Neural Nets:
Many possible refs
e.g., Mitchell Chapter 4

Simple Model Selection
Cross Validation
Regularization
Neural Networks

Machine Learning – 10701/15781

Carlos Guestrin

Carnegie Mellon University

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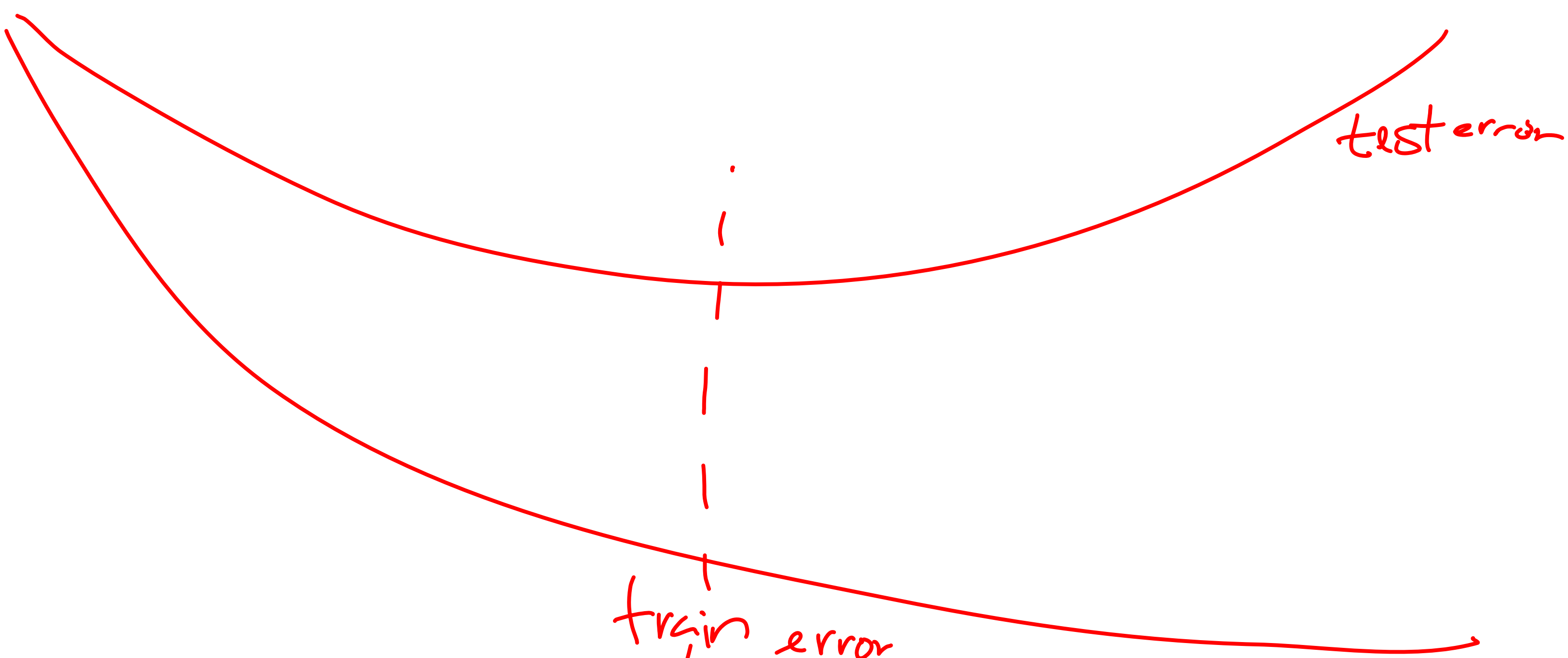
Announcements

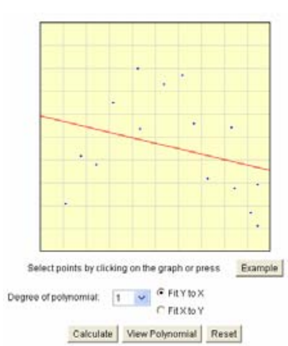
- Recitations stay on Thursdays
  - 5-6:30pm in Wean 5409
  - This week: Cross Validation and Neural Nets
- **Homework 2**
  - Due next Monday, Feb. 20^{th}
  - Updated version online with more hints
  - Start early

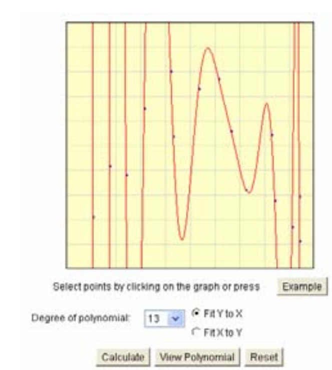
OK… now we'll learn to pick those darned parameters…

- **Selecting features (or basis functions)**
  - Linear regression
  - Naïve Bayes
  - Logistic regression
- **Selecting parameter value**
  - Prior strength
    - Naïve Bayes, linear and logistic regression
  - Regularization strength
    - Naïve Bayes, linear and logistic regression
  - Decision trees
    - MaxpChance, depth, number of leaves
  - Boosting
    - Number of rounds
- More generally, these are called **Model Selection** Problems
- Today:
  - Describe basic idea
  - Introduce very important concept for tuning learning approaches: **Cross-Validation**

Test set error as a function of model complexity







Simple greedy model selection algorithm

- Pick a dictionary of features (A hard part)
  - e.g., polynomials for linear regression $1, x, x^2, x^3, x^4, \dots$
- Greedy heuristic:
  - Start from empty (or simple) set of features $F_0 = \emptyset$ e.g., 1, x
  - Run learning algorithm for current set of features F_t β
    - Obtain h_t
  - Select **next best feature X_i**
    - e.g., X_j that results in lowest training error learner when learning with $F_t \cup \{X_j\}$ β
  - $F_{t+1} \leftarrow F_t \cup \{X_i\}$
  - Recurse

Greedy model selection

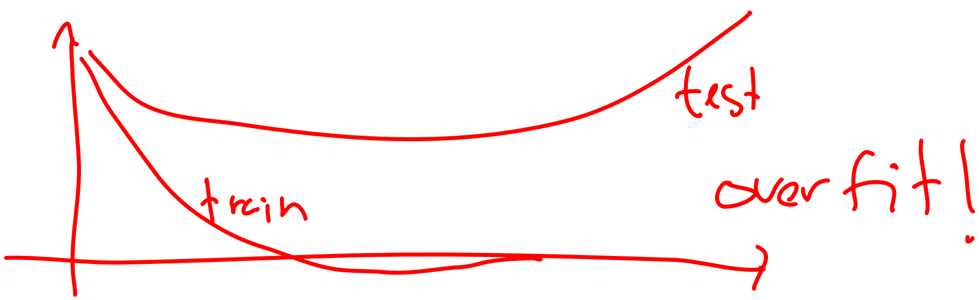
- Applicable in many settings:
  - Linear regression: Selecting basis functions
  - Naïve Bayes: Selecting (independent) features $P(X_i|Y)$
  - Logistic regression: Selecting features (basis functions)
  - Decision trees: Selecting leaves to expand
- Only a heuristic!
  - But, sometimes you can prove something cool about it
    - e.g., [Krause & Guestrin '05]: Near-optimal in some settings that include Naïve Bayes
- There are many more elaborate methods out there

Simple greedy model selection algorithm

- Greedy heuristic:
  - …
  - Select **next best feature X_i**
    - e.g., X_j that results in lowest training error learner when learning with $F_t \cup \{X_j\}$
  - $F_{t+1} \leftarrow F_t \cup \{X_i\}$
  - Recurse

When do you stop???

- When training error is low enough?



Simple greedy model selection algorithm

- Greedy heuristic:
  - …
  - Select **next best feature X_i**
    - e.g., X_j that results in lowest training error learner when learning with $F_t \cup \{X_j\}$
  - $F_{t+1} \leftarrow F_t \cup \{X_i\}$
  - Recurse

When do you stop???

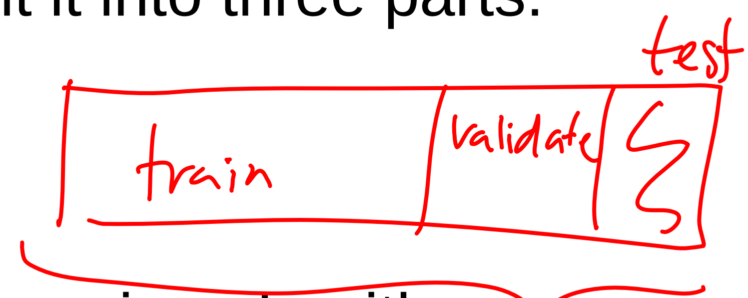
- ~~When training error is low enough?~~
- When test set error is low enough?

never ever ever learn on test data!!!

Validation set

- Thus far: Given a dataset, **randomly** split it into two parts:
  - Training data – $\{\mathbf{x}_1,\ldots,\mathbf{x}_{Ntrain}\}$
  - Test data – $\{\mathbf{x}_1,\ldots,\mathbf{x}_{Ntest}\}$

- But **Test data must always remain independent**!
  - Never ever ever ever learn on test data, including for model selection
- Given a dataset, **randomly** split it into three parts:
  - Training data – $\{\mathbf{x}_1,\ldots,\mathbf{x}_{Ntrain}\}$
  - Validation data – $\{\mathbf{x}_1,\ldots,\mathbf{x}_{Nvalid}\}$
  - Test data – $\{\mathbf{x}_1,\ldots,\mathbf{x}_{Ntest}\}$



- Use validation data for tuning learning algorithm, e.g., model selection
  - Save test data for very final evaluation

Simple greedy model selection algorithm

- Greedy heuristic:
  - …
  - Select **next best feature X_i**
    - e.g., X_j that results in lowest training error learner when learning with $F_t \cup \{X_j\}$
  - $F_{t+1} \leftarrow F_t \cup \{X_i\}$
  - Recurse

When do you stop???

- ~~When training error is low enough?~~
- ~~When test set error is low enough?~~
- When validation set error is low enough?

overfit to validation set.

Simple greedy model selection algorithm

- Greedy heuristic:
  - …
  - Select **next best feature X_i**
    - e.g., X_j that results in lowest training error learner when learning with $F_t \cup \{X_j\}$
  - $F_{t+1} \leftarrow F_t \cup \{X_i\}$
  - Recurse

When do you stop???

- ~~When training error is low enough?~~
- ~~When test set error is low enough?~~
- ~~When validation set error is low enough?~~
- Man!!! OK, should I just repeat until I get tired???
  - I am tired now…
  - **No, "There is a better way!"**

(LOO) Leave-one-out cross validation

- Consider a **validation set with 1 example**:
  - *D* – training data
  - *D*\i – training data with *i* th data point moved to validation set
- **Learn classifier $h_{D\backslash i}$ with *D*\i dataset**
- **Estimate true error** as:
  - 0 if $h_{D\backslash i}$ classifies *i* th data point correctly
  - 1 if $h_{D\backslash i}$ is wrong about *i* th data point
  - Seems really bad estimator, but wait!
- **LOO cross validation**: Average over all data points *i*:
  - **For each data point you leave out, learn a new classifier $h_{D\backslash i}$**
  - **Estimate error** as:

$$error_{LOO} = \frac{1}{m}\sum_{i=1}^{m} \mathbb{1}\left(h_{D\backslash i}(\mathbf{x}^i) \neq y^i\right)$$

set notation: $D\backslash i = D \setminus \{i\}$

overfit:

indicator func.

LOO cross validation is (almost) unbiased estimate of true error!

- When computing **LOOCV error, we only use *m-1* data points**
  - So it's not estimate of true error of learning with *m* data points!
  - Usually pessimistic, though – learning with less data typically gives worse answer
- **LOO is almost unbiased**!
  - Let $error_{true,m-1}$ be true error of learner when you only get *m-1* data points
  - In homework, you'll prove that LOO is unbiased estimate of $error_{true,m-1}$:

$$E_{\mathcal{D}}[error_{LOO}] = error_{true,m-1}$$

- **Great news!**
  - **Use LOO error for model selection!!!**

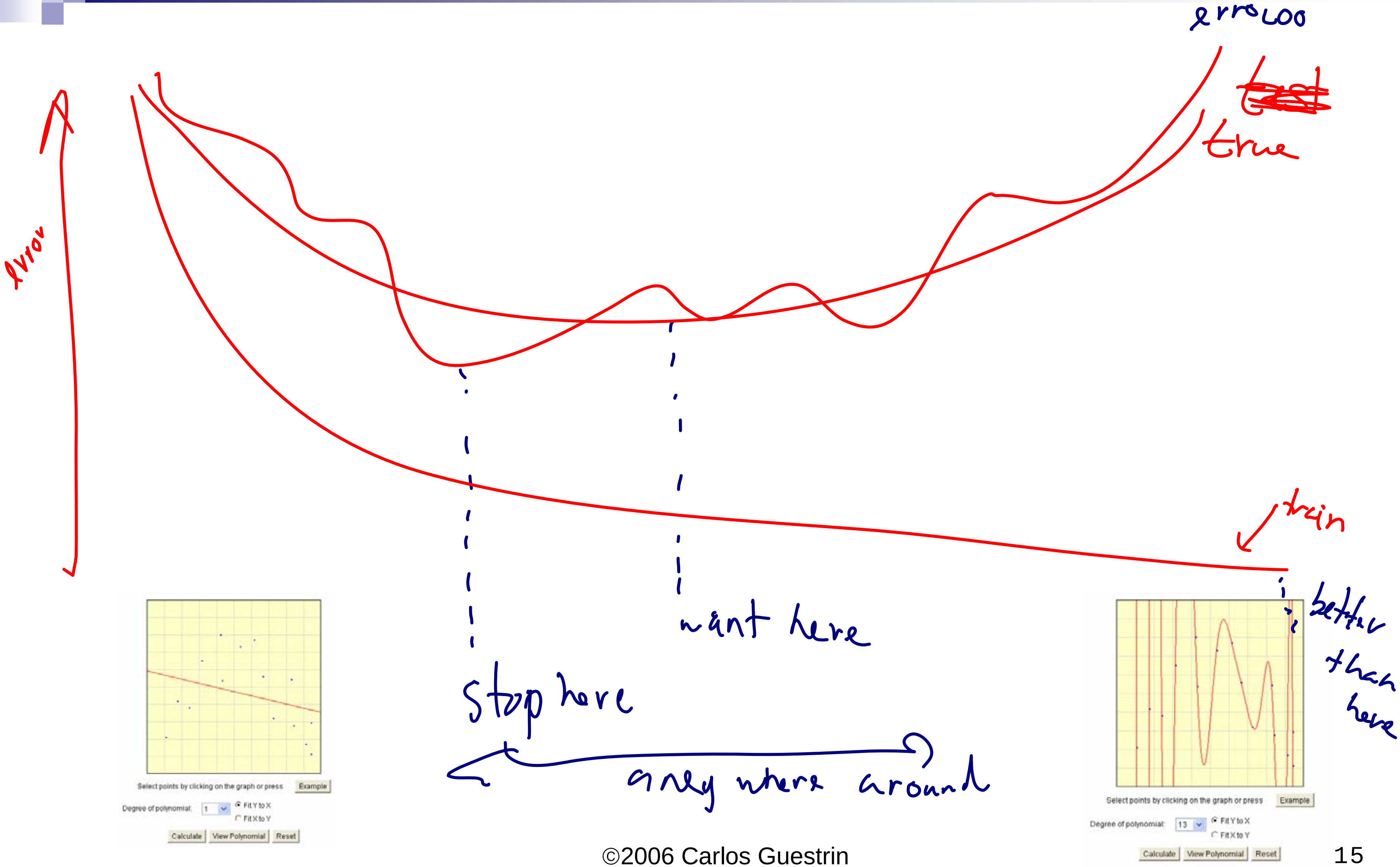
Simple greedy model selection algorithm

- Greedy heuristic:
  - …
  - Select **next best feature X_i**
    - e.g., X_j that results in lowest training error learner when learning with $F_t \cup \{X_j\}$
  - $F_{t+1} \leftarrow F_t \cup \{X_i\}$
  - Recurse

When do you stop???

- ~~When training error is low enough?~~
- ~~When test set error is low enough?~~
- ~~When validation set error is low enough?~~
- **STOP WHEN $error_{LOO}$ IS LOW!!!**

Using LOO error for model selection

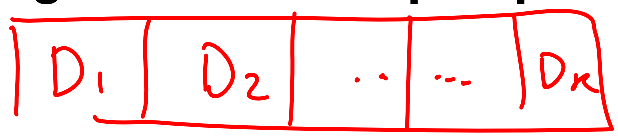


Computational cost of LOO

- Suppose you have 100,000 data points
- You implemented a great version of your learning algorithm
  - Learns in only 1 second
- Computing LOO will take about 1 day!!!
  - If you have to do for each choice of basis functions, it will take fooooooreeeve'!!!
- Solution 1: Preferred, but not usually possible
  - Find a cool trick to compute LOO (e.g., see homework)

Solution 2 to complexity of computing LOO: (More typical) **Use *k*-fold cross validation**

- Randomly **divide training data into *k* equal parts**
  - $D_1,\ldots,D_k$



- For each *i*
  - **Learn classifier $h_{D\backslash Di}$ using data point not in D_i**
  - **Estimate error of $h_{D\backslash Di}$ on validation set D_i:**

$$error_{\mathcal{D}_i} = \frac{k}{m} \sum_{(\mathbf{x}^j, y^j) \in \mathcal{D}_i} \mathbb{1}\left(h_{\mathcal{D}\backslash\mathcal{D}_i}(\mathbf{x}^j) \neq y^j\right)$$

- ***k*-fold cross validation error is average** over data splits:

$$error_{k-fold} = \frac{1}{k} \sum_{i=1}^{k} error_{\mathcal{D}_i}$$

- *k*-fold cross validation properties:
  - **Much faster to compute** than LOO
  - **More (pessimistically) biased** – using much less data, only *m(k-1)/k*
  - Usually, **k = 10** ☺

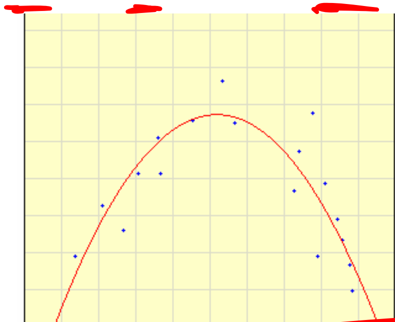
Regularization – Revisited

- Model selection 1: **Greedy**
  - Pick subset of features that have yield low LOO error
- Model selection 2: **Regularization**
  - Include **all possible features!**
  - **Penalize "complicated" hypothesis**

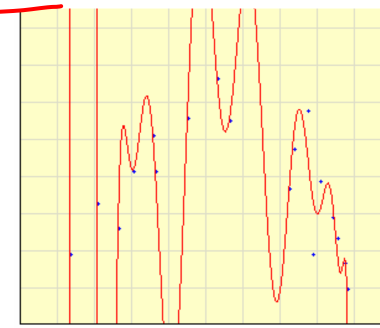
Regularization in linear regression

- Overfitting usually leads to very large parameter choices, e.g.:

-2.2 + 3.1 X – 0.30 X²



-1.1 + 4,700,910.7 X – 8,585,638.4 X² + …



degree 14

- Regularized least-squares (a.k.a. ridge regression), for $\lambda \geq 0$:

$$\mathbf{w}^* = \arg\min_{\mathbf{w}} \sum_j \left(t(\mathbf{x}_j) - \sum_i w_i h_i(\mathbf{x}_j) \right)^2 + \lambda \sum_{i=1}^{k} w_i^2$$

L2 error — penalty

use: all basis fns., penalize for large ws

Other regularization examples

- **Logistic regression** regularization
  - Maximize data likelihood minus **penalty for large parameters**

$$\arg\max_{\mathbf{w}} \sum_j \ln P(y^j|\mathbf{x}^j,\mathbf{w}) - \lambda \sum_i w_i^2$$

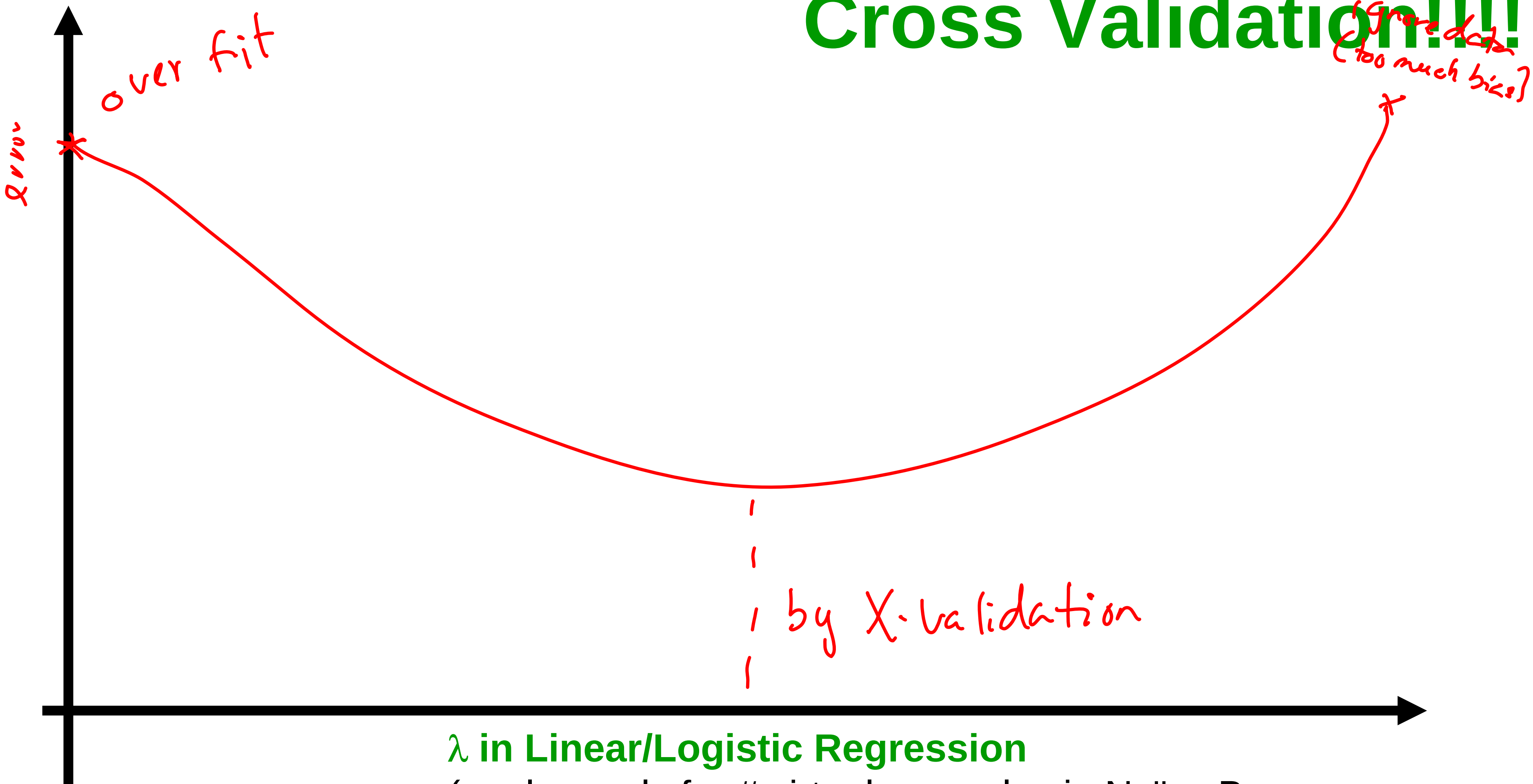
  - **Biases towards small parameter values**

- **Naïve Bayes** regularization
  - **Prior** over likelihood of features
  - **Biases away from zero probability** outcomes

- **Decision tree** regularization
  - Many possibilities, e.g., **Chi-Square test and MaxPvalue** parameter
  - **Biases towards smaller trees**

How do we pick magic parameter?

Cross Validation!!!!



λ in Linear/Logistic Regression
(analogously for # virtual examples in Naïve Bayes, MaxPvalue in Decision Trees)

Regularization and Bayesian learning

likelihood term — prior

$$p(\mathbf{w} \mid Y, \mathbf{X}) \propto P(Y \mid \mathbf{X}, \mathbf{w}) p(\mathbf{w})$$

- We already saw that **regularization for logistic regression** corresponds to **MAP for zero mean, Gaussian prior** for **w**

model selection: have prior over models.

- Similar interpretation for other learning approaches:
  - **Linear regression**: Also zero mean, Gaussian prior for **w**
  - **Naïve Bayes**: Directly defined as prior over parameters
  - **Decision trees**: Trickier to define… but we'll get back to this

polynomials for regression: prior: $P(degree = i) \propto e^{-i}$ — prefer lower degree polynomials a priori

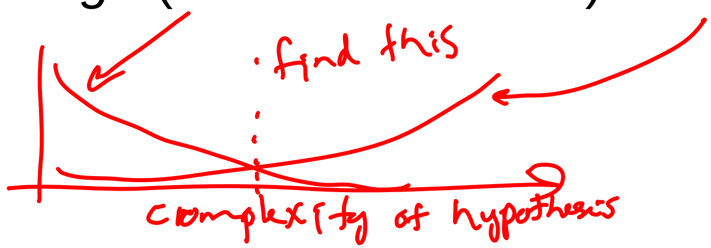
posterior: $P(degree = i \mid D) \propto P(D \mid degree) \cdot P(degree)$

when degree high: ↑ ↓

degree low: ↓ ↑

Occam's Razor

- William of Ockham (1285-1349) *Principle of Parsimony*:
  - "One should not increase, beyond what is necessary, the number of entities required to explain anything." over fitting....
- Regularization penalizes for *"complex explanations"*
- Alternatively (but pretty much the same), use *Minimum Description Length (MDL) Principle*:
  - minimize *length*(misclassifications) + *length*(hypothesis)



Describe data by a tree + exceptions

- *length*(misclassifications) – e.g., #wrong training examples
- *length*(hypothesis) – e.g., size of decision tree

Minimum Description Length Principle

- MDL prefers small hypothesis that fit data well:

$$h_{MDL} = \arg\min_h L_{C_1}(\mathcal{D} \mid h) + L_{C_2}(h)$$

misclassifications hyp.

  - $L_{C1}(D|h)$ – description length of data under code C_1 given *h*
    - Only need to describe points that *h* doesn't explain (classify correctly)
  - $L_{C2}(h)$ – description length of hypothesis *h*
- Decision tree example
  - $L_{C1}(D|h)$ – #bits required to describe data given *h*
    - If all points correctly classified, $L_{C1}(D|h) = 0$
  - $L_{C2}(h)$ – #bits necessary to encode tree
  - Trade off quality of classification with tree size

Bayesian interpretation of MDL Principle

- MAP estimate

$$h_{MAP} = \arg\max_h \left[P(\mathcal{D} \mid h)P(h)\right]$$
$$= \arg\max_h \left[\log_2 P(\mathcal{D} \mid h) + \log_2 P(h)\right]$$
$$= \arg\min_h \left[-\log_2 P(\mathcal{D} \mid h) - \log_2 P(h)\right]$$

- **Information theory fact**:
  - Smallest code for event of probability *p* requires $-\log_2 p$ bits
- MDL interpretation of MAP:
  - $-\log_2 P(D|h)$ – length of *D* under hypothesis *h*
  - $-\log_2 P(h)$ – length of hypothesis *h* (there is hidden parameter here)
  - MAP prefers simpler hypothesis:
    - minimize *length*(misclassifications) + *length*(hypothesis)

- **In general, Bayesian approach usually looks for simpler hypothesis** – Acts as a regularizer

What you need to know about Model Selection, Regularization and Cross Validation

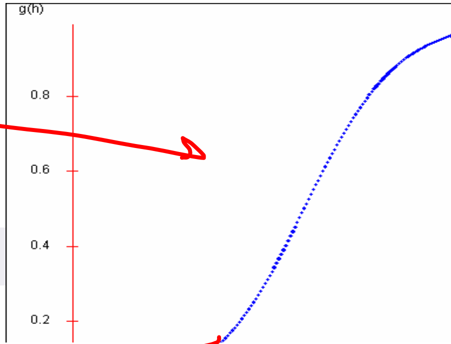
- Cross validation
  - (Mostly) Unbiased estimate of true error
  - LOOCV is great, but hard to compute
  - *k*-fold much more practical
  - Use for selecting parameter values!
- Model selection
  - Search for a model with low cross validation error
- Regularization
  - Penalizes for complex models
  - Select parameter with cross validation
  - Really a Bayesian approach
- Minimum description length
  - Information theoretic interpretation of regularization
  - Relationship to MAP

Logistic regression

- P(Y|X) represented by:

$$P(Y=1 \mid x, W) = \frac{1}{1+e^{-(w_0+\sum_i w_i x_i)}}$$

$$= g(w_0 + \sum_i w_i x_i)$$



logistic f. or sigmoid

- Learning rule – MLE:

$$\frac{\partial \ell(W)}{\partial w_i} = \sum_j x_i^j [y^j - P(Y^j = 1 \mid x^j, W)]$$

$$= \sum_j x_i^j [y^j - g(w_0 + \sum_i w_i x_i^j)]$$

$$w_i \leftarrow w_i + \eta \sum_j x_i^j \delta^j$$

learn rate; feature

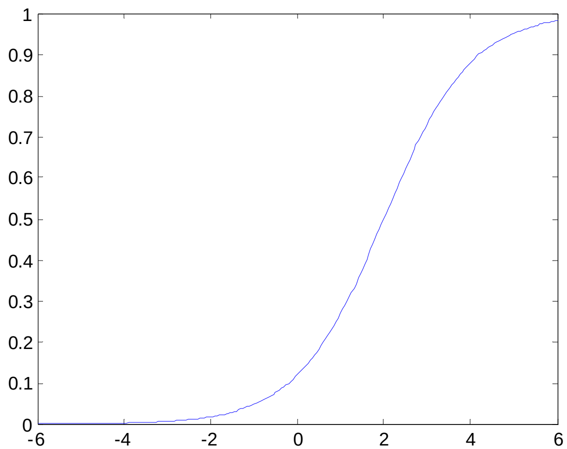
$$\delta^j = y^j - g(w_0 + \sum_i w_i x_i^j)$$

diff. true value – classifier value

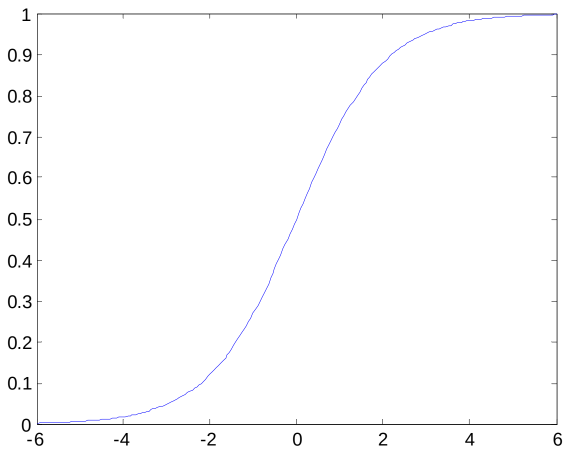
Sigmoid

$$g(w_0 + \sum_i w_i x_i) = \frac{1}{1 + e^{-(w_0 + \sum_i w_i x_i)}}$$

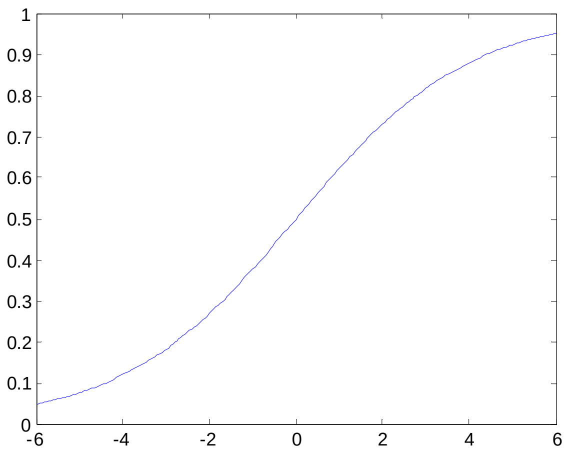
w_0=2, w_1=1



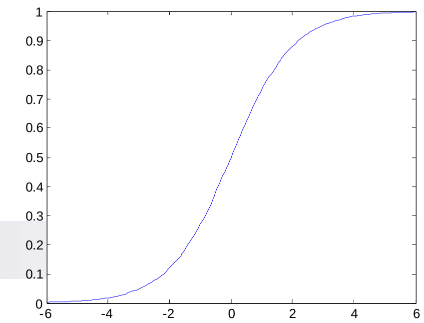
w_0=0, w_1=1



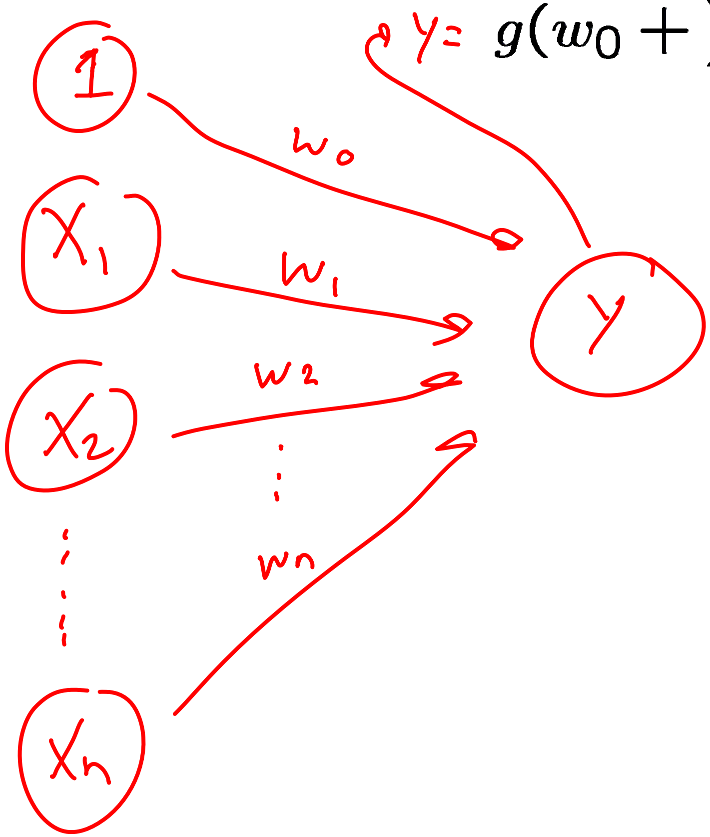
w_0=0, w_1=0.5



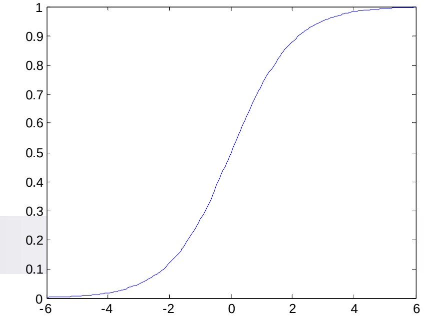
Perceptron as a graph



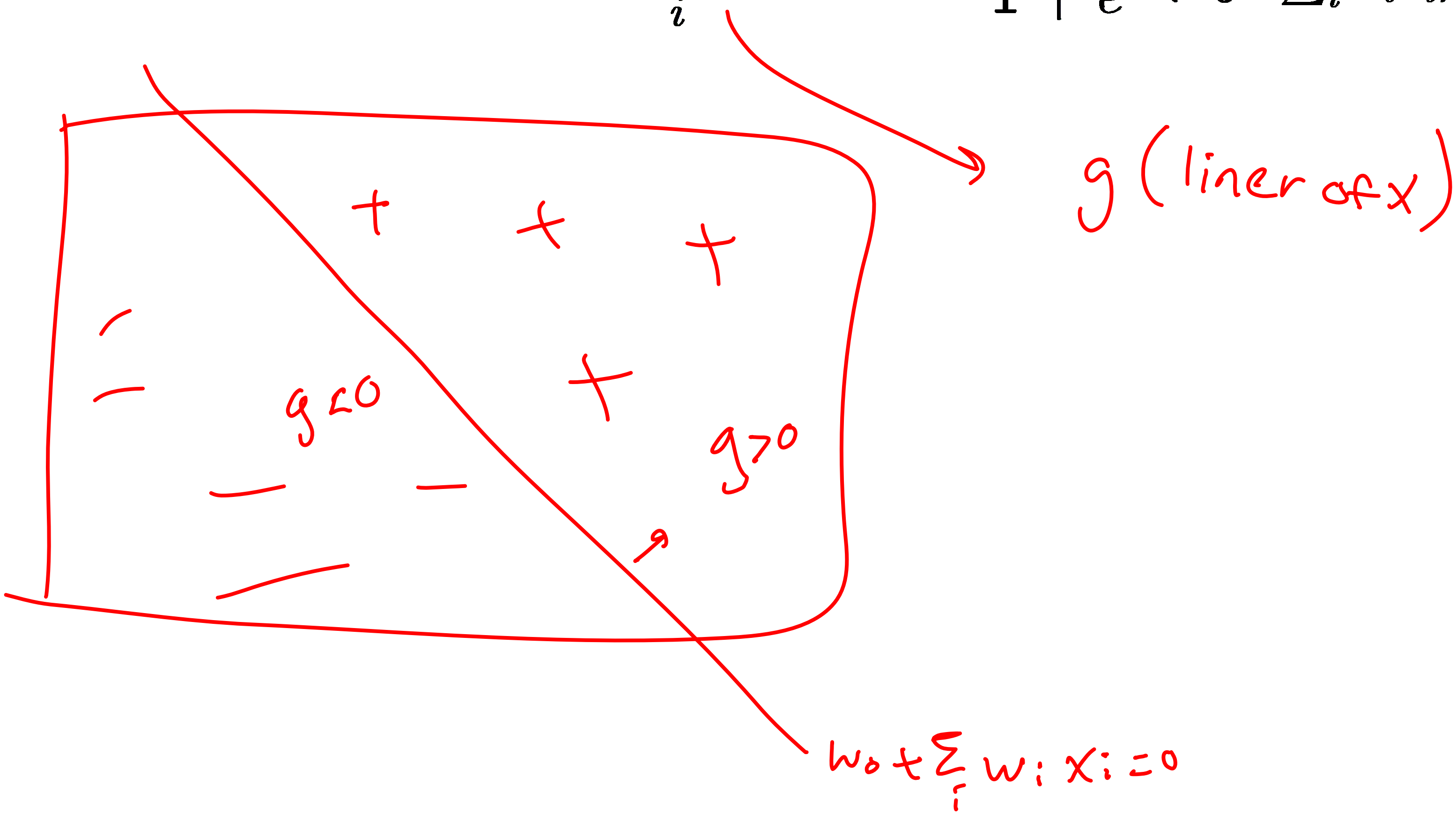
$$y = g(w_0 + \sum_i w_i x_i) = \frac{1}{1 + e^{-(w_0 + \sum_i w_i x_i)}}$$



Linear perceptron classification region



$$g(w_0 + \sum_i w_i x_i) = \frac{1}{1 + e^{-(w_0 + \sum_i w_i x_i)}}$$



Optimizing the perceptron

- Trained to minimize sum-squared error

$$\ell(W) = \frac{1}{2}\sum_j [y^j - g(w_0 + \sum_{i'} w_{i'} x^j_{i'})]^2$$

chain rule

$$\frac{\partial \ell(w)}{\partial w_i} = \sum_j -[y^j - g(w_0 + \sum_{i'} w_{i'} x^j_{i'})] \cdot \frac{\partial}{\partial w_i} g(w_0 + \sum_{i'} w_{i'} x^j_{i'})$$

derivative of sigmoid!

Derivative of sigmoid

$$\frac{\partial \ell(W)}{\partial w_i} = -\sum_j [y^j - g(w_0 + \sum_{i'} w_{i'} x_{i'}^j)]\; x_i^j\; g'(w_0 + \sum_{i'} w_{i'} x_{i'}^j)$$

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

$$\frac{\partial g(w_0 + \sum_i w_i x_i)}{\partial w_i} = w_i \cdot \frac{\partial g(w_0 + \sum_i w_i x_i)}{\partial (w_0 + \sum_i w_i x_i)}$$

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

$$= -(1+e^{-x})^{-2} \cdot \frac{\partial}{\partial x}(1+e^{-x})$$

$$= (1+e^{-x})^{-2} \cdot e^{-x}$$

$$= \frac{e^{-x}}{(1+e^{-x})^2} = \frac{1+e^{-x}-1}{(1+e^{-x})^2} =$$

$$= \frac{1}{1+e^{-x}} - \frac{1}{(1+e^{-x})^2} = g(x) - g(x)^2$$

$$= g(x)(1-g(x))$$

The perceptron learning rule

$$w_i \leftarrow w_i + \eta \sum_j x_i^j \delta^j$$

$$\delta^j = [y^j - g(w_0 + \sum_i w_i x_i^j)] g^j (1 - g^j)$$

$$g^j = g(w_0 + \sum_i w_i x_i^j)$$

perceptron

loss function: squared error

learn rate

example

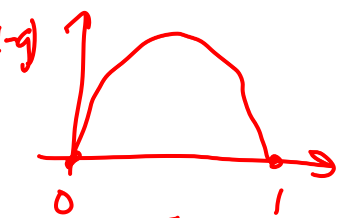
delta

how well classify

extra term

loss function: Cond. likelihood

logistic regression



more: unhappy with 50/50 classification

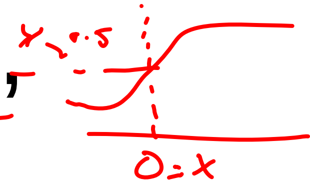
- Compare to MLE:

$$w_i \leftarrow w_i + \eta \sum_j x_i^j \delta^j$$

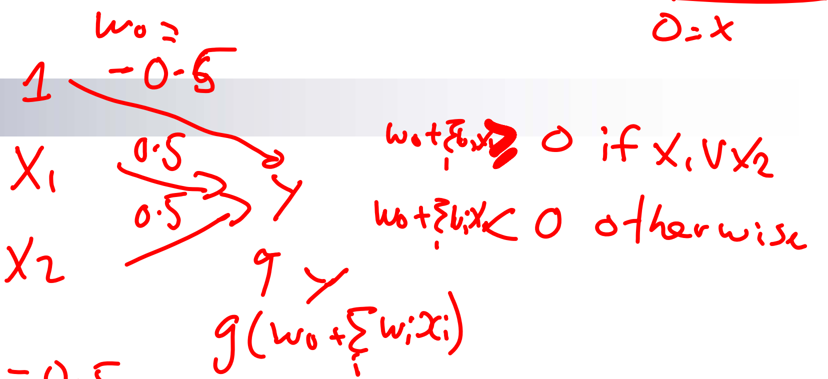
$$\delta^j = [y^j - g(w_0 + \sum_i w_i x_i^j)]$$

also unhappy with 50/50

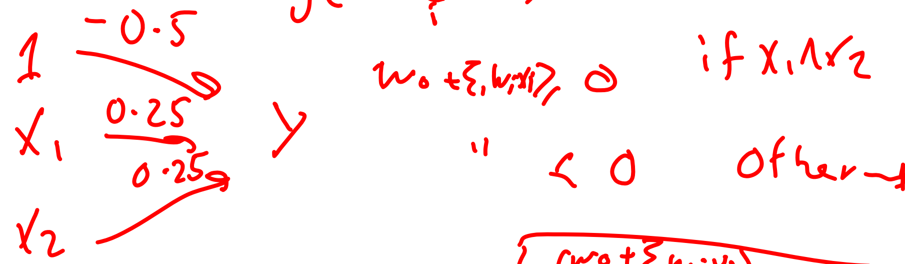
Percepton, linear classification, Boolean functions



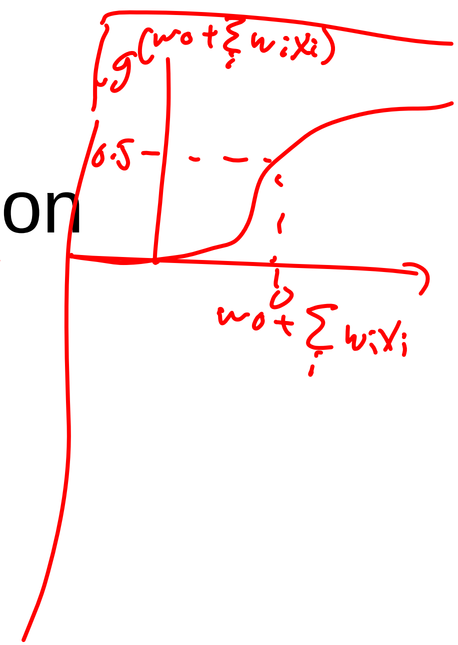
- Can learn $x_1 \vee x_2$

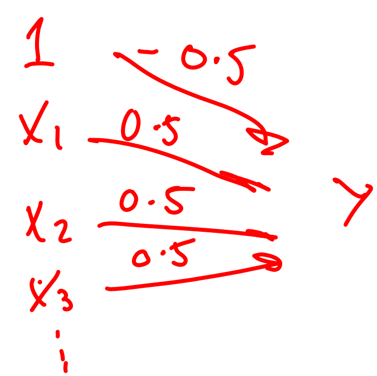


- Can learn $x_1 \wedge x_2$



- Can learn any conjunction or disjunction

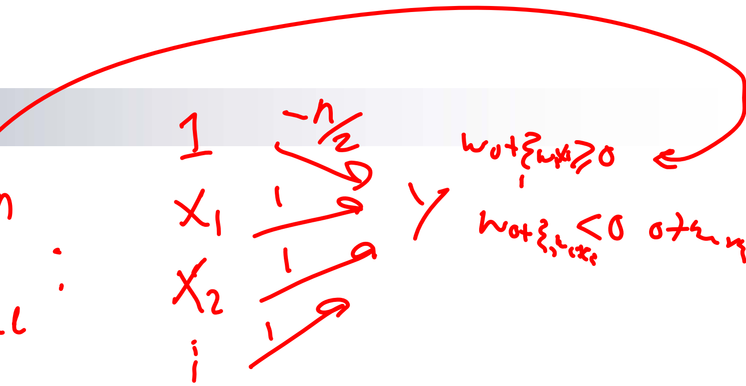




Percepton, linear classification, Boolean functions

- Can learn majority

more than half xi are true:



- Can perceptrons do everything?

cannot learn XOR

Going beyond linear classification

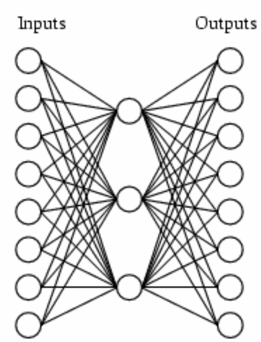
- Solving the XOR problem

Hidden layer

- Perceptron: $$out(\mathbf{x}) = g(w_0 + \sum_i w_i x_i)$$
- 1-hidden layer:

$$out(\mathbf{x}) = g\left(w_0 + \sum_k w_k g(w_0^k + \sum_i w_i^k x_i)\right)$$

Example data for NN with hidden layer



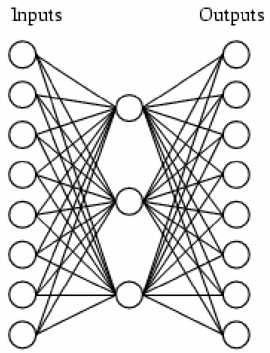
A target function:

Input		Output
10000000	→	10000000
01000000	→	01000000
00100000	→	00100000
00010000	→	00010000
00001000	→	00001000
00000100	→	00000100
00000010	→	00000010
00000001	→	00000001

Can this be learned??

Learned weights for hidden layer

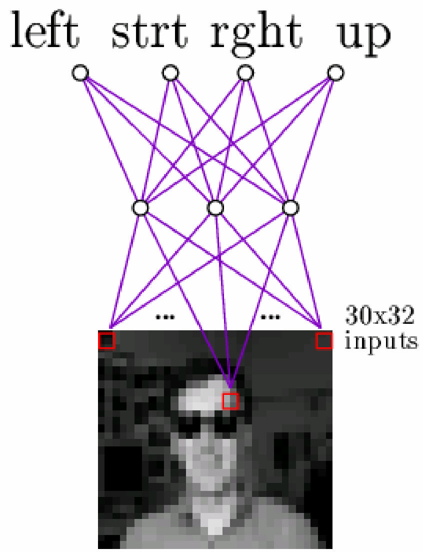
A network:

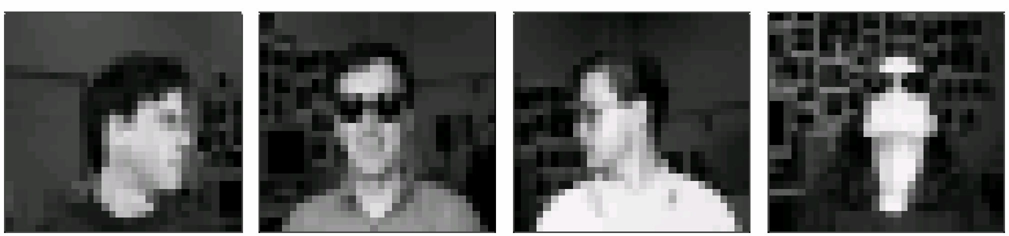


Learned hidden layer representation:

Input		Hidden Values				Output
10000000	→	.89	.04	.08	→	10000000
01000000	→	.01	.11	.88	→	01000000
00100000	→	.01	.97	.27	→	00100000
00010000	→	.99	.97	.71	→	00010000
00001000	→	.03	.05	.02	→	00001000
00000100	→	.22	.99	.99	→	00000100
00000010	→	.80	.01	.98	→	00000010
00000001	→	.60	.94	.01	→	00000001

NN for images

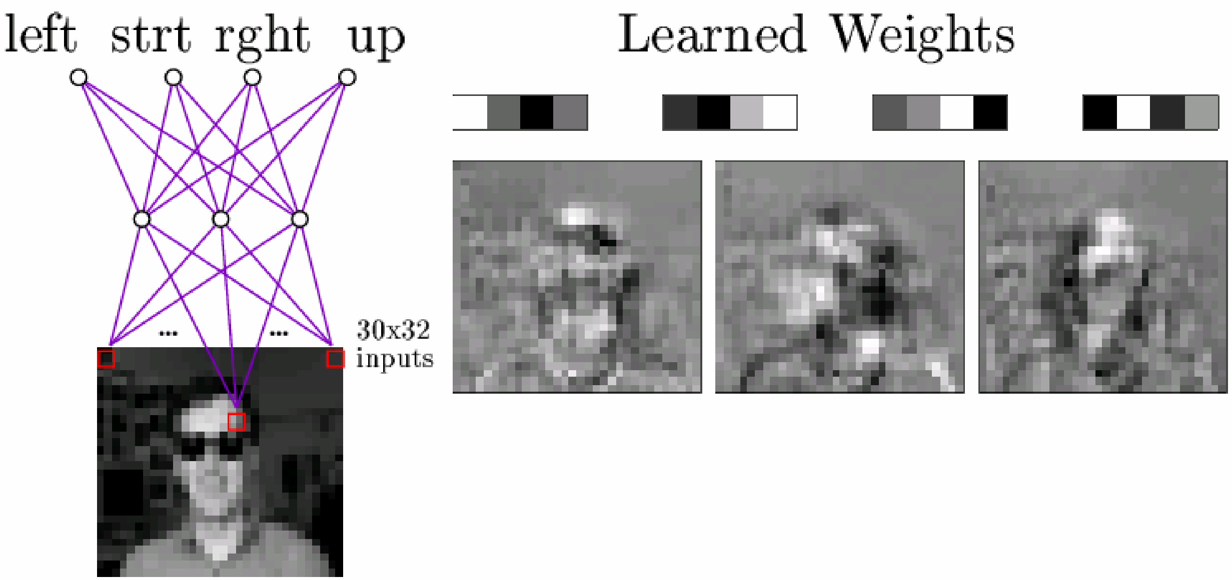


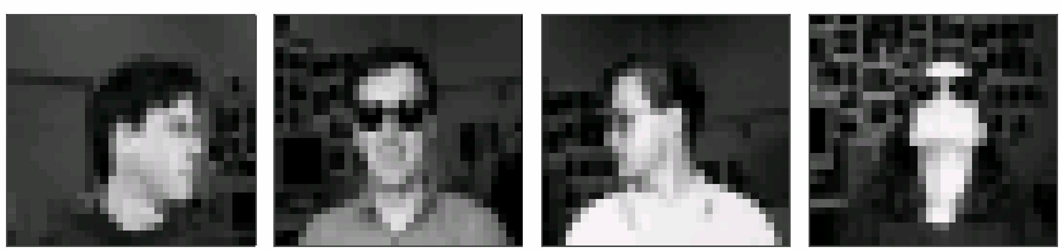


Typical input images

90% accurate learning head pose, and recognizing 1-of-20 faces

Weights in NN for images





Typical input images

Forward propagation for 1-hidden layer - Prediction

- 1-hidden layer:

$$out(\mathbf{x}) = g\left(w_0 + \sum_k w_k g(w_0^k + \sum_i w_i^k x_i)\right)$$

Gradient descent for 1-hidden layer – Back-propagation: Computing $\frac{\partial \ell(W)}{\partial w_k}$

Dropped w_0 to make derivation simpler

$$\ell(W) = \frac{1}{2}\sum_j [y^j - out(\mathbf{x}^j)]^2$$

$$out(\mathbf{x}) = g\left(\sum_{k'} w_{k'} g(\sum_{i'} w_{i'}^{k'} x_{i'})\right)$$

$$\frac{\partial \ell(W)}{\partial w_k} = -[y - out(\mathbf{x})]\frac{\partial out(\mathbf{x})}{\partial w_k}$$

Gradient descent for 1-hidden layer – Back-propagation: Computing $\frac{\partial \ell(W)}{\partial w_i^k}$

Dropped w_0 to make derivation simpler

$$\ell(W) = \frac{1}{2}\sum_j [y^j - out(\mathbf{x}^j)]^2$$

$$out(\mathbf{x}) = g\left(\sum_{k'} w_{k'} g(\sum_{i'} w_{i'}^{k'} x_{i'})\right)$$

$$\frac{\partial \ell(W)}{\partial w_i^k} = -[y - out(\mathbf{x})]\frac{\partial out(\mathbf{x})}{\partial w_i^k}$$

Multilayer neural networks

Forward propagation – prediction

- Recursive algorithm
- Start from input layer
- Output of node V_k with parents $U_1, U_2, \ldots$:

$$V_k = g\left(\sum_i w_i^k U_i\right)$$

Back-propagation – learning

- Just gradient descent!!!
- Recursive algorithm for computing gradient
- For each example
  - Perform forward propagation
  - Start from output layer
  - Compute gradient of node V_k with parents U_1,U_2,…
  - Update weight w_i^k

Many possible response functions

- Sigmoid
- Linear
- Exponential
- Gaussian
- …

Convergence of backprop

- Perceptron leads to convex optimization
  - Gradient descent reaches **global minima**
- Multilayer neural nets **not convex**
  - Gradient descent gets stuck in local minima
  - Hard to set learning rate
  - Selecting number of hidden units and layers = fuzzy process
  - NNs falling in disfavor in last few years
  - We'll see later in semester, *kernel trick* is a good alternative
  - Nonetheless, neural nets are one of the most used ML approaches

Training set error

- Neural nets represent complex functions
  - Output becomes more complex with gradient steps
- Training set error

What about test set error?

Overfitting

- Output fits training data "too well"
  - Poor test set accuracy
- Overfitting the training data
  - Related to bias-variance tradeoff
  - One of central problems of ML
- Avoiding overfitting?
  - More training data
  - Regularization
  - Early stopping

What you need to know

- Perceptron:
  - Representation
  - Perceptron learning rule
  - Derivation
- Multilayer neural nets
  - Representation
  - Derivation of backprop
  - Learning rule
- Overfitting
  - Definition
  - Training set versus test set
  - Learning curve