Aprendizaje Supervisado

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RoadMap

- **Short review of topics from previous course**
  Classification / Regression / Perceptron
- **What supervised learning is**
- **SVMs**
- **Ensemble methods**
  Bagging: Random Forests / Boosting
- **Neural Networks**

Motivation

Example 1

- **A credit card company receives applications for new credit cards. Each one has information about an applicant:**
  - salary
  - age
  - marital status
  - Veraz
  - Credit report from BCRA
  - ...
- **Problem: determine if an application should be approved or rejected**

Example 2

- **Problem: classify an email as SPAM or not**

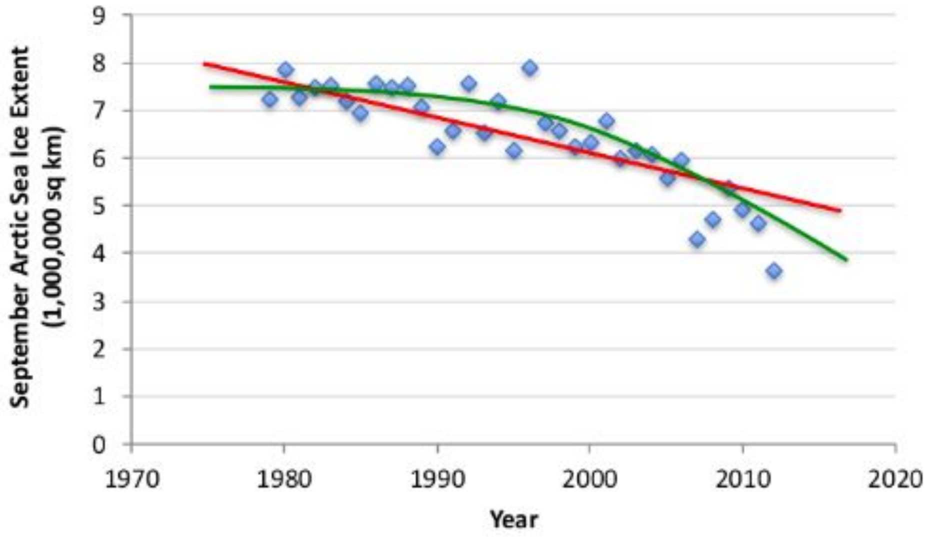
Describing the problem

- **Data:** A set of records (or samples, instances) described by n attributes: A1, A2, … An and each sample is labelled with a class (Like SPAM or NOT) or a "score" (like the credit score)

- **Goal:** To learn a model (or a function) from the data that can be used to predict the labels that the records have (and labels for new unlabelled records)

Aprendizaje supervisado: regresión

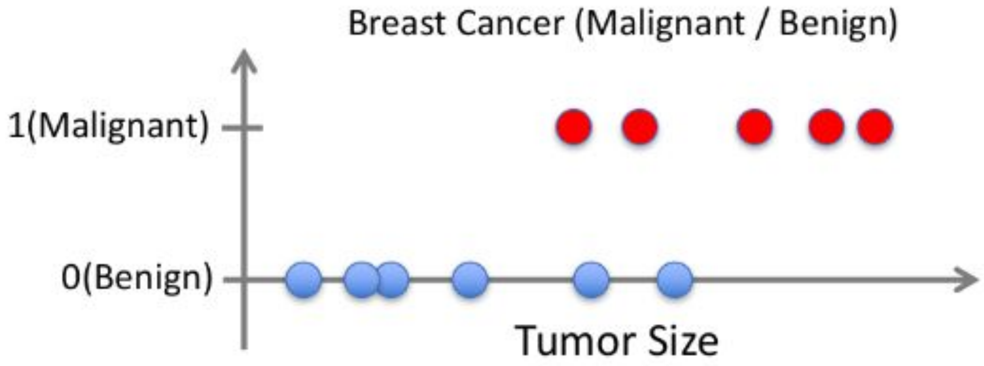
- Dados $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$
- Aprender una $f(x)$ que permita predecir y a partir de x
    - Si y está en $\mathbb{R}^n$ $\rightarrow$ **regresión**



Slides from the previous course

Aprendizaje supervisado: clasificación

- Dados $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$
- Aprender una $f(x)$ que permita predecir y a partir de x
    - Si y es categórica $\rightarrow$ **clasificación**



Slides from the previous course

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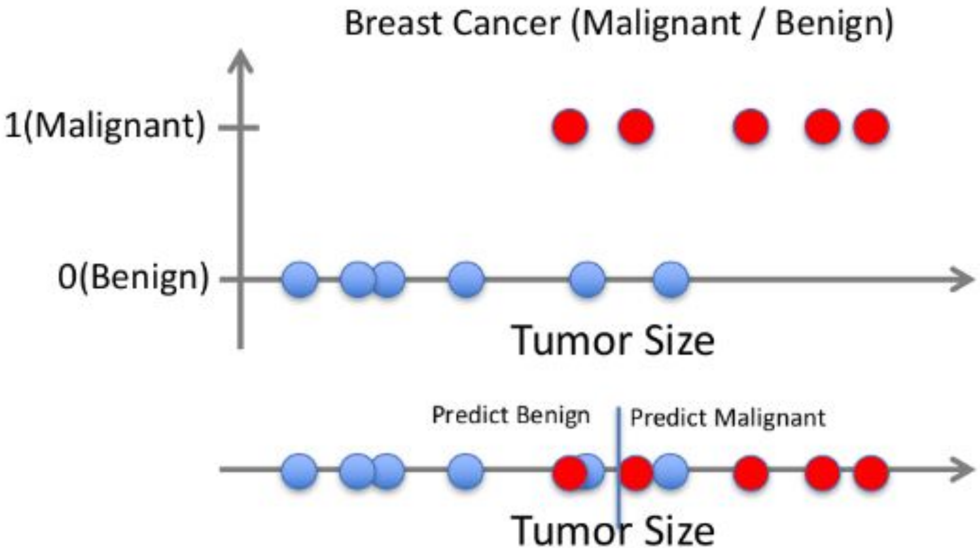
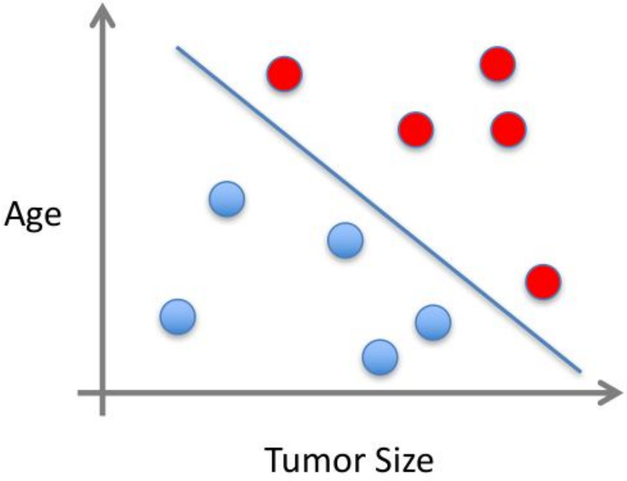


Slides from the previous course

Supervised Learning

- x can be multi-dimensional
  – Each dimension corresponds to an attribute



- Clump Thickness
- Uniformity of Cell Size
- Uniformity of Cell Shape

…

Based on example by Andrew Ng

Slides from the previous course

Aprendizaje supervisado

Functions $\mathcal{F}$

$f : \mathcal{X} \to \mathcal{Y}$

Training data

$\{(x_i, y_i) \in \mathcal{X} \times \mathcal{Y}\}$

LEARNING

$\boxed{\begin{array}{l} \text{find } \hat{f} \in \mathcal{F} \\ \text{s.t. } y_i \approx \hat{f}(x_i) \end{array}}$

Learning machine

New data

PREDICTION

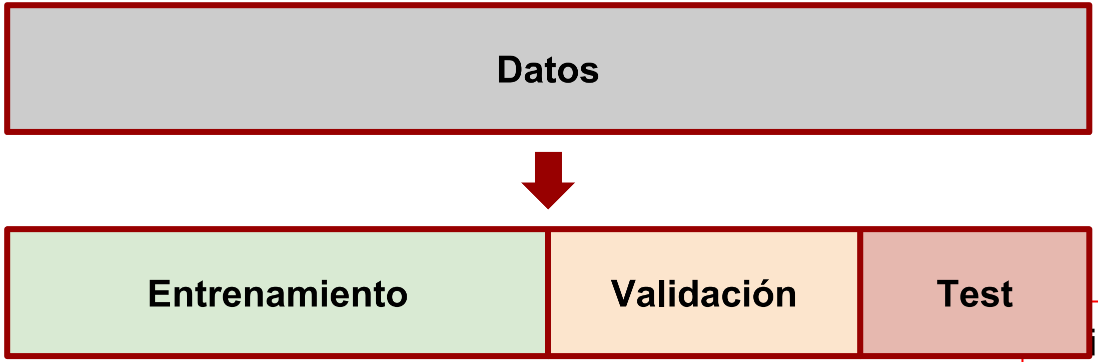
$\boxed{y = \hat{f}(x)} \Leftarrow \boxed{x}$

Slides from the previous course

Elección de *hiperparámetros*

Dividir el conjunto total de ejemplos en tres subconjuntos

- **Entrenamiento**: aprendizaje de variables del modelo
- **Validación**: ajuste/elección de hiperparámetros
- **Test**: estimación final de la performance del modelo entrenado (y con hiperparámetros elegidos adecuadamente



ides from the previous course

El algoritmo del "perceptrón"

- Propuesto por Rosemblatt en 1958
- El objetivo es encontrar un hiperplano de separación
  - Si los datos son linealmente separables, lo encuentra
- Es un algoritmo *online* (procesa un ejemplo a la vez)
- Muchas variantes ...

Slides from the previous course

El algoritmo del "perceptrón"

Entrada:

- una secuencia de pares de entrenamiento (x_1,y_1), (x_2, y_2) ...
- Una tasa de aprendizaje r

Algoritmo:

- Inicializar $w^{(0)} \in \mathbb{R}^{n}$
- Para cada ejemplo (x_i,y_i)
  - Predecir $y_i' = sign(w^{T} x_i + w_0)$
  - Si $y_i' \neq y_i$:

    $w^{(t+1)} \leftarrow w^{(t)} + r\,(y_i x_i)$

Slides from the previous course

El algoritmo del "perceptrón"

Entrada:

- una secuencia de pares de entrenamiento (x_1,y_1), (x_2, y_2) ...
- Una tasa de aprendizaje r (número pequeño y menor a 1)

Algoritmo:

- Inicializar $w^{(0)} \epsilon \mathbb{R}^n$
- Para cada ejemplo (x_i,y_i)
  - Predecir $y_i' = sign(w^T x_i)$
  - Si $y_i' \neq y_i$:

    $w^{(t+1)} \leftarrow w^{(t)} + r\,(y_i x_i)$

Actualiza solo cuando comete un error

Error en positivos:

$$w^{(t+1)} \leftarrow w^{(t)} + r\,x_i$$

Error en negativos:

$$w^{(t+1)} \leftarrow w^{(t)} - r\,x_i$$

Si $y_i w^T x_i \leq 0 \rightarrow$ error

Slides from the previous course

Demo Time (demo 1) …

Support Vector Machines

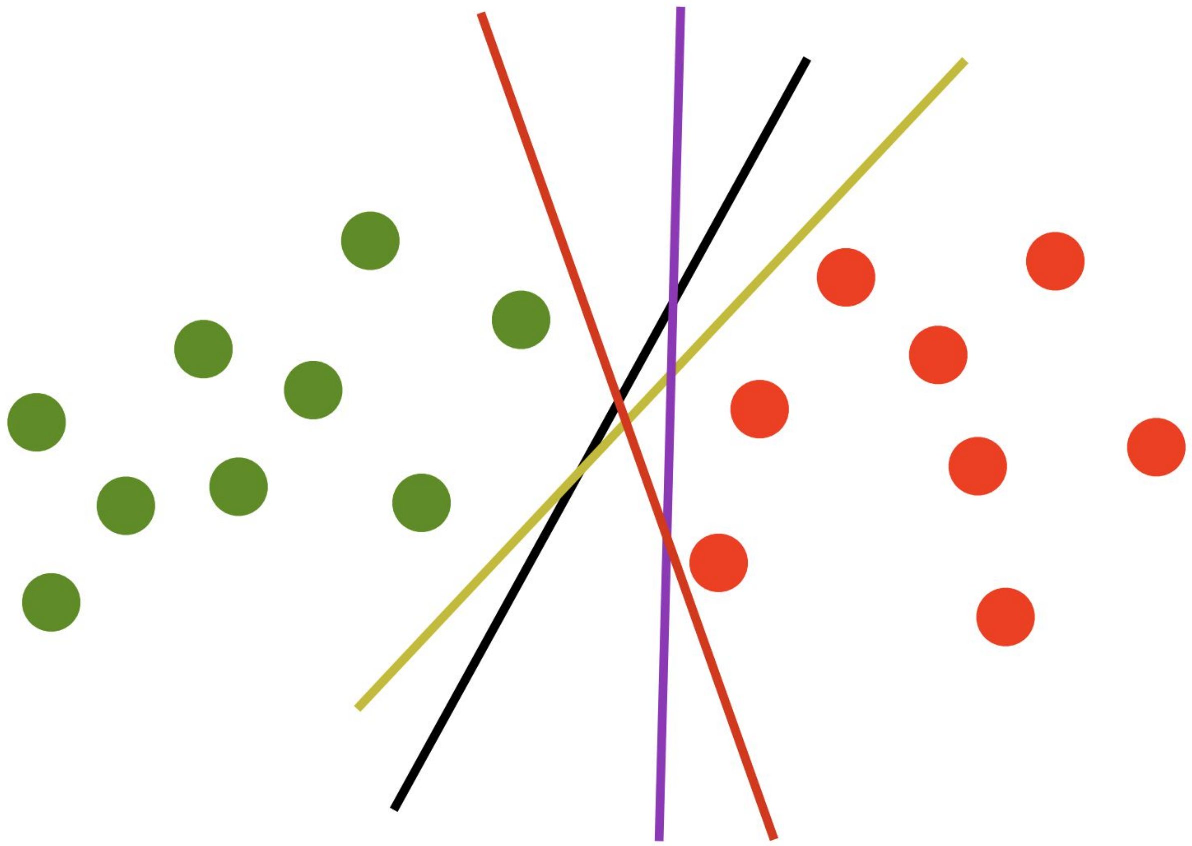
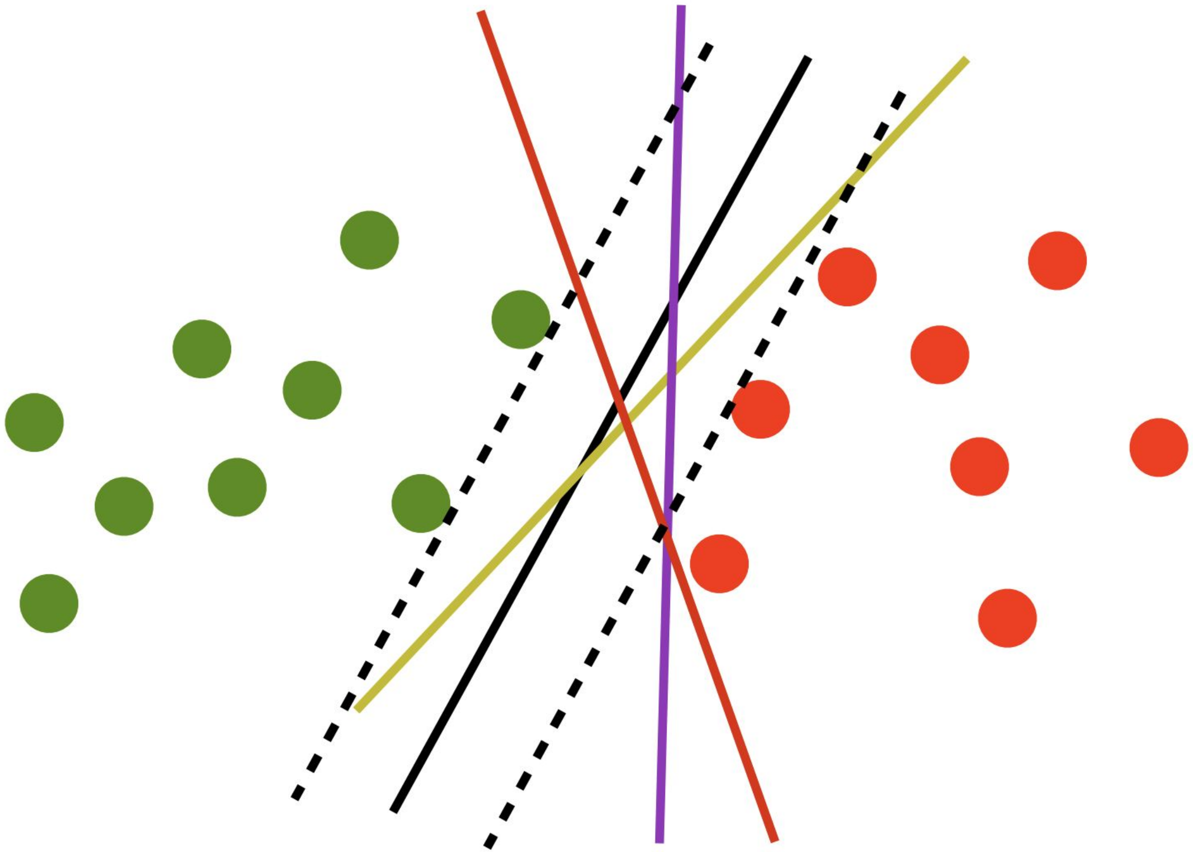


Image by Alex Smola

Support Vector Machines



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Support Vector Machines

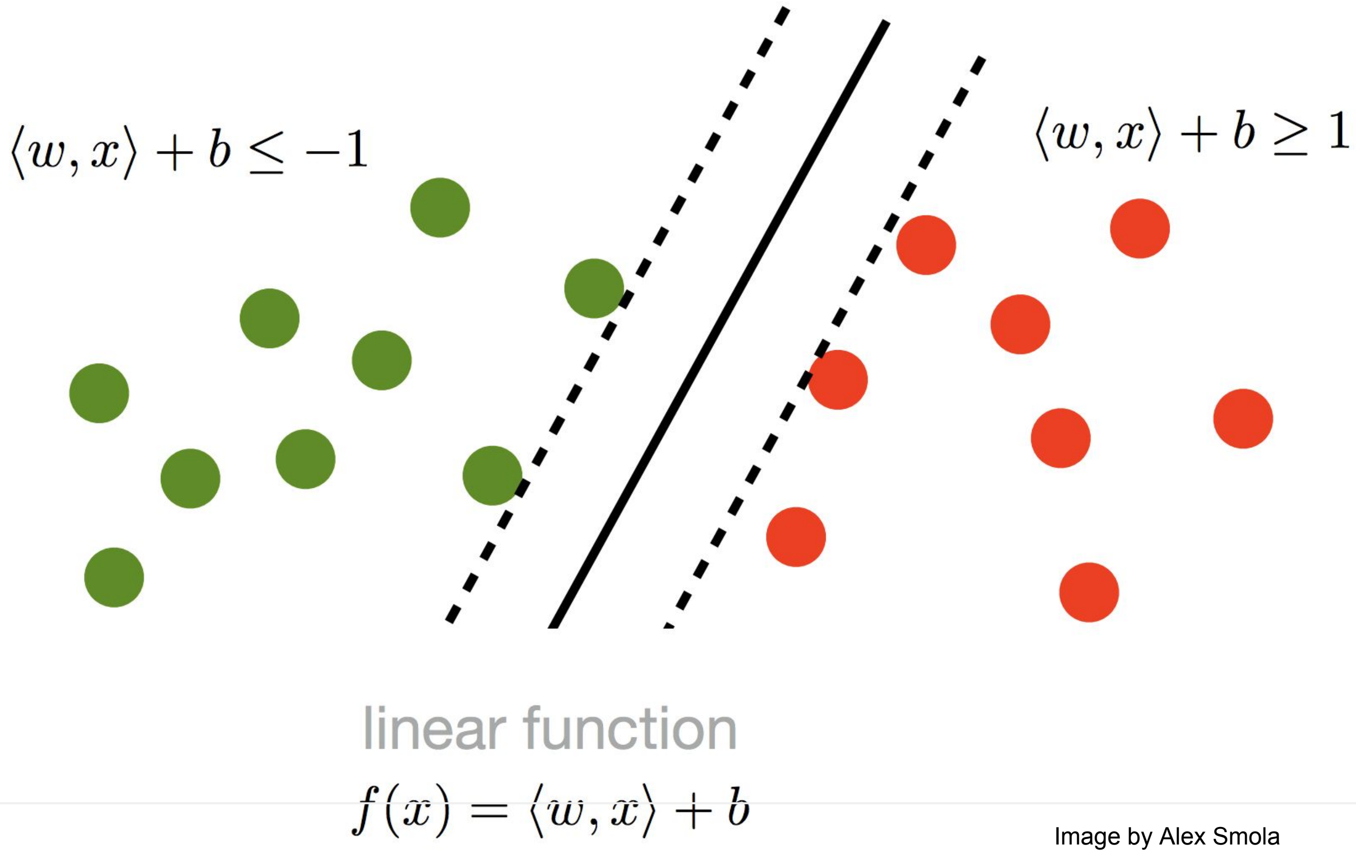

Image by Alex Smola

Whiteboard Time

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Support Vector Machines, Deriving the Equations

Support Vector Machines

Some Interesting Properties we have found:

- $w = \sum_i \alpha_i y_i x_i$
- Just the points on the margin used to define the hyperplane

Demo Time (demo 2)

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SVMs: slack variables

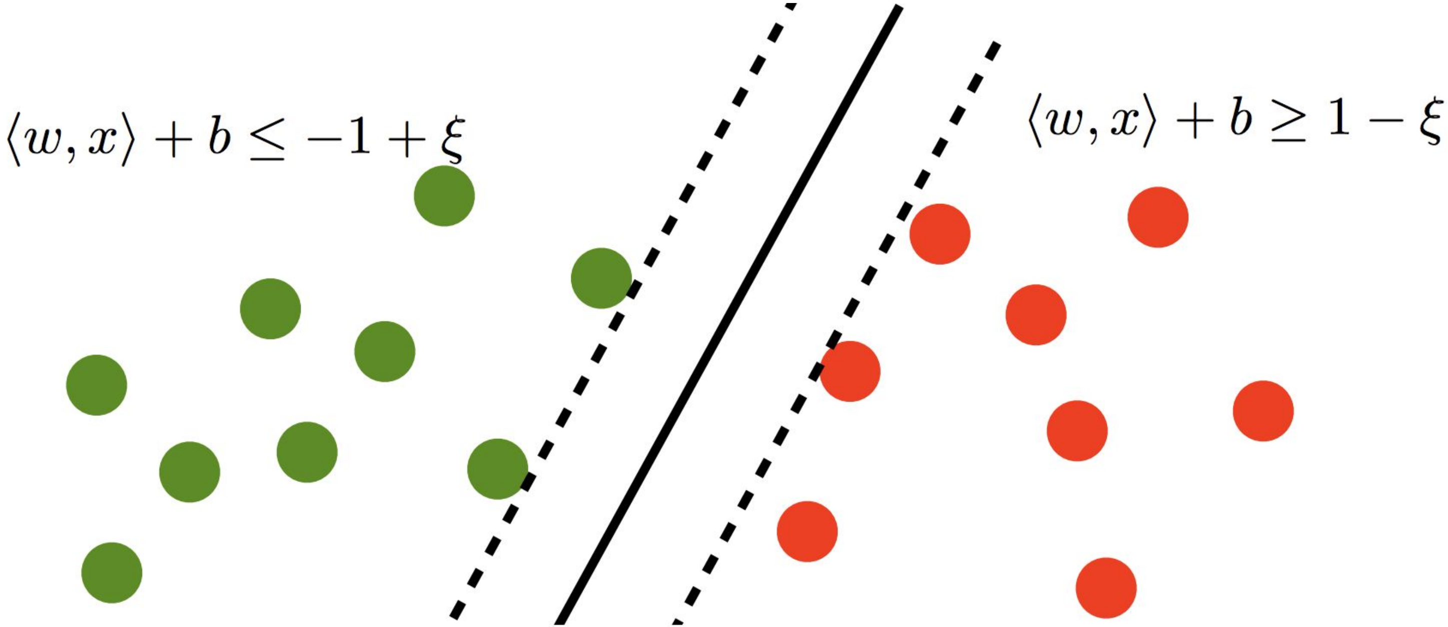

Image by Alex Smola

Demo Time (demo 3)

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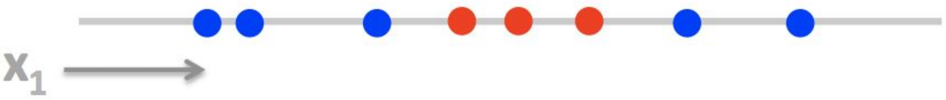
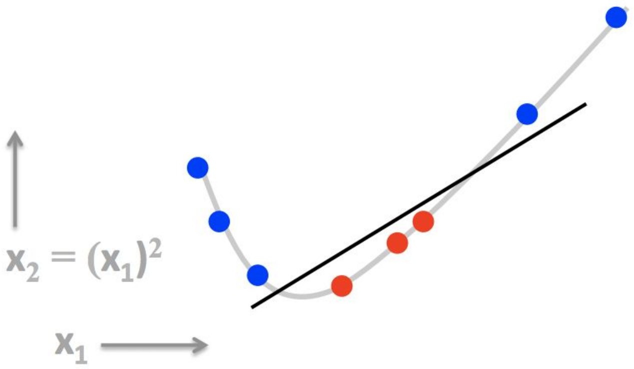
SVMs: Kernels

Images by Alex Ihler

SVMs: Kernels





Images by Alex Ihler

Whiteboard Time

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SVMs: Kernels

Some common kernels:

- Polynomial
  $$K(x,z) = (1 + \sum_j x_j z_j)^d$$
- Radial Basis Functions (RBF aka Gaussian Similarity Functions)
  $$K(x,z) = \exp(-(x-z)^2/2\sigma^2)$$
- Sigmoid
  $$K(x,z) = \tanh(c < x,z > +h)$$
- Specific for certain types of problems

Demo Time (demo 4)

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Multiclass SVMs

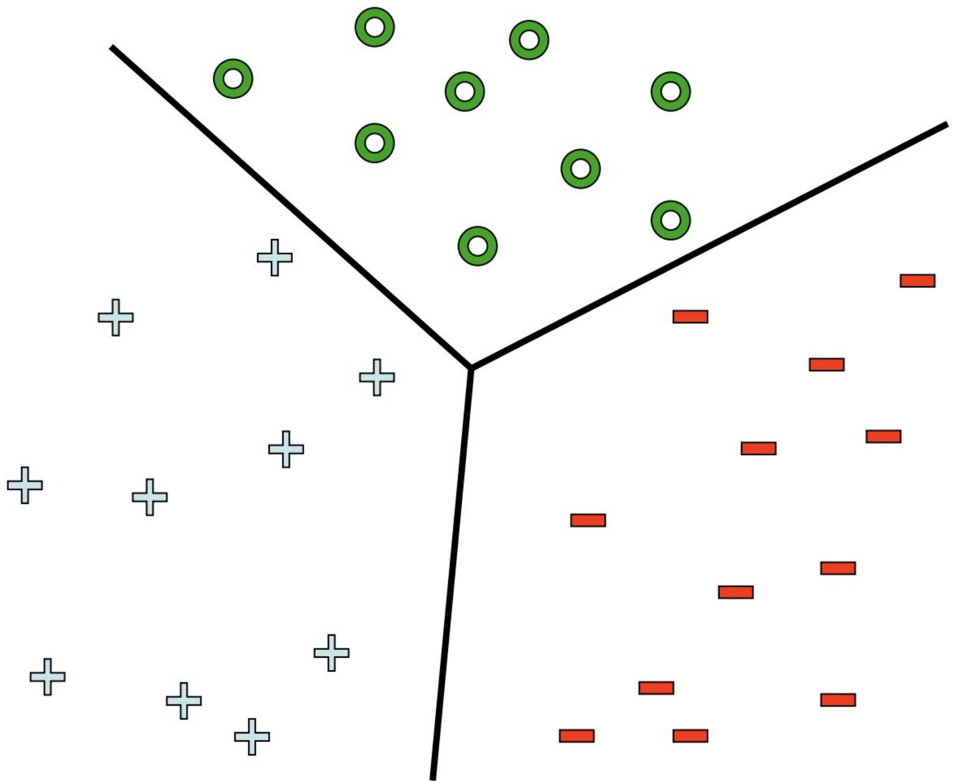

Image by David Sontag

Multiclass SVMs: one vs the rest (one vs all)

- **Training:** how could we do it?

Multiclass SVMs: one vs the rest (one vs all)

- **Training:** For M classes:

  construct a hyperplane between class k and the other M − 1 classes => M SVMs

- **Classification:** how could we do it?

Multiclass SVMs: one vs the rest

- **Training:** For M classes:

  construct a hyperplane between class k and the other $M - 1$ classes => M SVMs

- **Classification:** make M predictions (one for each SVMs) and find out the one getting more hits into its positive region.

Multiclass SVMs: one vs one (all vs all)

Multiclass SVMs: one vs one (all vs all)

- **Training:** For M classes:

  construct a hyperplane between class i and class j. => M(M-1)/2 SVMs

- **Classification:** If f_{ij} is the classifier where i are the positive samples and j the negative ones,, the classification of x is given by

$$f(x) = \text{argmin}_i \left(\sum_j f_{ij}(x)\right)$$

Support Vector Regressions

- Idea based on support vectors like in SVMs, but now y_i is a real number.
- Uses soft margins in the regression process instead of classification
- Additional parameter ε, to compute the loss function

Support Vector Regressions

- Idea based on support vectors like in SVMs, but now y_i is a real number.
- Uses soft margins in the regression process instead of classification
- Additional parameter ε, to compute the loss function
- Not frequently used, logistic regression is more popular

Whiteboard Time

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Decision Trees (review)

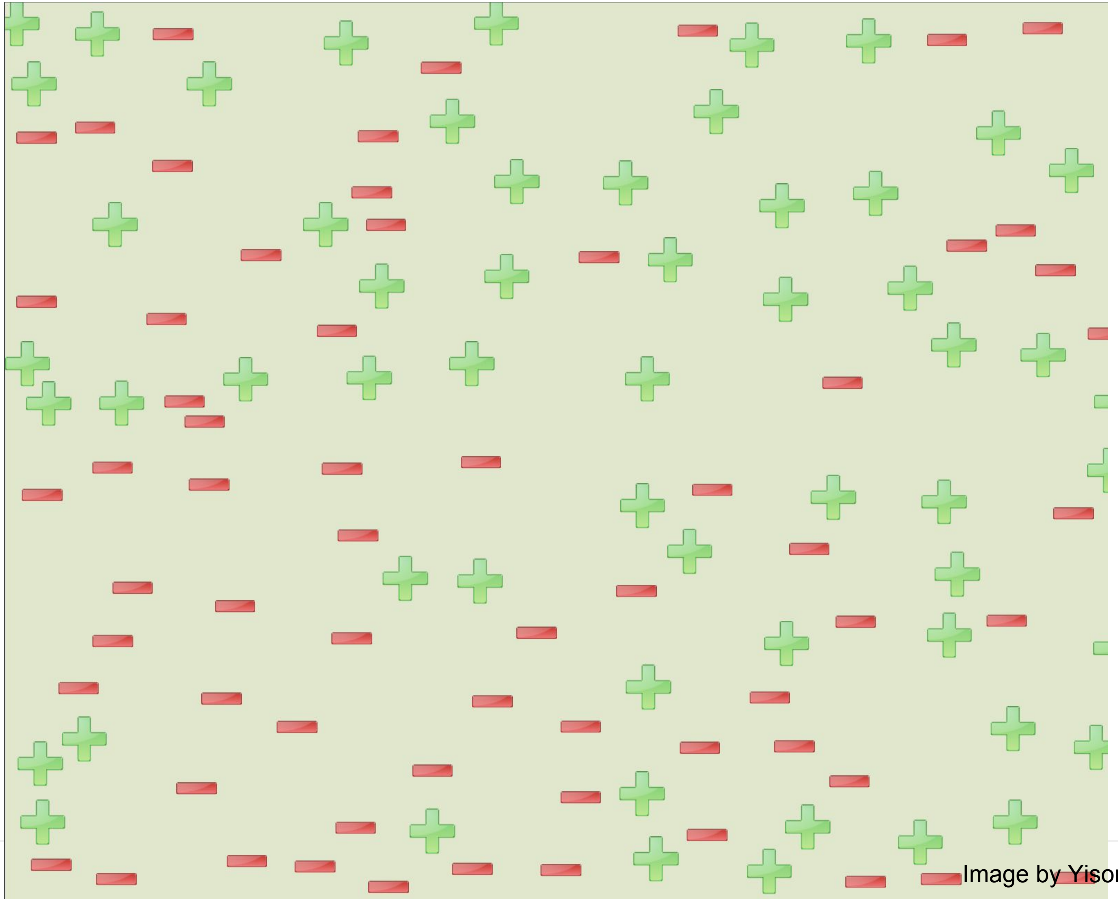

Image by Yisong Yue

Decision Trees (review)

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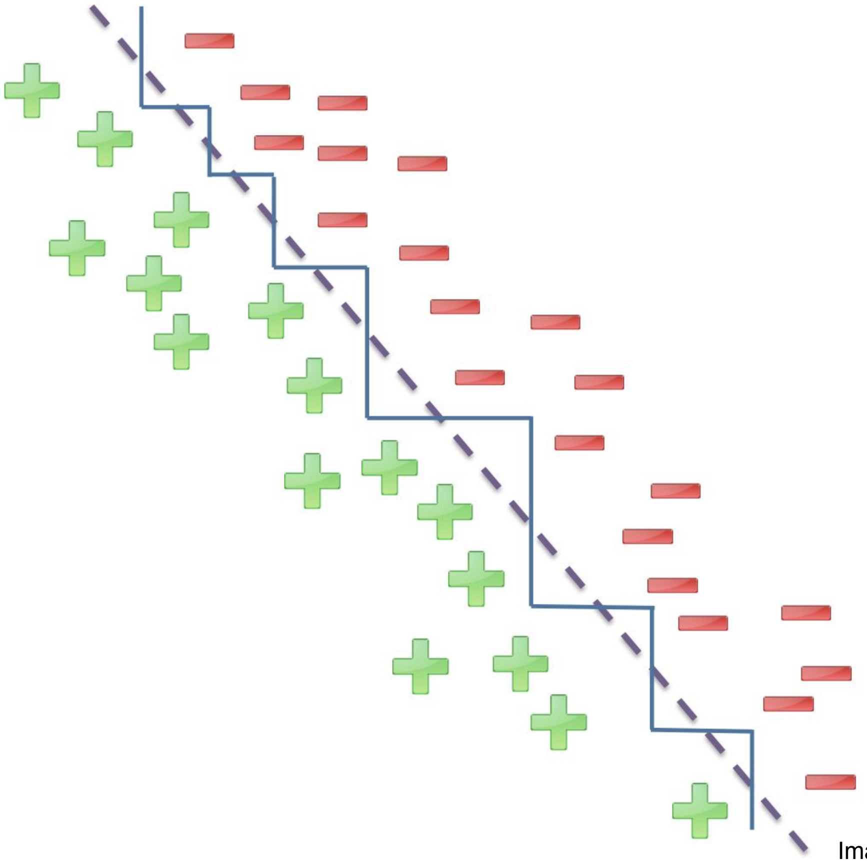
Decision Trees (review)



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Demo Time (demo 5)

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Ensemble Learning

- Generate a set of "learners" that, when combined, have higher accuracy.
- Assuming we have three learners: L1, L2, L3
- The predictions from them may differ
- What would we do? Who do we trust?
    - Believe the model that we know is best?
    - Go with the majority?

Ensemble Learning

- **An ensemble model is a model that is a combination of several different models**
- **Usually, an ensemble is more accurate than all its constituent models**
- **Why?**
  - **Intuition:** "two know more than one"

Ensemble Learning. First approach: Voting

- Given n classifiers m1, m2, … mn
- Consider a new classifier M that, given a datum x, M computes m1(x), m2(x), …, counts the predictions and returns the most predicted class
- How well would M work?

Ensemble Learning. First approach: Voting

- To answer the question, let's make some assumptions:
    - All the classifiers m1, …, mn are equally accurate (with p being their accuracy)
    - The errors in the classification made by each classifier are independent
        - P(mj wrong | mk wrong) = P(mj wrong)
- How well would M work?

Ensemble Learning. First approach: Voting

- **Example**
  - **p = 0.8**
  - **n = 5**
  - **P(majority of 5 models is correct) =**

$$= \binom{5}{5}0.8^5 0.2^0 + \binom{5}{4}0.8^4 0.2^1 + \binom{5}{3}0.8^3 0.2^2$$
$$= 0.942$$

- **Need empirical validation if assumptions not valid**

Ensemble Learning. First approach: Voting

- **Example**
  - **p = 0.8**
  - **n = 5**
  - **P(majority of 5 models is correct) =**

$$
\begin{aligned}
&= \binom{5}{5} 0.8^5 0.2^0 + \binom{5}{4} 0.8^4 0.2^1 + \binom{5}{3} 0.8^3 0.2^2 \\
&= 0.942
\end{aligned}
$$

- **Need empirical validation if assumptions not valid**

Ensemble Learning

- We know how to build decision trees
- How can we build different trees for the same data?
  - This may result on the same tree
- Do we introduce some variations?

Bagging

- Let D be the dataset
- Repeat k times:
  - Create D' from D by randomly selecting |D| instances of D with replacement
  - Learn a new model m
- Return a model that selects the most frequent prediction among m1, …, mk predictions

Bagging

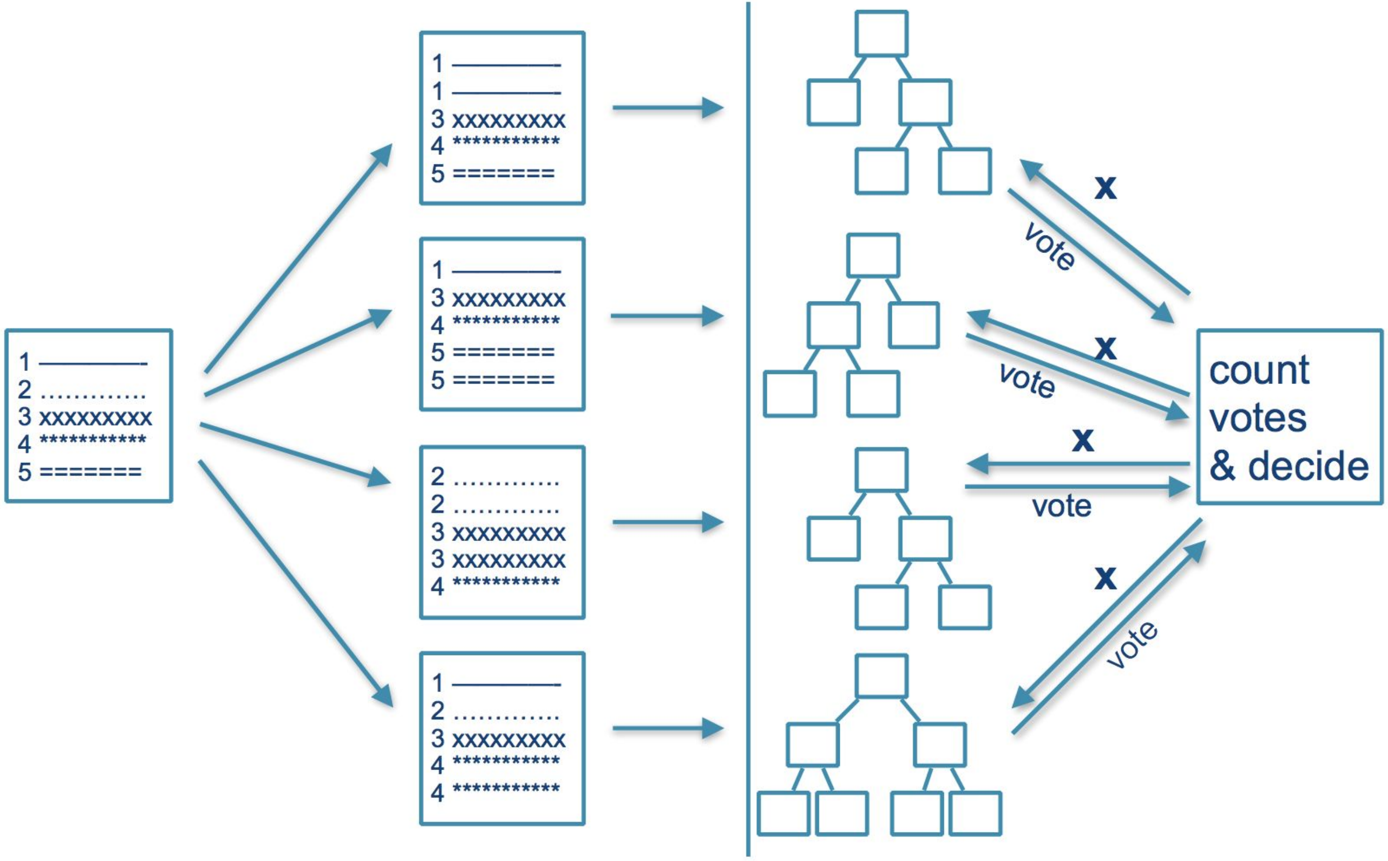


Image by Hendrik Blockeel

Bagging for Decision Trees

- Bagging generally works well for unstable learners
  - A learner is unstable if small changes in the dataset can give very different resulting models
  - It turns out that decision tree learners are indeed unstable

- Disadvantage: learning k trees is k times as expensive as learning one tree

Random Forests

- Like bagging, with one improvement
  - For trees, ALL the features are considered to create a split node (inner node)
  - For random forests, at each node consider only M randomly chosen attributes (not all)
  - Usually take $M = \sqrt{\text{number of attributes}}$

Random Forests

Common Steps

- Build a random forest considering M attributes
- Predict the value of "Out-of-bag" samples using the random forest
- Estimate the accuracy
- Determine the optimal M (hyperparameter)

Random Forests

- **Random Forests is one of the most efficient and most accurate learning methods to date (2008)** (Caruana+: An empirical evaluation of supervised learning in high dimensions. ICML 2008)

- **Easy to use with little parameter tuning**

- **Easy to debug, but, compared with Decision Trees, the model is less interpretable**

Demo Time (demo 6)

...

Boosting

- **Bagging goal:** fit large trees to resampled versions of the training data, and classify by majority vote

- **Boosting:** fit large or small trees to "**reweighted**" versions of the training data and classify by **weighted** majority vote

Boosting

- **Each model, defines the features that the next model will focus on**
- **Uses bootstrapping like bagging, but here we weight each sample of data**
    - **Some samples will be used more frequently**
- **Process:**
    - Given a model, track the samples that are more "erroneous" and give them heavier weights (considered to be data that have more complexity and requires more steps)
    - Given a model, track the error rate so that better models are given more weights

Neural Networks Warm-up

Why neural?

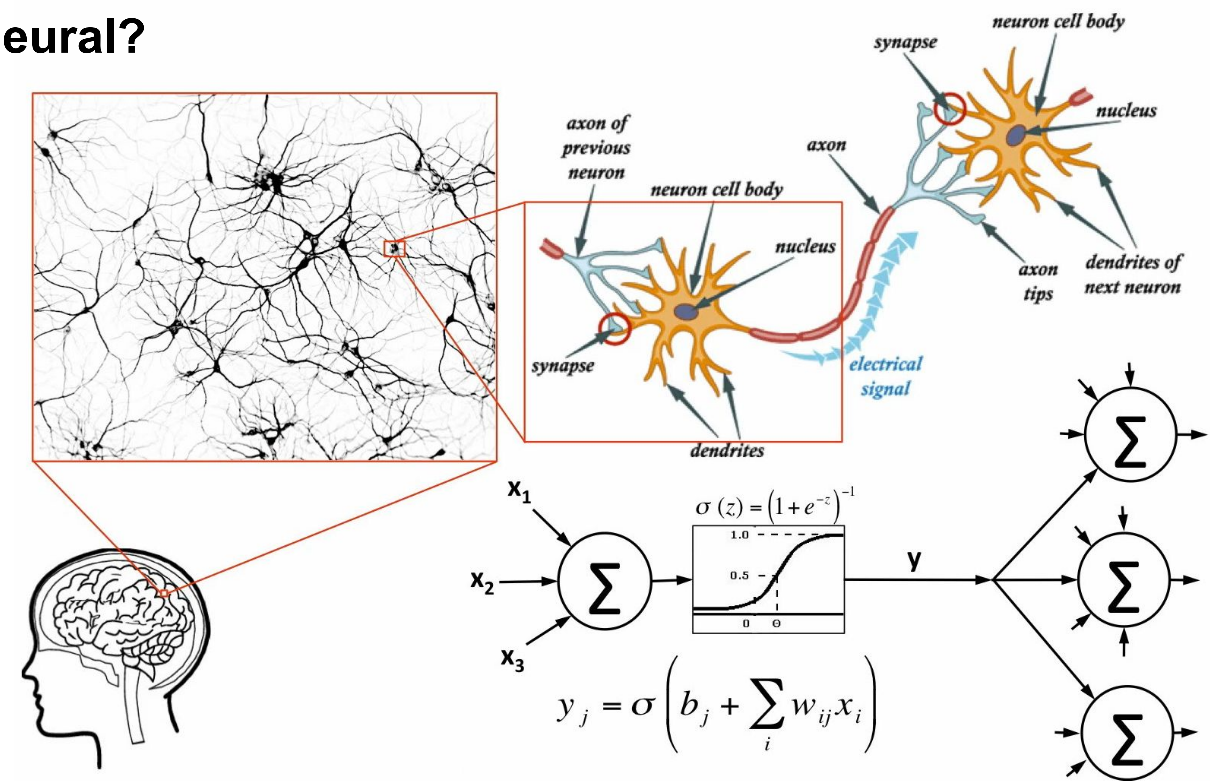


Image by Victor Lavrenko

Neural Networks Warm-up

Logistic Regression Review

Given x, we would like to find $\hat{y} = P(y = 1|x)$

What is the easiest way to transform x?

Neural Networks Warm-up

Logistic Regression Review

Given x, we would like to find $\hat{y} = P(y = 1|x)$

What is the easiest way to transform x?

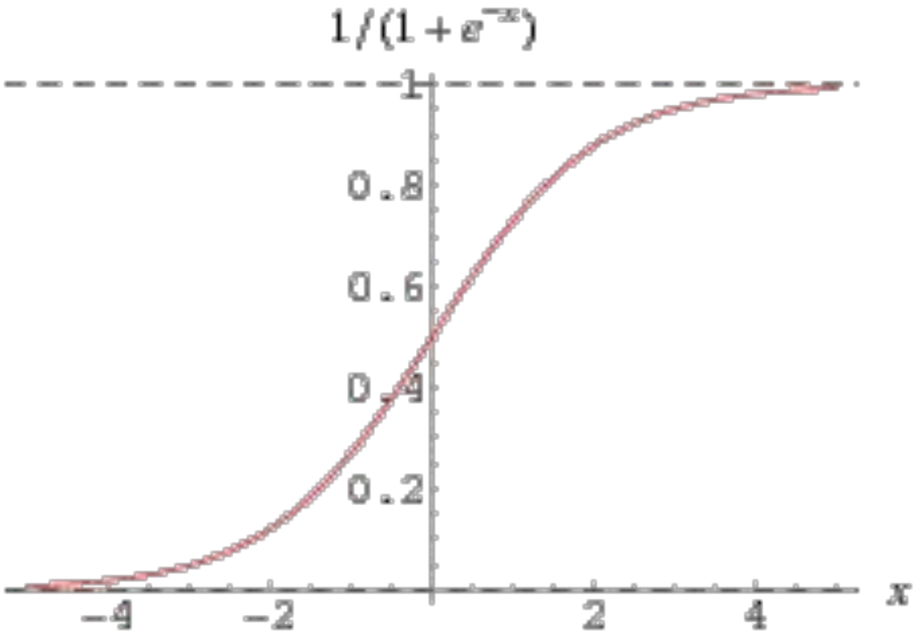
$$\hat{y} = w^T x + b$$

But we would like ŷ to be a probability: $0 \leq \hat{y} \leq 1$

Neural Networks Warm-up

Sigmoid function

$$f(x) = \frac{1}{1+\exp(-x)}$$



Neural Networks Warm-up

Cost function (for Logistic Regression)

- **m training samples:** $\{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \dots (x^{(m)}, y^{(m)})\}$
- **want to find:** $\hat{y}^{(i)} \approx y^{(i)}$
- **Popular loss function:**

$$\mathcal{L}(\hat{y}, y) = \frac{1}{2}(\hat{y} - y)^2$$

Neural Networks Warm-up

Cost function (for Logistic Regression)

- **m training samples:** $\{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \dots (x^{(m)}, y^{(m)})\}$
- **want to find:** $\hat{y}^{(i)} \approx y^{(i)}$
- **~~Popular~~ loss function:**
$$\mathcal{L}(\hat{y}, y) = -[y \log \hat{y} + (1-y) \log (1-\hat{y})]$$
- **Cost function:**
$$\mathcal{J}(w, b) = \frac{1}{m} \sum_{i=1}^{m} \mathcal{L}(\hat{y}^{(i)}, y^{(i)})$$

Neural Networks Warm-up

Logistic Regression

$$z = w^T x + b$$

$$\hat{y} = \sigma(w^T x + b)(\text{activation function; we usually use } a \text{ instead of } \hat{(}y)$$

$$\mathcal{L}(a, y) = -[y \log a + (1 - y) \log (1 - a)]$$

The goal is to minimize $\mathcal{J}$, to do so we compute

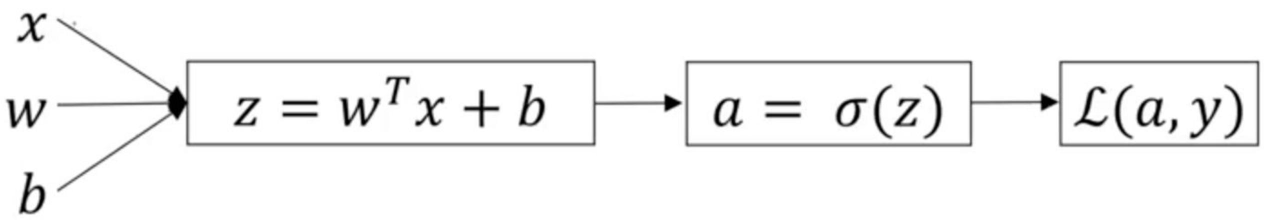
$$\frac{\partial}{\partial w_1} \mathcal{J}(w, b) = \frac{1}{m} \sum_{i=1}^{m} \frac{\partial}{\partial w_1} \mathcal{L}(a^{(i)}, y^{(i)})$$

Whiteboard Time

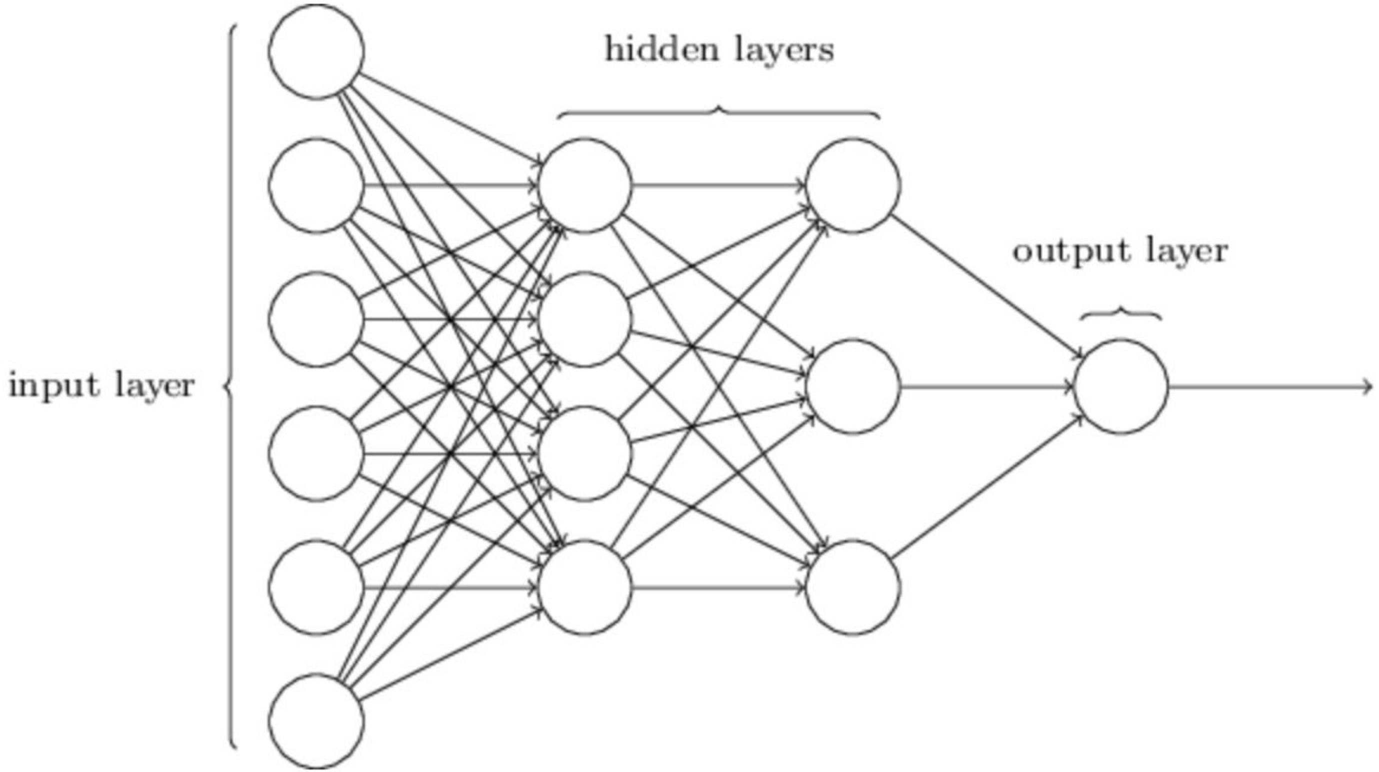
Computation graph for backpropagation
&
Logistic Regression minimization

Neural Networks Warm-up

Logistic Regression Gradient Descent



Neural Networks



Neural Networks

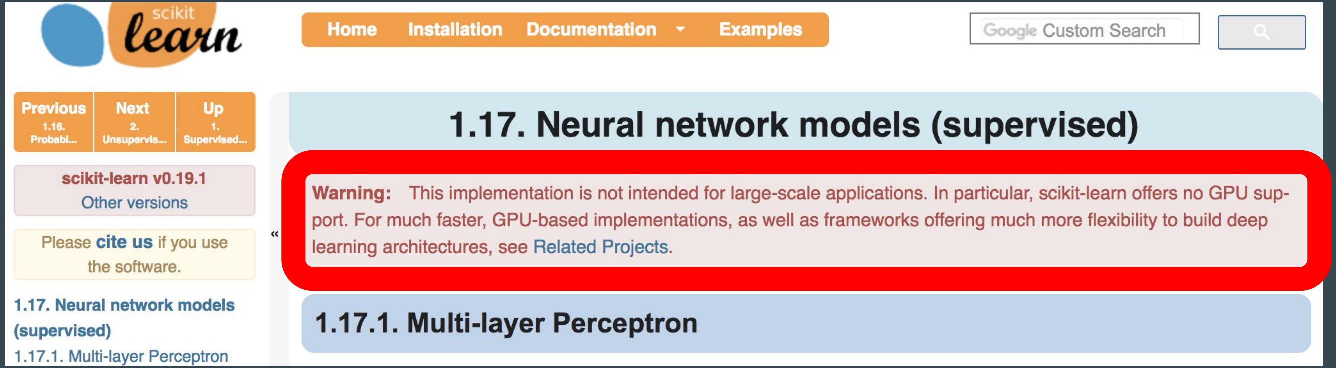
Activation Functions

- **Sigmoid function (as in Logistic regression)**
- **tanh:** $\frac{\exp(x)-\exp(-x)}{\exp(x)+\exp(-x)}$
- **Rectified Linear Unit (ReLU):** $\max(0, x)$
- **Leaky ReLU**

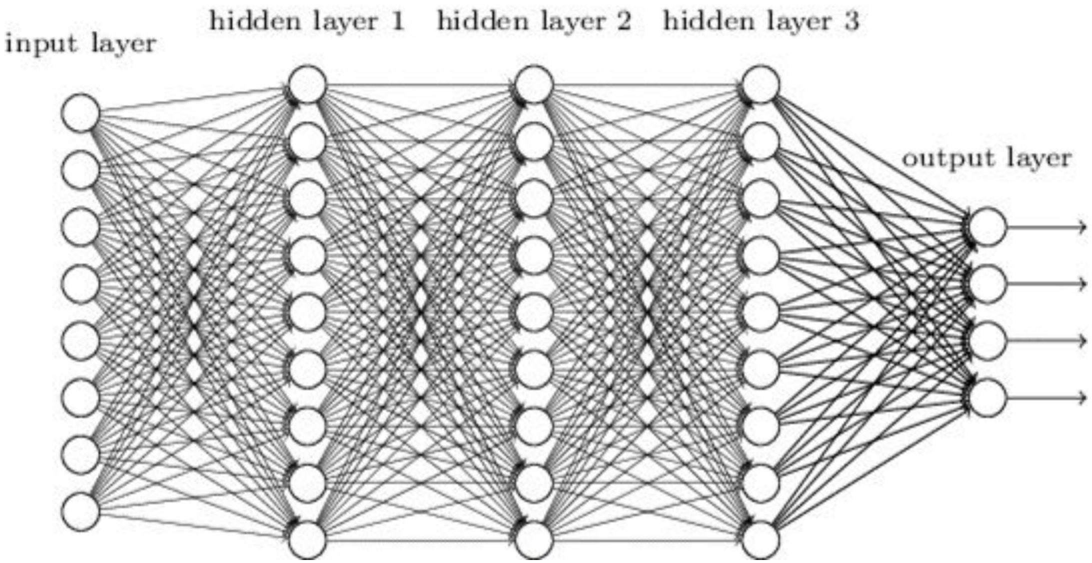
Demo Time (demo 7)

...

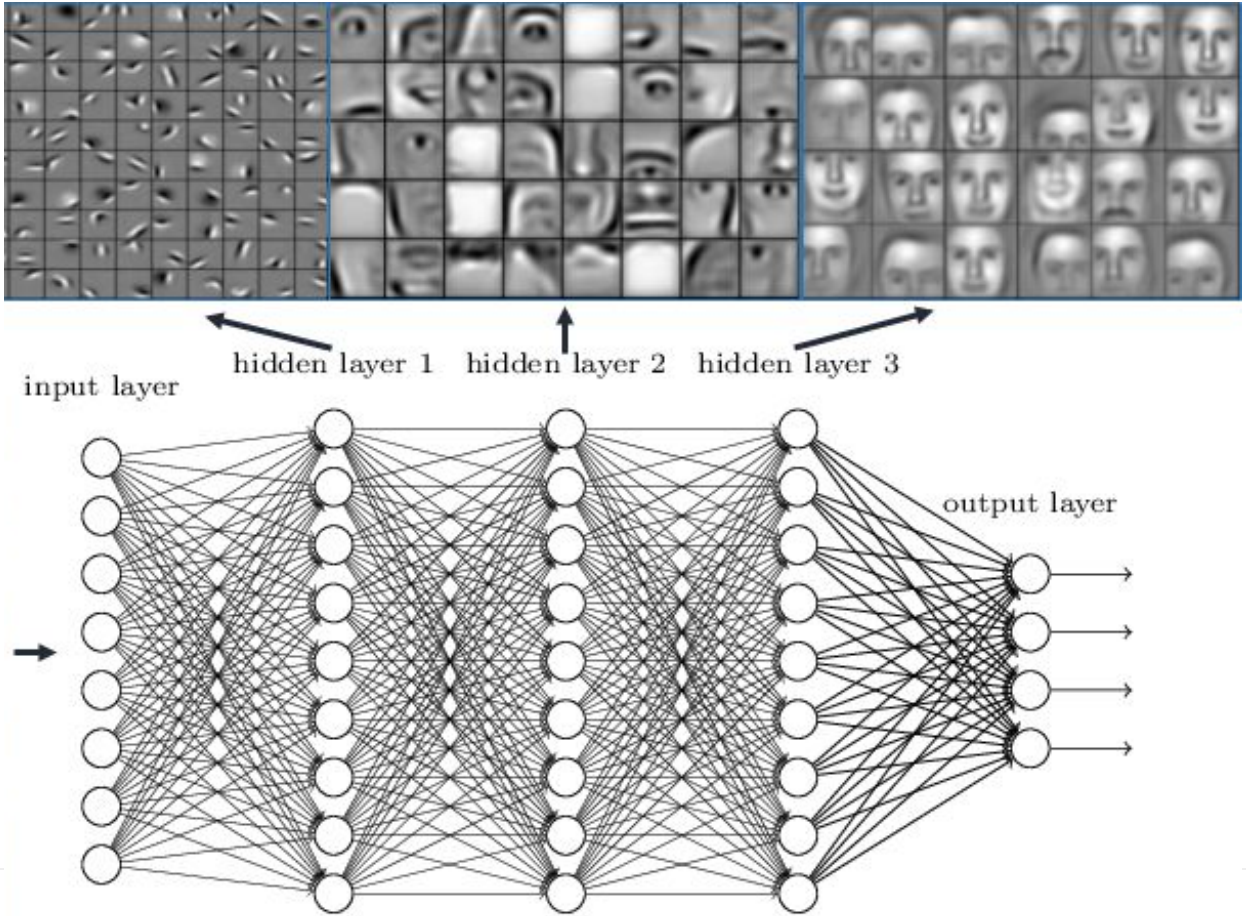
Demo Time (demo 7) …



Deep Neural Networks



Deep Neural Networks



Deep Neural Networks

How to split the data?

- **Train / Test / Validation**

Deep Neural Networks

How to split the data?

- **Train / Test / Validation**

- **Now?**

Deep Neural Networks

How to split the data?

- **Train / Test / Validation**

- **Now?**
  - **Too much data (> 10.000.000 samples)**

Deep Neural Networks

How to split the data?

- **Train / Test / Validation**

- **Now?**
  - **Too much data (> 10.000.000 samples)**

Make sure your train/ test / validation come from the same distribution

Deep Neural Networks

Rule of thumb to deal with bias/variance?

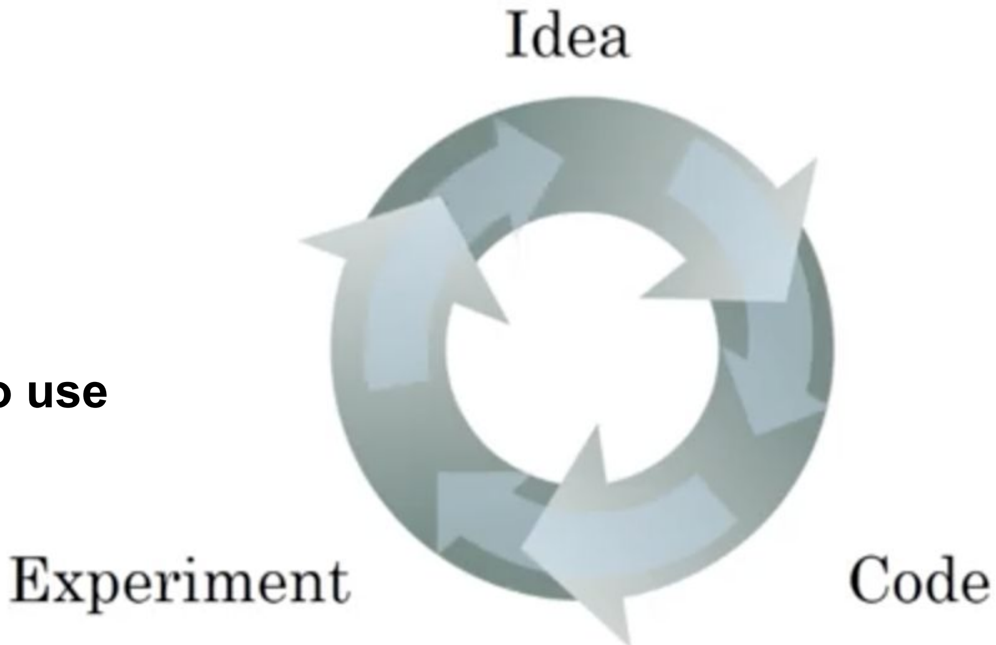
- **High Bias:**
  - **Bigger Network**
  - **Different Network Architecture**

- **High Variance:**
  - **More data**
  - **Regularization**
  - **Different Network Architecture**

Neural Networks

How to decide the size?

- **# hidden layers**
- **# hidden units**
- **What activation function to use**



Neural Networks Regularization

Logistic regression:

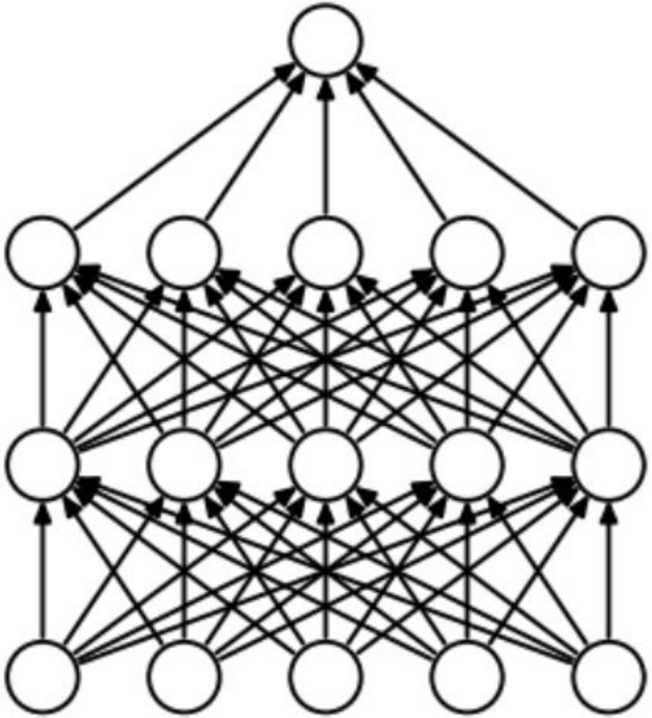
$$J(\theta) = -\frac{1}{m}\left[\sum_{i=1}^{m} y^{(i)}\log h_\theta(x^{(i)}) + (1-y^{(i)})\log(1-h_\theta(x^{(i)}))\right] + \frac{\lambda}{2m}\sum_{j=1}^{n}\theta_j^2$$

Neural network:

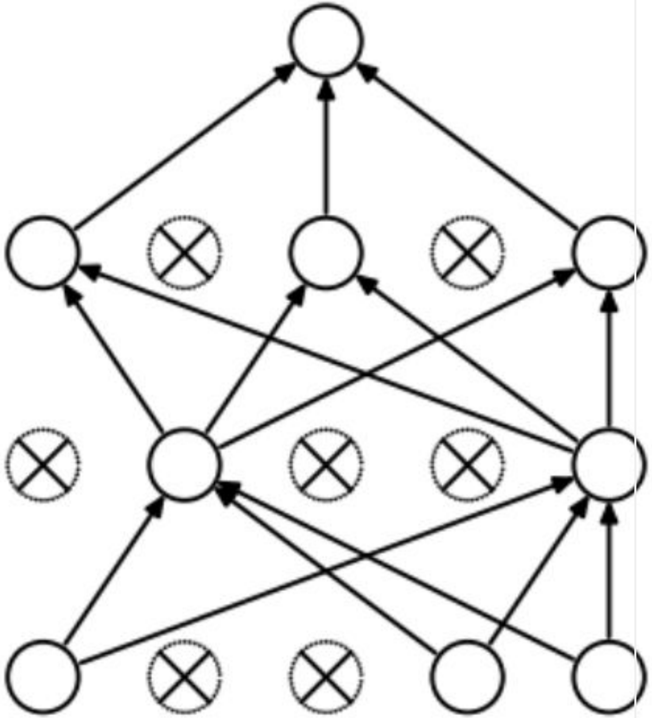
$$h_\Theta(x) \in \mathbb{R}^K \quad (h_\Theta(x))_i = i^{th} \text{ output}$$

$$J(\Theta) = -\frac{1}{m}\left[\sum_{i=1}^{m}\sum_{k=1}^{K} y_k^{(i)}\log(h_\Theta(x^{(i)}))_k + (1-y_k^{(i)})\log(1-(h_\Theta(x^{(i)}))_k)\right]$$
$$+\frac{\lambda}{2m}\sum_{l=1}^{L-1}\sum_{i=1}^{s_l}\sum_{j=1}^{s_{l+1}}(\Theta_{ji}^{(l)})^2$$

Neural Networks Dropout



(a) Standard Neural Net



(b) After applying dropout.

Neural Networks Momentum

- **Mini-batch Gradient Descent**

- **Gradient Descent optimization**
  - **with Momentum**
  - **RMSprop**
  - **Adam**

Resources (shown in class)

- **Multiclass classification (graphs):** https://jermwatt.github.io/mlrefined/blog_posts/Linear_Supervised_Learning/Part_5_One_versus_all.html
- **SVMs on fraud detection:** https://www.kaggle.com/pierra/credit-card-dataset-svm-classification
- **SVM kernels:** https://www.youtube.com/watch?v=3liCbRZPrZA
- **Random Forests on Titanic:** https://www.kaggle.com/zlatankr/titanic-random-forest-82-78/notebook
- **AdaBoost:** (slides 13 to 23) http://media.nips.cc/Conferences/2007/Tutorials/Slides/schapire-NIPS-07-tutorial.pdf
- **Computation graphs video:** (minute 6:00) https://www.youtube.com/watch?v=u2OeYrlAx_A&t=836s
- **CNNs vizualization:** (someone asked in class about this, the one below is one I found, not the one I had in mind, but it should be similar) https://github.com/InFoCusp/tf_cnnvis
- **Pydata :)** https://pydata.org/cordoba2018/