# CSCE 970 Lecture 3: Regularization

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## Introduction

- Machine learning can generally be distilled to an optimization problem
- Choose a classifier (function, hypothesis) from a set of functions that minimizes an objective function
- Clearly we want part of this function to measure performance on the training set, but this is insufficient





## Outline

- Types of machine learning problems
- Loss functions
- Generalization performance vs training set performance
- Overfitting
- Regularization
- Estimating generalization performance





## Machine Learning Problems

- **Supervised Learning:** Algorithm is given labeled *training data* and is asked to infer a function (*hypothesis*) from a family of functions (e.g., set of all ANNs) that is able to predict well on new, unseen examples
  - **Classification:** Labels come from a finite, discrete set
  - **Regression:** Labels are real-valued
- **Unsupervised Learning:** Algorithm is given data without labels and is asked to model its structure
  - Clustering, density estimation
- **Reinforcement Learning:** Algorithm controls an agent that interacts with its environment and learns good actions in various situations





## Measuring Performance
### Loss

- In any learning problem, need to be able to quantify performance of an algorithm
- In supervised learning, we often use a **loss function** (or error function) $\mathcal{J}$ for this task
- Given instance $\boldsymbol{x}$ with true label $y$, if the learner's prediction on $\boldsymbol{x}$ is $\hat{y}$, then

$$\mathcal{J}(y, \hat{y})$$

is the loss on that instance





## Measuring Performance
### Examples of Loss Functions

- **0-1 Loss:** $\mathcal{J}(y, \hat{y}) = 1$ if $y \neq \hat{y}$, 0 otherwise
- **Square Loss:** $\mathcal{J}(y, \hat{y}) = (y - \hat{y})^2$
- **Cross-Entropy:** $\mathcal{J}(y, \hat{y}) = -y \ln \hat{y} - (1 - y) \ln (1 - \hat{y})$ ($y$ and $\hat{y}$ are considered probabilities of a '1' label; generalizes to multi-class.)
- **Hinge Loss:** $\mathcal{J}(y, \hat{y}) = \max(0, 1 - y\,\hat{y})$ (used sometimes for large margin classifiers like SVMs)

All non-negative

## Measuring Performance
### Training Loss

- Given a loss function $\mathcal{J}$ and a training set $\mathcal{X}$, the total loss of the classifier $h$ on $\mathcal{X}$ is

$$error_{\mathcal{X}}(h) = \sum_{x \in \mathcal{X}} \mathcal{J}(y_{\boldsymbol{x}}, \hat{y}_{\boldsymbol{x}}) \ ,$$

where $y_{\boldsymbol{x}}$ is $\boldsymbol{x}$'s label and $\hat{y}_{\boldsymbol{x}}$ is $h$'s prediction



## Measuring Performance
### Expected Loss

- More importantly, the learner needs to **generalize** well: Given a new example drawn iid according to unknown probability distribution $\mathcal{D}$, we want to minimize $h$'s **expected loss**:

$$error_{\mathcal{D}}(h) = \mathbb{E}_{\boldsymbol{x} \sim \mathcal{D}} \left[ \mathcal{J}(y_{\boldsymbol{x}}, \hat{y}_{\boldsymbol{x}}) \right]$$

- Is minimizing training loss the same as minimizing expected loss?



## Measuring Performance
### Expected vs Training Loss

- Sufficiently sophisticated learners (decision trees, multi-layer ANNs) can often achieve arbitrarily small (or zero) loss on a training set
- A hypothesis (e.g., ANN with specific parameters) $h$ *overfits* the training data $\mathcal{X}$ if there is an alternative hypothesis $h'$ such that

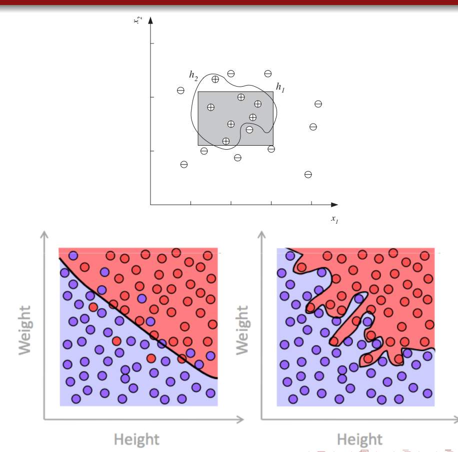
$$error_{\mathcal{X}}(h) < error_{\mathcal{X}}(h')$$

and

$$error_{\mathcal{D}}(h) > error_{\mathcal{D}}(h')$$

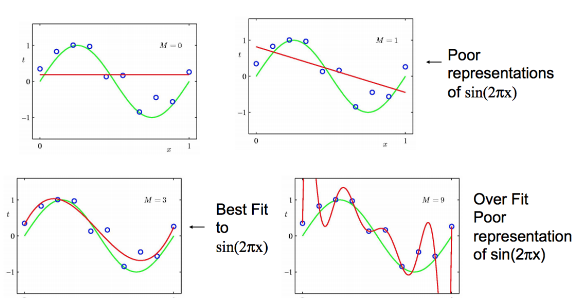


## Measuring Performance
### Overfitting






## Measuring Performance
### Overfitting



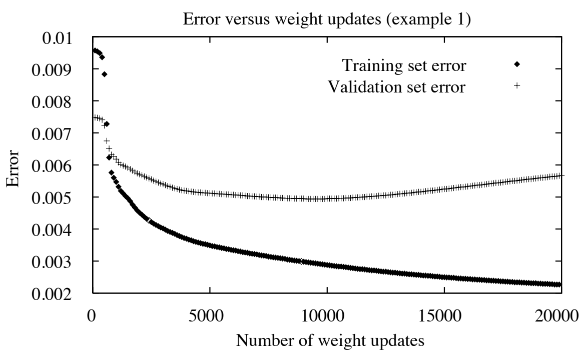

To generalize well, need to balance **training accuracy** with **simplicity**



## Regularization
### Causes of Overfitting

- Generally, if the set of functions $\mathcal{H}$ the learner has to choose from is complex relative to what is required for correctly predicting the labels of $\mathcal{X}$, there's a larger chance of overfitting due to the large number of "wrong" choices in $\mathcal{H}$
  - Could be due to an overly sophisticated set of functions
    - E.g., can fit any set of $n$ real-valued points with an $(n-1)$-degree polynomial, but perhaps only degree 2 is needed
    - E.g., using an ANN with 5 hidden layers to solve the logical AND problem
  - Could be due to training an ANN too long
    - Over-training an ANN often leads to weights deviating far from zero
    - Makes the function more non-linear, and more complex
- Often, a larger data set mitigates the problem

# Regularization
## Causes of Overfitting: Overtraining



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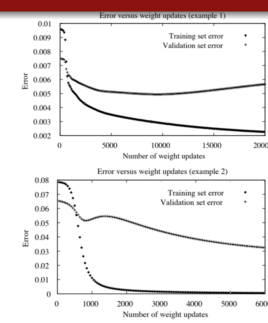
# Regularization
## Early Stopping




- Danger of stopping too soon
  - "Patience" parameter determines how long to wait
- Can re-start and track best one on separate validation set



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# Regularization
## Parameter Norm Penalties

- Still want to minimize training loss, but balance it against a complexity penalty on the parameters used:

$$\tilde{\mathcal{J}}(\boldsymbol{\theta};\mathcal{X},\boldsymbol{y}) = \mathcal{J}(\boldsymbol{\theta};\mathcal{X},\boldsymbol{y}) + \alpha\,\Omega(\boldsymbol{\theta})$$

- $\alpha \in [0,\infty)$ weights loss $\mathcal{J}$ against penalty $\Omega$



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# Regularization
## Parameter Norm Penalties: $L^2$ Norm

- $\Omega(\boldsymbol{\theta}) = (1/2)\|\boldsymbol{\theta}\|_2^2$, i.e., sum of squares of network's weights
- Since $\boldsymbol{\theta} = \boldsymbol{w}$, this becomes

$$\tilde{\mathcal{J}}(\boldsymbol{w};\mathcal{X},\boldsymbol{y}) = (\alpha/2)\boldsymbol{w}^\top\boldsymbol{w} + \mathcal{J}(\boldsymbol{w};\mathcal{X},\boldsymbol{y})$$

- As weights deviate from zero, activation functions become more nonlinear, which is higher risk of overfitting



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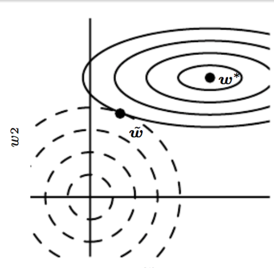
# Regularization
## Parameter Norm Penalties: $L^2$ Norm




- $\boldsymbol{w}^*$ is optimal for $\mathcal{J}$, $\boldsymbol{0}$ optimal for regularizer
- $\mathcal{J}$ less sensitive to $w_1$, so $\tilde{\boldsymbol{w}}$ (optimal for $\tilde{\mathcal{J}}$) closer to $w_2$ axis than $w_1$



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# Regularization
## Parameter Norm Penalties: $L^1$ Norm

- $\Omega(\boldsymbol{\theta}) = \|\boldsymbol{\theta}\|_1$, i.e., sum of absolute values of network's weights

$$\tilde{\mathcal{J}}(\boldsymbol{w};\mathcal{X},\boldsymbol{y}) = \alpha\|\boldsymbol{w}\|_1 + \mathcal{J}(\boldsymbol{w};\mathcal{X},\boldsymbol{y})$$

- As with $L^2$ regularization, penalizes large weights
- Unlike $L^2$ regularization, can drive some weights to zero
  - **Sparse** solution
  - Sometimes used in **feature selection** (e.g., LASSO algorithm)

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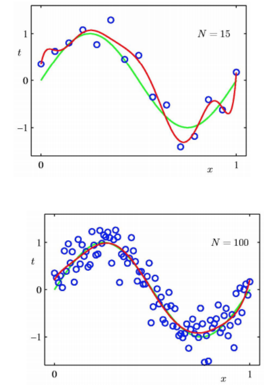
# Regularization
## Data Augmentation

- If $\mathcal{H}$ powerful and $\mathcal{X}$ small, then learner can choose some $h \in \mathcal{H}$ that fits idiosyncrasies or noise in data
- Deep ANNs would like to have at least thousands or tens of thousands of data points
- In classification of high-dimensional data (e.g., image classification), expect the classifier to tolerate transformations and noise
  - $\Rightarrow$ Can artificially enlarge data set by duplicating existing instances and applying transformations
    - Translating, rotating, scaling
    - Don't change the class, e.g., "b" vs "d" or "6" vs "9"
    - **Don't let duplicates lie in both training and testing sets**
  - $\Rightarrow$ Can also apply noise injection to input or hidden layers



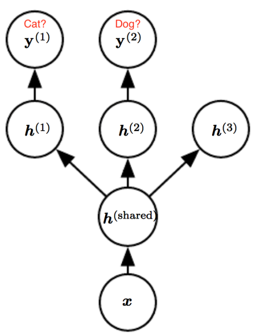
# Regularization
## Data Augmentation






# Regularization
## Multitask Learning

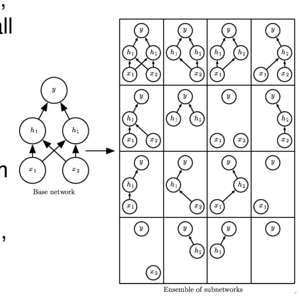
- If multiple tasks share **generic parameters**, initially process inputs via shared nodes, then do final processing via task-specific nodes
- Backpropagation works as before with multiple output nodes
- Serves as a regularizer since parameter tuning of shared nodes is based on backpropagated error from multiple tasks






# Regularization
## Dropout

- Imagine if, for a network, we could average over all networks with each subset of nodes deleted
- Analogous to **bagging**, where we average over ANNs trained on random samples of $\mathcal{X}$
- In each training iteration, sample a random bit vector $\boldsymbol{\mu}$, which determines which nodes are used (e.g., $\mathrm{P}(\mu_i = 1) = 0.8$ for input unit, 0.5 for hidden unit)
- When training done, re-scale weights by $\mathrm{P}(\mu_i = 1)$






# Regularization
## Other Approaches

- **Parameter Tying:** If two learners are learning the same task but different scenarios (distributions, etc.), can tie their parameters together
  - If $\boldsymbol{w}^{(A)}$ are weights for task $A$ and $\boldsymbol{w}^{(B)}$ are weights for task $B$, then can use regularization term $\Omega(\boldsymbol{w}^{(A)}, \boldsymbol{w}^{(B)}) = \|\boldsymbol{w}^{(A)} - \boldsymbol{w}^{(B)}\|_2^2$
  - E.g., $A$ is supervised and $B$ is unsupervised
- **Parameter Sharing:** When detecting objects in an image, the same recognizer should apply invariant to translation
  - Train a single detector (subnetwork) for an object (e.g., cat) by training full network on multiple images with translated cats, where the cat detector subnets share parameters (single copy, used multiple times)



# Regularization
## Other Approaches (cont'd)

- **Sparse Representations:** Instead of penalizing large weights, penalize large outputs of hidden nodes:

$$\tilde{\mathcal{J}}(\boldsymbol{\theta}; \mathcal{X}, \boldsymbol{y}) = \mathcal{J}(\boldsymbol{\theta}; \mathcal{X}, \boldsymbol{y}) + \alpha\, \Omega(\boldsymbol{h}) \ ,$$

where $\boldsymbol{h}$ is the vector of hidden unit outputs

## Estimating Generalization Performance

### Setting Goals

- Before setting up an experiment, need to understand exactly what the goal is
  - Estimate the generalization performance of a hypothesis
  - Tuning a learning algorithm's parameters
  - Comparing two learning algorithms on a specific task
  - Etc.
- Will never be able to answer the question with 100% certainty
  - Due to variances in training set selection, test set selection, etc.
  - Will choose an **estimator** for the quantity in question, determine the probability distribution of the estimator, and bound the probability that the estimator is way off
  - Estimator needs to work regardless of distribution of training/testing data





## Estimating Generalization Performance

### Setting Goals

- Need to note that, in addition to statistical variations, what we determine is limited to the application that we are studying
  - E.g., if $\text{ANN}_1$ better than $\text{ANN}_2$ on speech recognition, that means nothing about video analysis
- In planning experiments, need to ensure that training data not used for evaluation
  - I.e., **don't test on the training set!**
  - Will bias the performance estimator
  - If using data augmentation, **don't let duplicates lie in both training and testing sets**
  - Also holds for **validation set** used for early stopping, tuning parameters, etc.
    - Validation set serves as part of training set, but not used for model building





## Confidence Intervals

Let $error_{\mathcal{D}}(h)$ be 0-1 loss of hypothesis $h$ on instances drawn according to distribution $\mathcal{D}$. If

- Test set $\mathcal{V}$ contains $N$ examples, drawn independently of $h$ and each other
- $N \geq 30$

Then with approximately 95% probability, $error_{\mathcal{D}}(h)$ lies in

$$error_{\mathcal{V}}(h) \pm 1.96\sqrt{\frac{error_{\mathcal{V}}(h)(1 - error_{\mathcal{V}}(h))}{N}}$$

E.g. hypothesis $h$ misclassifies 12 of the 40 examples in test set $\mathcal{V}$:

$$error_{\mathcal{V}}(h) = \frac{12}{40} = 0.30$$

Then with approx. 95% confidence, $error_{\mathcal{D}}(h) \in [0.158, 0.442]$





## Confidence Intervals (cont'd)

Let $error_{\mathcal{D}}(h)$ be 0-1 loss of $h$ on instances drawn according to distribution $\mathcal{D}$. If

- Test set $\mathcal{V}$ contains $N$ examples, drawn independently of $h$ and each other
- $N \geq 30$

Then with approximately c% probability, $error_{\mathcal{D}}(h)$ lies in

$$error_{\mathcal{V}}(h) \pm z_c\sqrt{\frac{error_{\mathcal{V}}(h)(1 - error_{\mathcal{V}}(h))}{N}}$$

| $N\%$: | 50% | 68% | 80% | 90% | 95% | 98% | 99% |
|---|---|---|---|---|---|---|---|
| $z_c$: | 0.67 | 1.00 | 1.28 | 1.64 | 1.96 | 2.33 | 2.58 |

**Why?**

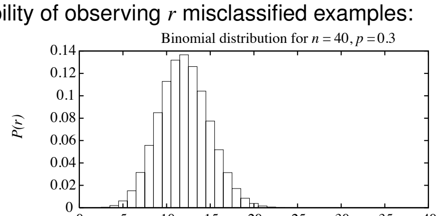




## $error_{\mathcal{V}}(h)$ is a Random Variable

Repeatedly run the experiment, each with different randomly drawn $\mathcal{V}$ (each of size $N$)

Probability of observing $r$ misclassified examples:




$$P(r) = \binom{N}{r} error_{\mathcal{D}}(h)^r (1 - error_{\mathcal{D}}(h))^{N-r}$$

I.e., let $error_{\mathcal{D}}(h)$ be probability of heads in biased coin, then $P(r) =$ prob. of getting $r$ heads out of $N$ flips





## Binomial Probability Distribution

$$P(r) = \binom{N}{r} p^r (1-p)^{N-r} = \frac{N!}{r!(N-r)!} p^r (1-p)^{N-r}$$

Probability $P(r)$ of $r$ heads in $N$ coin flips, if $p = \Pr(heads)$

- Expected, or mean value of $X$, $\mathbb{E}[X]$ (= # heads on $N$ flips = # mistakes on $N$ test exs), is

$$\mathbb{E}[X] \equiv \sum_{i=0}^{N} iP(i) = Np = N \cdot error_{\mathcal{D}}(h)$$

- Variance of $X$ is

$$Var(X) \equiv \mathbb{E}[(X - \mathbb{E}[X])^2] = Np(1-p)$$

- Standard deviation of $X$, $\sigma_X$, is

$$\sigma_X \equiv \sqrt{\mathbb{E}[(X - \mathbb{E}[X])^2]} = \sqrt{Np(1-p)}$$

## Approximate Binomial Dist. with Normal

$error_{\mathcal{V}}(h) = r/N$ is binomially distributed, with

- mean $\mu_{error_{\mathcal{V}}(h)} = error_{\mathcal{D}}(h)$ (i.e., unbiased est.)
- standard deviation $\sigma_{error_{\mathcal{V}}(h)}$

$$\sigma_{error_{\mathcal{V}}(h)} = \sqrt{\frac{error_{\mathcal{D}}(h)(1 - error_{\mathcal{D}}(h))}{N}}$$

(increasing $N$ decreases variance)

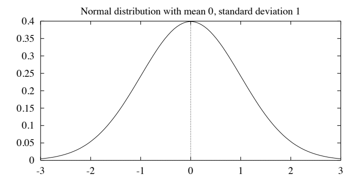
Want to compute confidence interval = interval centered at $error_{\mathcal{D}}(h)$ containing $c$% of the weight under the distribution

Approximate binomial by **normal** (Gaussian) dist:
- mean $\mu_{error_{\mathcal{V}}(h)} = error_{\mathcal{D}}(h)$
- standard deviation $\sigma_{error_{\mathcal{V}}(h)}$

$$\sigma_{error_{\mathcal{V}}(h)} \approx \sqrt{\frac{error_{\mathcal{V}}(h)(1 - error_{\mathcal{V}}(h))}{N}}$$



## Normal Probability Distribution

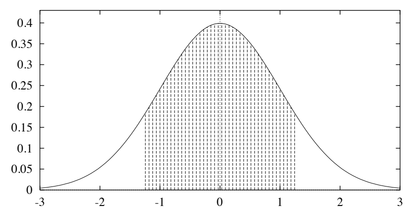



$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2\right)$$

- The probability that $X$ will fall into the interval $(a, b)$ is given by $\int_a^b p(x)\,dx$
- Expected, or mean value of $X$, $\mathbb{E}[X]$, is $\mathbb{E}[X] = \mu$
- Variance is $Var(X) = \sigma^2$, standard deviation is $\sigma_X = \sigma$



## Normal Probability Distribution (cont'd)



80% of area (probability) lies in $\mu \pm 1.28\sigma$

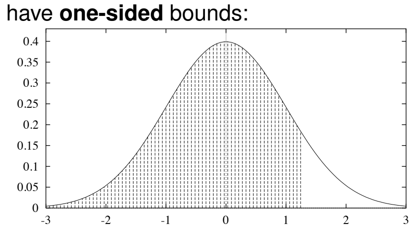
$c$% of area (probability) lies in $\mu \pm z_c\,\sigma$

| $c$%: | 50% | 68% | 80% | 90% | 95% | 98% | 99% |
|---|---|---|---|---|---|---|---|
| $z_c$: | 0.67 | 1.00 | 1.28 | 1.64 | 1.96 | 2.33 | 2.58 |



## Normal Probability Distribution (cont'd)

Can also have **one-sided** bounds:



$c$% of area lies $< \mu + z'_c\,\sigma$ or $> \mu - z'_c\sigma$, where $z'_c = z_{100-(100-c)/2}$

| $c$%: | 50% | 68% | 80% | 90% | 95% | 98% | 99% |
|---|---|---|---|---|---|---|---|
| $z'_c$: | 0.0 | 0.47 | 0.84 | 1.28 | 1.64 | 2.05 | 2.33 |



## Confidence Intervals Revisited

If $\mathcal{V}$ contains $N \geq 30$ examples, indep. of $h$ and each other

Then with approximately 95% probability, $error_{\mathcal{V}}(h)$ lies in

$$error_{\mathcal{D}}(h) \pm 1.96\sqrt{\frac{error_{\mathcal{D}}(h)(1 - error_{\mathcal{D}}(h))}{N}}$$

Equivalently, $error_{\mathcal{D}}(h)$ lies in

$$error_{\mathcal{V}}(h) \pm 1.96\sqrt{\frac{error_{\mathcal{D}}(h)(1 - error_{\mathcal{D}}(h))}{N}}$$

which is approximately

$$error_{\mathcal{V}}(h) \pm 1.96\sqrt{\frac{error_{\mathcal{V}}(h)(1 - error_{\mathcal{V}}(h))}{N}}$$

(**One-sided bounds yield upper or lower error bounds**)



## Central Limit Theorem

How can we justify approximation?

Consider set of iid random variables $Y_1, \ldots, Y_N$, all from **arbitrary** probability distribution with mean $\mu$ and finite variance $\sigma^2$. Define sample mean $\bar{Y} \equiv (1/N)\sum_{i=1}^{n} Y_i$

$\bar{Y}$ is itself a random variable, i.e., result of an experiment (e.g., $error_S(h) = r/N$)

**Central Limit Theorem**: As $N \to \infty$, the distribution governing $\bar{Y}$ approaches normal distribution with mean $\mu$ and variance $\sigma^2/N$

Thus the distribution of $error_S(h)$ is approximately normal for large $N$, and its expected value is $error_{\mathcal{D}}(h)$

(**Rule of thumb:** $N \geq 30$ when estimator's distribution is binomial; might need to be larger for other distributions)

## Calculating Confidence Intervals

1. Pick parameter to estimate: $error_{\mathcal{D}}(h)$ (0-1 loss on distribution $\mathcal{D}$)
2. Choose an estimator: $error_{\mathcal{V}}(h)$ (0-1 loss on independent test set $\mathcal{V}$)
3. Determine probability distribution that governs estimator: $error_{\mathcal{V}}(h)$ governed by binomial distribution, approximated by normal when $N \geq 30$
4. Find interval $(L, U)$ such that $c$% of probability mass falls in the interval
   - Could have $L = -\infty$ or $U = \infty$
   - Use table of $z_c$ or $z'_c$ values (if distribution normal)





## Comparing Learning Algorithms

- What if we want to compare two learning algorithms $L^1$ and $L^2$ (e.g., two ANN architectures, two regularizers, etc.) on a specific application?
- Insufficient to simply compare error rates on a single test set
- Use **$K$-fold cross validation** and a **paired $t$ test**





## $K$-Fold Cross Validation

1. Partition data set $\mathcal{X}$ into $K$ equal-sized subsets $\mathcal{X}_1, \mathcal{X}_2, \ldots, \mathcal{X}_K$, where $|\mathcal{X}_i| \geq 30$
2. For $i$ from 1 to $K$, do (Use $\mathcal{X}_i$ for testing, and rest for training)
   1. $\mathcal{V}_i = \mathcal{X}_i$
   2. $\mathcal{T}_i = \mathcal{X} \setminus \mathcal{X}_i$
   3. Train learning algorithm $L^1$ on $\mathcal{T}_i$ to get $h_i^1$
   4. Train learning algorithm $L^2$ on $\mathcal{T}_i$ to get $h_i^2$
   5. Let $p_i^j$ be error of $h_i^j$ on test set $\mathcal{V}_i$
   6. $p_i = p_i^1 - p_i^2$
3. Error difference estimate $p = (1/K) \sum_i^K p_i$





## $K$-Fold Cross Validation (cont'd)

- Now estimate confidence that true expected error difference $< 0$
- ⇒ Confidence that $L^1$ is better than $L^2$ on learning task
- Use **one-sided test**, with confidence derived from **student's $t$ distribution** with $K - 1$ **degrees of freedom**
- With approximately $c$% probability, true difference of expected error between $L^1$ and $L^2$ is at most

$$p + t_{c,K-1}\, s_p$$

where

$$s_p \equiv \sqrt{\frac{1}{K(K-1)} \sum_{i=1}^{K} (p_i - p)^2}$$





## Student's $t$ Distribution (One-Sided Test)

| df | 0.600 | 0.700 | 0.800 | 0.900 | 0.950 | 0.975 | 0.990 | 0.995 |
|---|---|---|---|---|---|---|---|---|
| 1 | 0.325 | 0.727 | 1.376 | 3.078 | 6.314 | 12.706 | 31.821 | 63.657 |
| 2 | 0.289 | 0.617 | 1.061 | 1.886 | 2.920 | 4.303 | 6.965 | 9.925 |
| 3 | 0.277 | 0.584 | 0.978 | 1.638 | 2.353 | 3.182 | 4.541 | 5.841 |
| 4 | 0.271 | 0.569 | 0.941 | 1.533 | 2.132 | 2.776 | 3.747 | 4.604 |
| 5 | 0.267 | 0.559 | 0.920 | 1.476 | 2.015 | 2.571 | 3.365 | 4.032 |
| 6 | 0.265 | 0.553 | 0.906 | 1.440 | 1.943 | 2.447 | 3.143 | 3.707 |
| 7 | 0.263 | 0.549 | 0.896 | 1.415 | 1.895 | 2.365 | 2.998 | 3.499 |
| 8 | 0.262 | 0.546 | 0.889 | 1.397 | 1.860 | 2.306 | 2.896 | 3.355 |
| 9 | 0.261 | 0.543 | 0.883 | 1.383 | 1.833 | 2.262 | 2.821 | 3.250 |
| 10 | 0.260 | 0.542 | 0.879 | 1.372 | 1.812 | 2.228 | 2.764 | 3.169 |
| 11 | 0.260 | 0.540 | 0.876 | 1.363 | 1.796 | 2.201 | 2.718 | 3.106 |
| 12 | 0.259 | 0.539 | 0.873 | 1.356 | 1.782 | 2.179 | 2.681 | 3.055 |
| 13 | 0.259 | 0.538 | 0.870 | 1.350 | 1.771 | 2.160 | 2.650 | 3.012 |

If $p + t_{c,K-1}\, s_p < 0$ our assertion that $L^1$ has less error than $L^2$ is supported with confidence $c$

So if $K$-fold CV used, compute $p$, look up $t_{c,K-1}$ and check if $p < -t_{c,K-1}\, s_p$

**One-sided test; says nothing about $L^2$ over $L^1$**





## Caveat

- Say you want to show that learning algorithm $L^1$ performs better than algorithms $L^2, L^3, L^4, L^5$
- If you use $K$-fold CV to show superior performance of $L^1$ over each of $L^2, \ldots, L^5$ at 95% confidence, there's a 5% chance each one is wrong
- ⇒ There's an over 18.5% chance that at least one is wrong
- ⇒ Our overall confidence is only just over 81%
- Need to account for this, or use more appropriate test

## More Specific Performance Measures

- So far, we've looked at a single error rate to compare hypotheses/learning algorithms/etc.
- This may not tell the whole story:
  - 1000 test examples: 20 positive, 980 negative
  - $h^1$ gets 2/20 pos correct, 965/980 neg correct, for accuracy of $(2+965)/(20+980) = 0.967$
  - Pretty impressive, except that always predicting negative yields accuracy $= 0.980$
  - Would we rather have $h^2$, which gets 19/20 pos correct and 930/980 neg, for accuracy $= 0.949$?
  - Depends on how important the positives are, i.e., frequency in practice and/or cost (e.g., cancer diagnosis)

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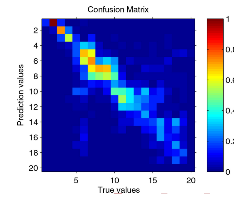
## Confusion Matrices

Break down error into type: true positive, etc.

| | Predicted Class | | |
|---|---|---|---|
| **True Class** | Positive | Negative | Total |
| Positive | $tp$ : true positive | $fn$ : false negative | $p$ |
| Negative | $fp$ : false positive | $tn$ : true negative | $n$ |
| Total | $p'$ | $n'$ | $N$ |

- Generalizes to multiple classes
- Allows one to quickly assess which classes are missed the most, and into what other class

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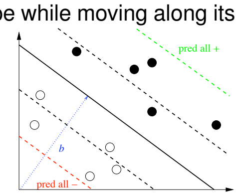
## ROC Curves

- Consider classification via ANN + linear threshold unit
- Normally threshold $f(\boldsymbol{x}; \boldsymbol{w}, b)$ at 0, but what if we changed it?
- Keeping $\boldsymbol{w}$ fixed while changing threshold = fixing hyperplane's slope while moving along its normal vector




- Get a **set** of classifiers, one per labeling of test set
- Similar situation with any classifier with confidence value, e.g., probability-based

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## ROC Curves
### Plotting $tp$ versus $fp$

- Consider the "always –" hyp. What is $fp$? What is $tp$? What about the "always +" hyp?
- In between the extremes, we plot TP versus FP by sorting the test examples by the confidence values

| Ex | Confidence | label | Ex | Confidence | label |
|---|---|---|---|---|---|
| $x_1$ | 169.752 | + | $x_6$ | $-12.640$ | – |
| $x_2$ | 109.200 | + | $x_7$ | $-29.124$ | – |
| $x_3$ | 19.210 | – | $x_8$ | $-83.222$ | – |
| $x_4$ | 1.905 | + | $x_9$ | $-91.554$ | + |
| $x_5$ | $-2.75$ | + | $x_{10}$ | $-128.212$ | – |

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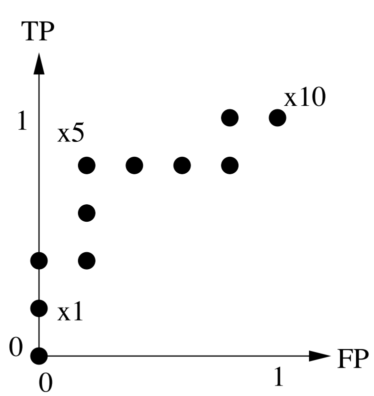
## ROC Curves
### Plotting $tp$ versus $fp$ (cont'd)

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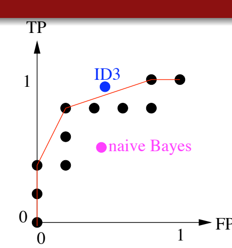
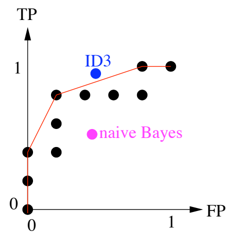
## ROC Curves
### Convex Hull




- The **convex hull** of the ROC curve yields a collection of classifiers, each optimal under different conditions
  - If FP cost = FN cost, then draw a line with slope $|N|/|P|$ at $(0, 1)$ and drag it towards convex hull until you touch it; that's your **operating point**
  - Can use as a classifier any part of the hull since can randomly select between two classifiers

## ROC Curves
### Convex Hull






- Can also compare curves against "single-point" classifiers when no curves
  - In plot, ID3 better than our SVM iff negatives scarce; nB never better



## ROC Curves
### Miscellany

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- What is the worst possible ROC curve?
- One metric for measuring a curve's goodness: **area under curve** (AUC):

$$\frac{\sum_{x_+ \in P} \sum_{x_- \in N} I(h(x_+) > h(x_-))}{|P|\,|N|}$$

  i.e., rank all examples by confidence in "+" prediction, count the number of times a positively-labeled example (from $P$) is ranked above a negatively-labeled one (from $N$), then normalize
  - What is the best value?
  - Distribution approximately normal if $|P|, |N| > 10$, so can find confidence intervals
  - Catching on as a better scalar measure of performance than error rate
- Possible (though tricky) with multi-class problems



## Precision-Recall Curves

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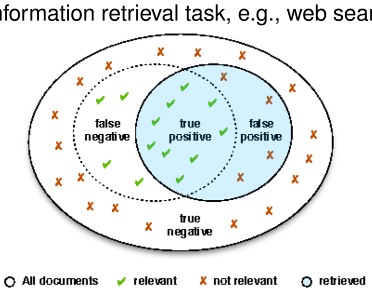
Consider information retrieval task, e.g., web search




**precision** $= tp/p' =$ fraction of retrieved that are positive

**recall** $= tp/p =$ fraction of positives retrieved



## Precision-Recall Curves (cont'd)

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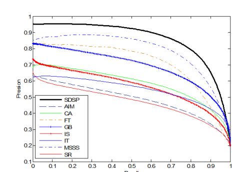
- As with ROC, vary threshold to trade precision and recall
- Can compare curves based on containment
- More suitable than ROC for large numbers of negatives




- Use $F_\beta$-measure to combine at a specific point, where $\beta$ weights precision vs recall:

$$F_\beta \equiv (1+\beta^2)\frac{precision \cdot recall}{(\beta^2 \cdot precision) + recall}$$