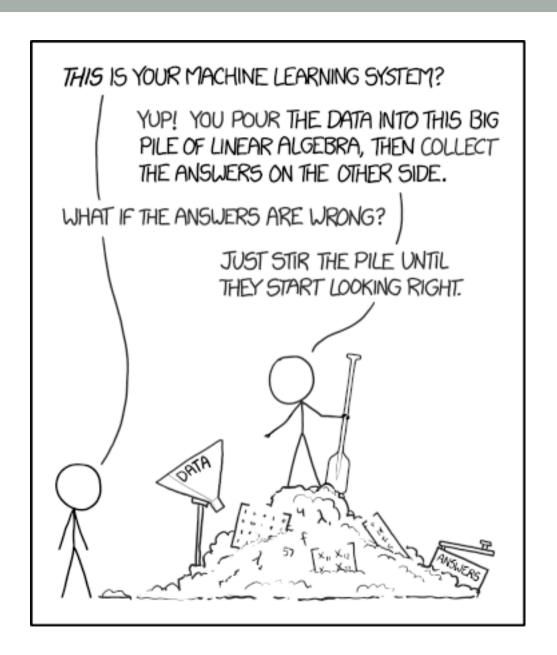
$$\Sigma = \begin{pmatrix} \sigma^2 & 0 \\ 0 & \sigma^2 \end{pmatrix} \qquad \Sigma = \begin{pmatrix} \sigma_x^2 & 0 \\ 0 & \sigma_y^2 \end{pmatrix} \qquad \Sigma = \begin{pmatrix} \sigma_x^2 & \rho \sigma_x \sigma_y \\ \rho \sigma_x \sigma_y & \sigma_y^2 \end{pmatrix}$$

Whitening and GMM fitting

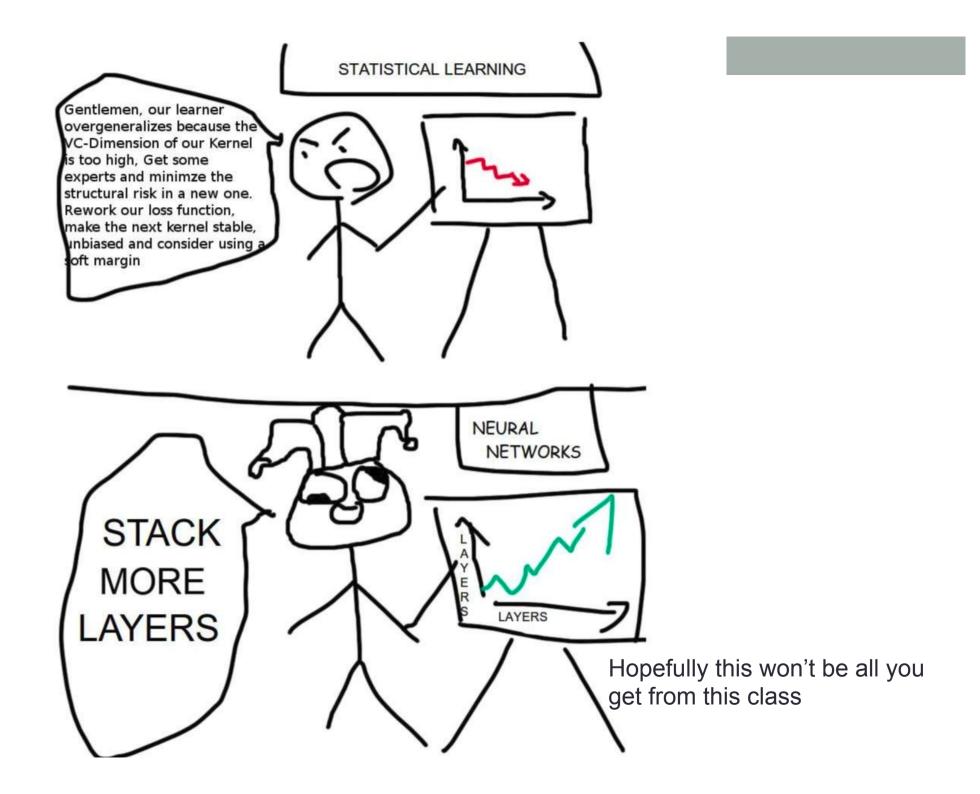
- Spherical/diagonal covariance are less prone to overfitting (less parameters)
- Data are not always distributed like that
- Use whitening to help make them spherical/diagonal distributed
 - Still not quite true, but oh well

NEURAL NETWORKS

Deep learning = Deep neural networks = neural networks



https://xkcd.com/1838/



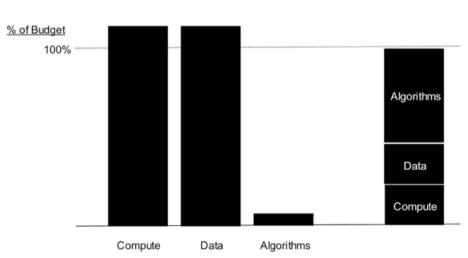
DNNs (Deep Neural Networks)

- Why deep learning?
- Greatly improved performance in ASR and other tasks (Computer Vision, Robotics, Machine Translation, NLP, etc.)
- Surpassed human performance in many tasks

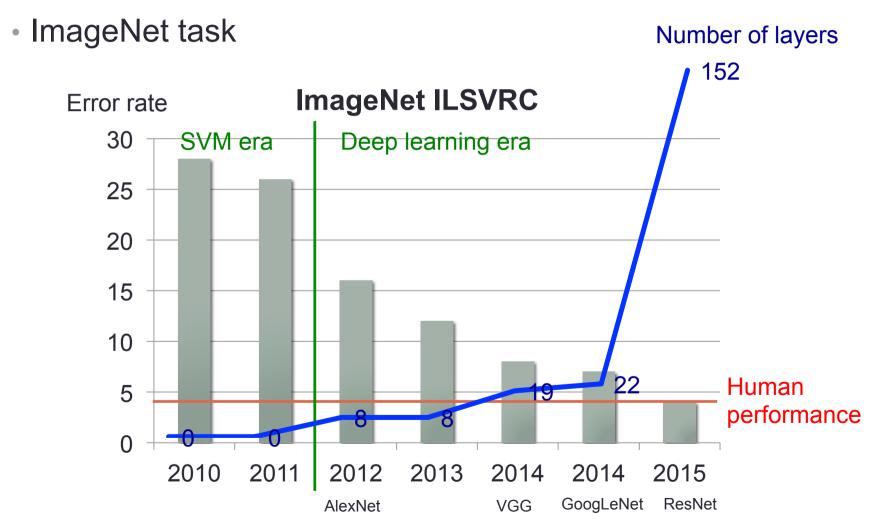
Task	Previous state-of-the-art	Deep learning (2012)	Deep learning (2017)
TIMIT	24.4%	20.0%	17.0%
Switchboard	23.6%	16.1%	5.5%
Google voice search	16.0%	12.3%	4.9%

Why now

- Neural Networks has been around since 1990s
- Big data DNN can take advantage of large amounts of data better than other models
- GPU Enable training bigger models possible
- Deep Easier to avoid bad local minima when the model is large



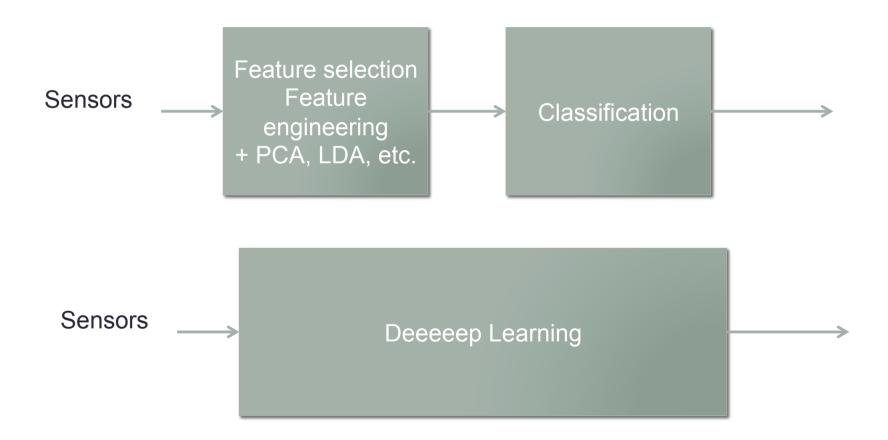
Wider and deeper networks



Why is deep learning good

- Traditional machine learning approaches need feature engineering
 - Features are based on human understanding of the phenomena
 - Have some simplifying assumptions
- Human knowledge captures known knowns, and Known unknowns NOT unknown unknowns
- Deep learning has enough parameters and model freedom to automatically learn the unknown unknowns
- Deep learning combines features engineering and modeling into one single optimization problem

Traditional VS Deep learning

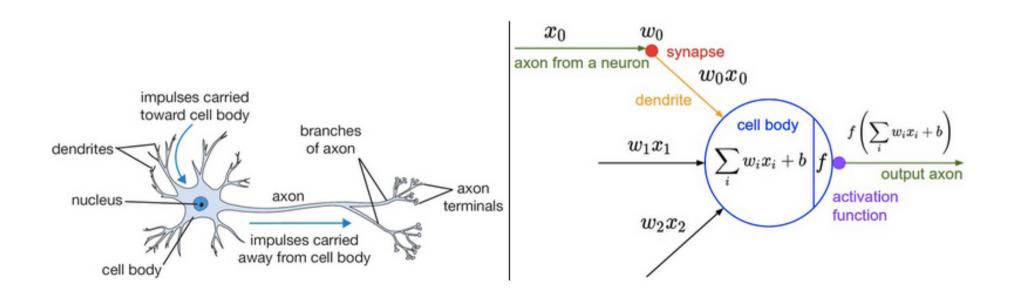


Neural networks

- Fully connected networks
 - Neuron
 - Non-linearity
 - Softmax layer
- DNN training
 - Loss function and regularization
 - SGD and backprop
 - Learning rate
 - Overfitting dropout, batchnorm
- t-SNE
- Demos
 - Tensorflow, Gcloud, Keras
- CNN, RNN, LSTM, GRU <- Next class

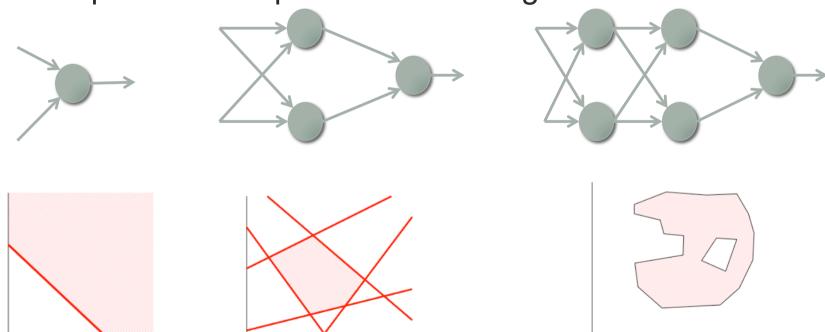
Fully connected networks

- Many names: feed forward networks or deep neural networks or multilayer perceptron or artificial neural networks
- Composed of multiple neurons



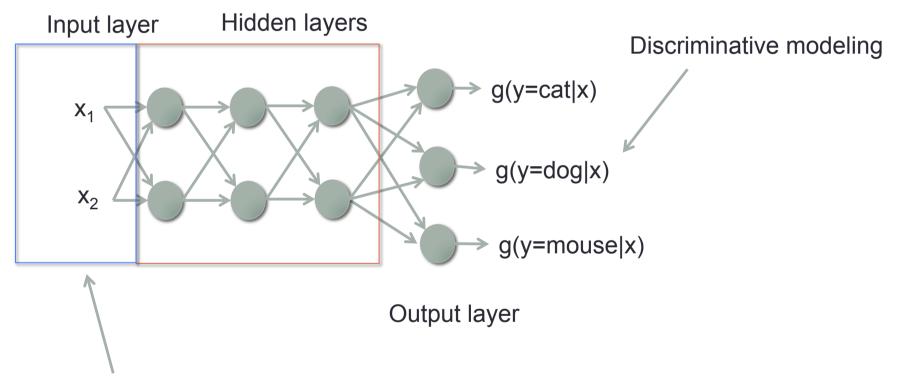
Combining neurons

- Each neuron splits the feature space with a hyperplane
- Stacking neuron creates more complicated decision boundaries
- More powerful but prone to overfitting



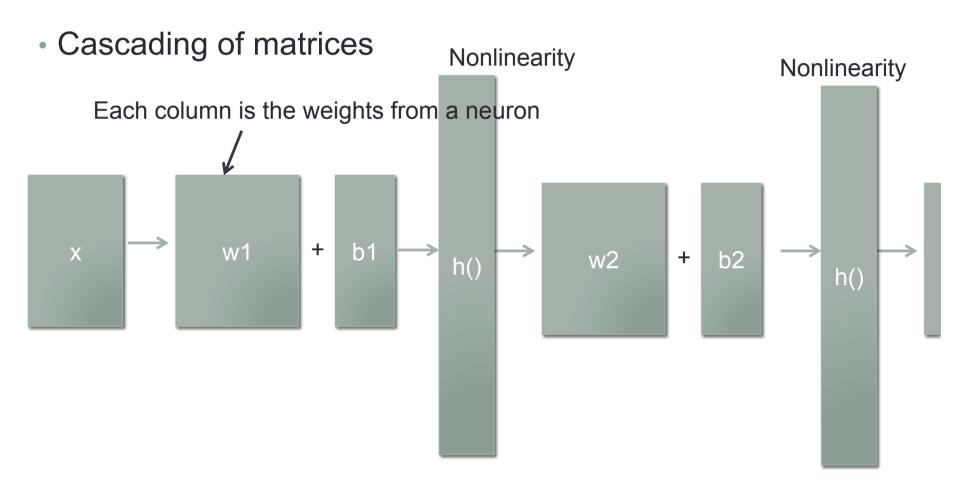
Terminology

Deep in Deep neural networks means many hidden layers



Input should be scaled to have zero mean unit variance

More linear algebra



$$h(W_2^T h(W_1^T X + \mathbf{b_1}) + \mathbf{b_2})$$

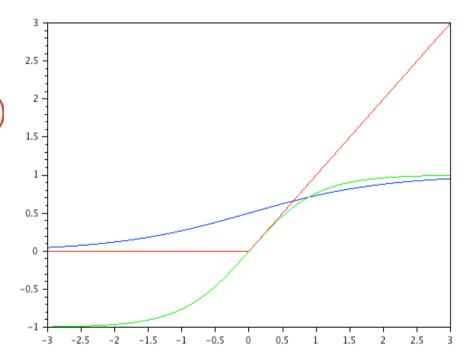
Computation graph

 Passing inputs through a series of computation Nonlinearity Nonlinearity b1 w1 b2 w2 h()

$$h(W_2^T h(W_1^T X + b_1) + b_2)$$

Non-linearity

- The Non-linearity is important in order to stack neurons
 - If F is linear, a multi layered network can be collapsed as a single layer (by just multiplying weights together)
- Sigmoid or logistic function
- tanh
- Rectified Linear Unit (ReLU)
- Most popular is ReLU and its variants (Fast to train, and more stable)

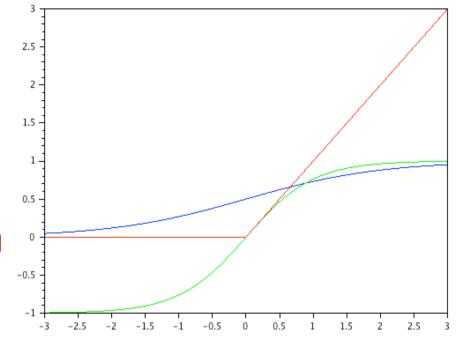


Non-linearity

• Sigmoid
$$\frac{1}{1 + e^{-x}}$$

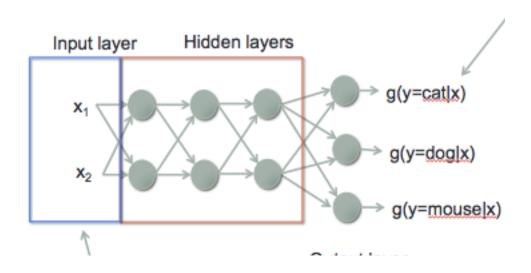
tanh

Rectified Linear Unit (ReLU)



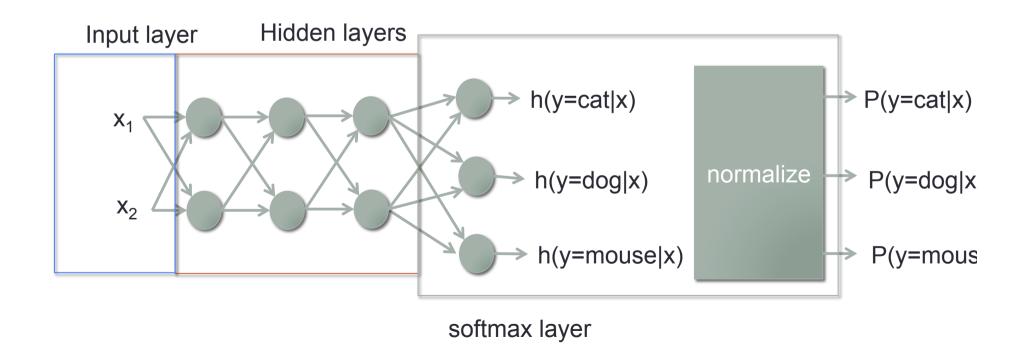
Output layer – Softmax layer

- We usually wants the output to mimic a probability function (0<=P<=1,sums to 1)
- Current setup has no such constraint
- The current output should have highest value for the correct class.
 - Value can be positive or negative number
- Takes the exponent
- Add a normalization



Softmax layer

$$P(y = j|x) = \frac{e^{h(y=j|x)}}{\sum_{y} e^{h(y|x)}}$$

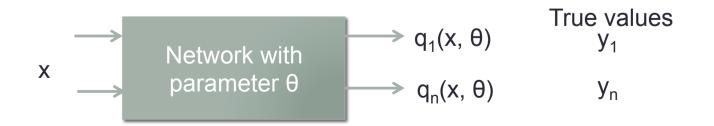


Neural networks

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Objective function (Loss function)

- Can be any function that summarizes the performance into a single number
- Cross entropy
- Sum of square errors



Cross entropy loss

Used for softmax outputs (probabilities), or classification tasks

$$L = -\Sigma_n y_n log q_n(x, \theta)$$

- Where y_n is 1 if data x comes from class n
 0 otherwise
- L only has the term from the correct class
- L is non negative with highest value when the output matches the true values, a "loss" function

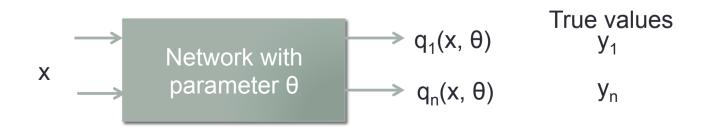
$$x \longrightarrow q_1(x, \theta)$$
 True values $y_1 = 1$ $y_1 = 0$ $y_2 = 0$

Sum of square errors

Used for any real valued outputs such as regression

$$L = \frac{1}{2}\Sigma_n(y_n - q_n(x, \theta))^2$$

Non negative, the better the lower the loss



Regularization terms

Regularization in one slide

- What?
 - Regularization is a method to lower the model variance (and thereby increasing the model bias)
- Why?
 - Gives more generalizability (lower variance)
 - Better for lower amounts of data (reduce overfiting)
- How?
 - Introducing regularizing terms in the original loss function
 - Can be anything that make sense

$$\mathbf{w}^{\mathsf{T}}\mathbf{w} + \mathsf{C}\Sigma \varepsilon_{\mathsf{i}}$$

MAP estimate is MLE with regularization (the prior term)

Famous types of regularization

L1 regularization: Regularizing term is a sum

•
$$\mathbf{w}^{\mathsf{T}}\mathbf{w} + \mathsf{C}\Sigma \epsilon_{\mathsf{i}}$$

L2 regularization: Regularizing term is a sum of squares

•
$$\mathbf{w}^{\mathsf{T}}\mathbf{w} + C\Sigma \epsilon_{\mathsf{i}}^{2}$$

L2 regularization	L1 regularization
Computational efficient due to having analytical solutions	Computational inefficient on non-sparse cases
Non-sparse outputs	Sparse outputs
No feature selection	Built-in feature selection

Regularization in neural networks L2

- We want to improve generalization somehow.
- Observation, models are better when the weights are spread out (no peaky weights).
 - Try to use every part of the model.
- Add a cost if we put some value to the weights
- Regularized loss = Original loss + 0.5 CΣw²
- we sum the square of weights of the whole model
- 0.5 is for prettiness when we take derivative
- C is a hyperparameter weighting the regularization term

Regularization in neural networks

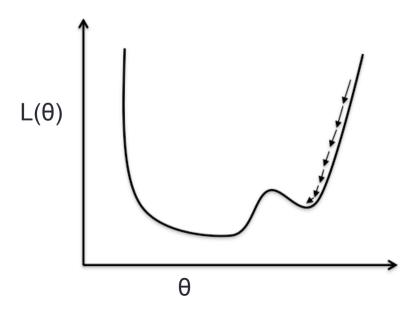
- We want to improve generalization somehow.
- Observation, models behave better when we force the weights to be sparse.
 - Sparse means many weights are zero or close to zero
 - Force the model to focus on only important parts
 - Less prone to noise
- Add a cost if we put some value to the weights
- Regularized loss = Original loss + 0.5 CΣ|w|
- we sum the absolute weights of the whole model
- 0.5 is for prettiness when we take derivative
- C is a hyperparameter weighting the regularization term

L1 L2 regularization notes

- Can use both at the same time
 - People claim L2 is superior
- I found them useless in practice for deep neural networks
 - Maybe there are some tasks out there that benefit from this? I don't know
- Other regularization methods exist (we will go over these later)

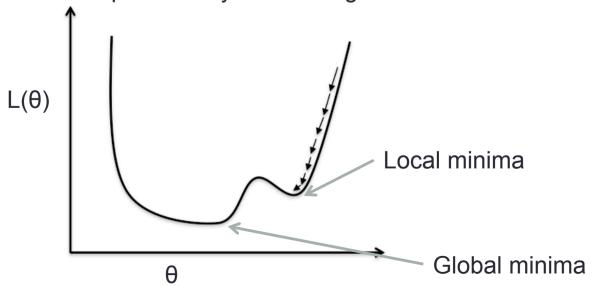
Minimization using gradient descent

- We want to minimize L with respect to θ (weights and biases)
 - Differentiate with respect to θ
 - Gradients passes through the network by Back Propagation



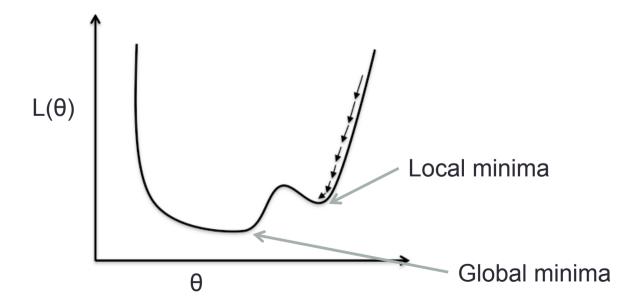
Deep vs Shallow

- The loss function of neural network is non-convex (and non-concave)
 - Local minimas can be avoided with convexity
 - Linear regression, SVM are convex optimization
 - Convexity gives easier training
 - Does not imply anything about the generalization of the model
 - The loss is optimized by the training set



Deep vs Shallow

- If deep, most local minimas are the global minima!
 - Always a way to lower the loss in the network with millions of paramters
 - Enough parameters to remember every training examples
 - Does not imply anything about generalization



Differentiating a neural network model

- We want to minimize loss by gradient descent
- A model is very complex and have many layers! How do we differentiate this!!?



Back propagation

- Forward pass
 - Pass the value of the input until the end of the network
- Backward pass
 - Compute the gradient starting from the end and passing down gradients using chain rule

Examples to read

https://alonalj.github.io/2016/12/10/What-is-Backpropagation/

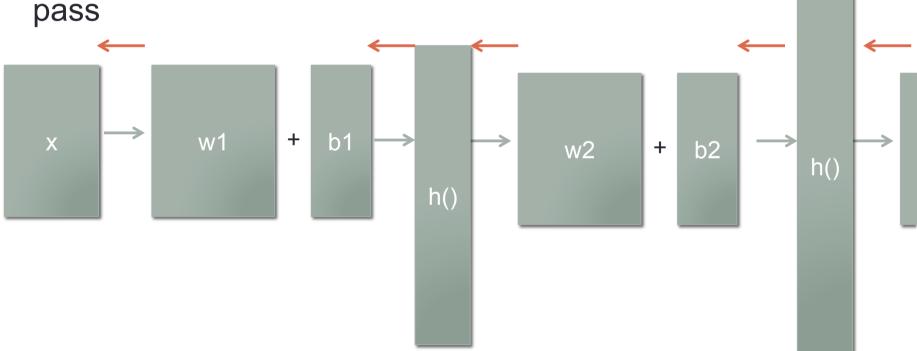
https://mattmazur.com/2015/03/17/a-step-by-step-backpropagation-example/

Back propagation

- Regularization terms only appears at the particular weights when doing the derivative
- What about cross entropy

Backprop and computation graph

 We can also define what happens to a computing graph when the gradient passes through during the backward



This lets us to build any neural networks without having to redo all the derivation as long as we define a forward and backward computation for the block.

Initialization

- The starting point of your descent
- Important due to local minimas
- Not as important with large networks AND big data (>100 hours for ASR)
- Now usually initialized randomly
 - One strategy

$$W \sim \text{Uniform}(0, \frac{1}{\sqrt{\text{FanIn} + \text{FanOut}}})$$

For ReLUs

$$w = np.random.randn(n) * sqrt(2.0/n)$$

Or use a pre-trained network as initialization

Initialization

- Bias
 - All Zeros is fine

Stochastic gradient descent (SGD)

- Consider you have one million training examples
 - Gradient descent computes the objective function of all samples, then decide direction of descent
 - Takes too long
 - SGD computes the objective function on subsets of samples
 - The subset should not be biased and properly randomized to ensure no correlation between samples
- The subset is called a mini-batch
- Size of the mini-batch determines the training speed and accuracy
 - Usually somewhere between 32-1024 samples per mini-batch
- Definition: 1 batch vs 1 epoch

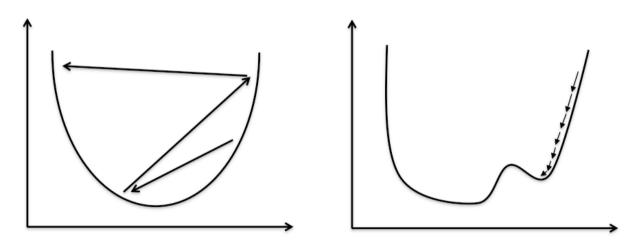
Self regularizaing property of SGD

- SGD by its randomized nature does not overfit (as fast)
 - Considered as an implicit regularization (no change in the loss)

https://cbmm.mit.edu/sites/default/files/publications/CBMM-Memo-067-v3.pdf

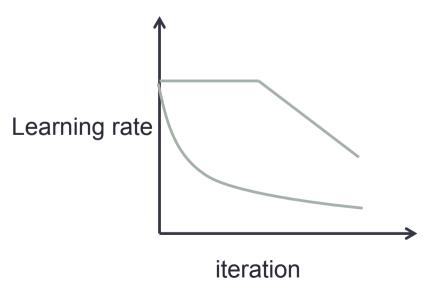
Learning rate

- How fast to go along the gradient direction is controlled by the learning rate
- Too large models diverge
- Too small the model get stuck in local minimas and takes too long to train



Learning rate scheduling

- Usually starts with a large learning rate then gets smaller later
- Depends on your task
- Automatic ways to adjust the learning rate: Adagrad,
 Adam, etc. (still need scheduleing still)

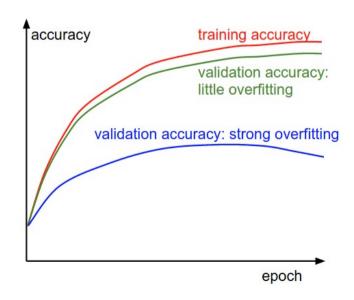


Learning rate strategies (annealing)

- Step decay: reduce learning rate by x after y epochs
- New bob method: half learning rate every time the validation error goes up. Only plausible in larger tasks
- Exponential decay: multiplies the learning rate by exp(rate*epoch number)

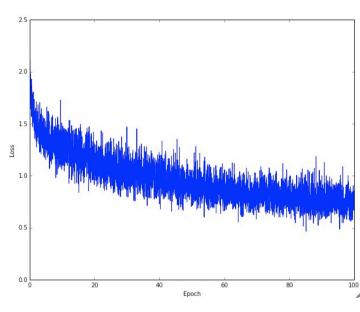
Overfitting

- You can keep doing back propagation forever!
- The training loss will always go down
- But it overfits
- Need to monitor performance on a held out set
- Stop or decrease learning rate when overfit happens



Monitoring performance

- Monitor performance on a dev/validation set
 - This is NOT the test set
- Can monitor many criterions
 - Loss function
 - Classification accuracy
- Sometimes these disagree
- Actual performance can be noisy, need to see the trend



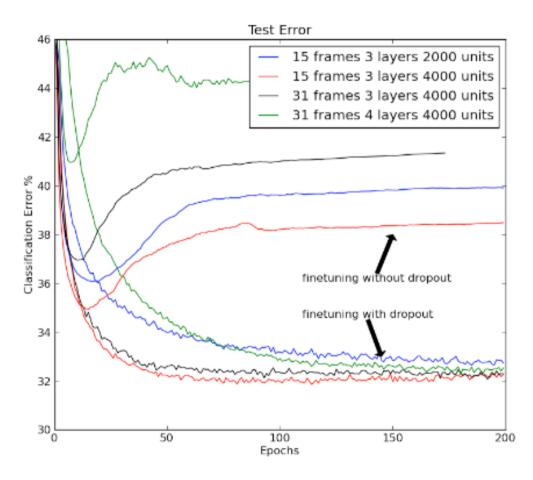
http://cs231n.github.io/neural-networks-3/

Reducing overfitting - dropout

- A RECENT (2012) regularization technique for reducing overfitting
- Randomly turn off different subset of neurons during training
 - Network no longer depend on any particular neuron
 - Force the model to have redundancy robust to any corruption in input data
 - A form of performing model averaging (assemble of experts)
- Now a standard technique

Dropout on TIMIT

A phoneme recognition task



Hinton, Geoffrey "Improving neural networks by preventing co-adaptation of feature detectors" 2012

Batch normalization

- Recent technique for (implicit) regularization
- Normalize every mini-batch at various batch norm layers to standard Gaussian (different from global normalization of the inputs)
- Place batch norm layers before non-linearities
- Faster training and better generalizations

Vanishing/Exploding gradient

- Backprop introduces many multiplications down chain
- The gradient value gets smaller and smaller
 - The deeper the network the smaller the gradient in the lower layers
 - Lower layers changes too slowly (or not at all)
 - Hard to train very deep networks (>6 layers)
- The opposite can also be true. The gradient explodes from repeated multiplication
 - Put a maximum value for the gradient (Gradient clipping)

- How to deal with this?
 - Next lectures

Neural networks

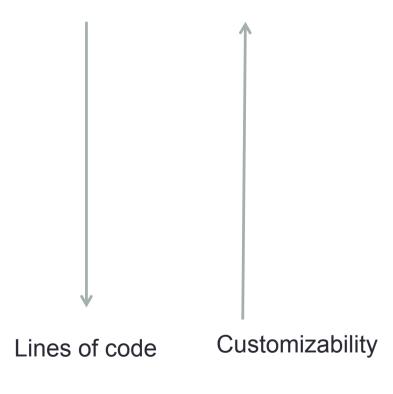
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t-distributed Stochastic Neighbor Embedding (t-SNE

- Non-linear dimensionality reduction technique that is good for reducing high dimensional data to 2-3 dimensions
 - Mainly for visualization
- Tries to preserve small pair-wise distances locally
 - Preserves relative order well
- Original features are distorted

What toolkit

- Tensorflow lower level
- Keras higher level





Demos

- Tensorboard
 - What's a tensor?
- Gcloud

Homework

- Part I out tonight
- Part II some time this week (this part needs Gcloud)
- Next week office hour is on Wednesday