Regularization and Performance Evaluation

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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
- Summary

Machine Learning Problems

- **Supervised Learning:** Algorithm given labeled **training data** and infers 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 algorithm
- In supervised learning, we often use **loss function** (or error function) J for this task
- Given instance $\boldsymbol{x}$ with true label y, if the learner's prediction on $\boldsymbol{x}$ is $\hat{y}$, then

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

is the loss on that instance

Measuring Performance

Examples of Loss Functions

- **0-1 Loss:** $J(y, \hat{y}) = 1$ if $y \neq \hat{y}$, 0 otherwise
- **Square Loss:** $J(y, \hat{y}) = (y - \hat{y})^2$
- **Cross-Entropy:** $J(y, \hat{y}) = -y \ln \hat{y} - (1 - y) \ln (1 - \hat{y})$ (y and $\hat{y}$ are considered probabilities of a ‘1’ label)
  - Generalizes to k classes ($i^* =$ correct class):

$$J(\boldsymbol{y}, \hat{\boldsymbol{y}}) = -\sum_{i=1}^{k} y_i \ln \hat{y}_i = -\ln \hat{y}_{i^*}$$

  ($\boldsymbol{y}$ is one-hot vector; $\hat{y}_i$ is predicted prob. of class i)
- **Hinge Loss:** $J(y, \hat{y}) = \max(0, 1 - y\,\hat{y})$ (used sometimes for large margin classifiers like SVMs)

All non-negative

Measuring Performance

Training Loss

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

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

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**:

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

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

Measuring Performance

Expected vs Training Loss

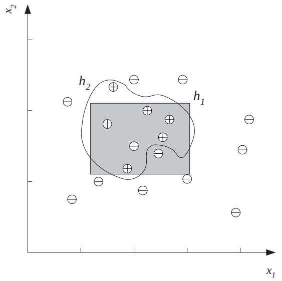
- Sufficiently sophisticated learners (decision trees, multi-layer ANNs) can often achieve arbitrarily small (or zero) loss on a training set
- A hypothesis (e.g., ANN with specific parameters) h **overfits** the training data $\mathcal{X}$ if there is an alternative hypothesis h' such that

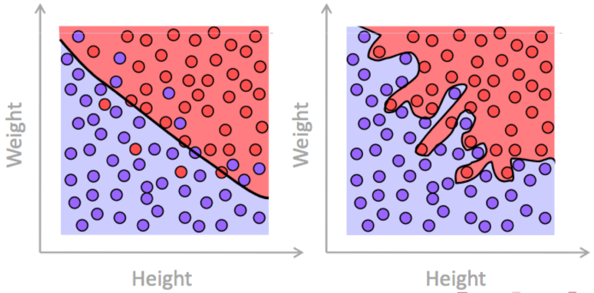
$$error_{\mathcal{X}}(h) < error_{\mathcal{X}}(h')$$

and

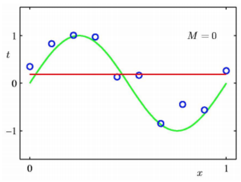
$$error_{\mathcal{D}}(h) > error_{\mathcal{D}}(h')$$

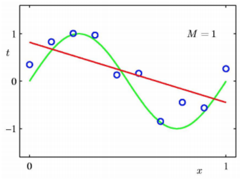
Measuring Performance
Overfitting



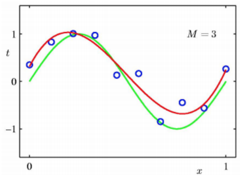


Measuring Performance
Overfitting

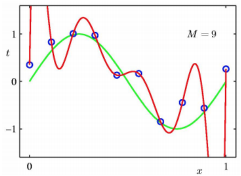




← Poor representations of $\sin(2\pi x)$



← Best Fit to $\sin(2\pi x)$



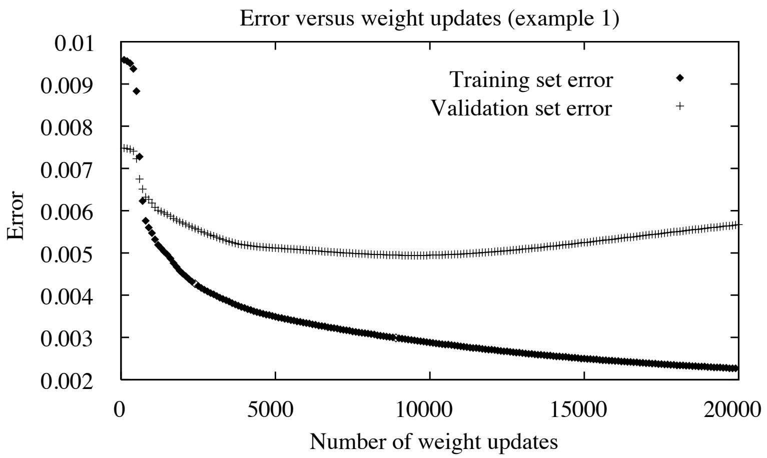
Over Fit Poor representation of $\sin(2\pi x)$

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

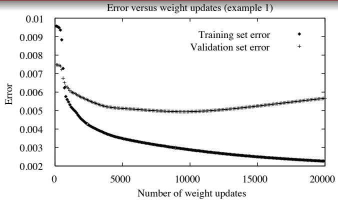
Regularization
Causes of Overfitting: Overtraining

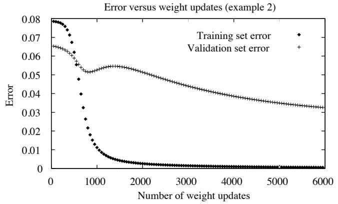


Nebraska Lincoln

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

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

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

- $\alpha \in [0, \infty)$ weights loss J against penalty Ω

Regularization

Parameter Norm Penalties: L^2 Norm

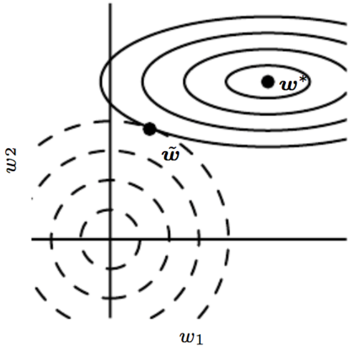
- $\Omega(\boldsymbol{\theta}) = (1/2)\|\boldsymbol{\theta}\|_2^2$, i.e., sum of squares of network's weights
- Since $\boldsymbol{\theta} = \boldsymbol{w}$, this becomes

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

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

Regularization

Parameter Norm Penalties: L^2 Norm



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

Regularization

Parameter Norm Penalties: L^1 Norm

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

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

- 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)

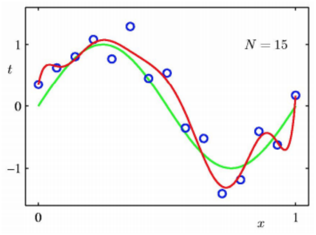
Regularization
Data Augmentation

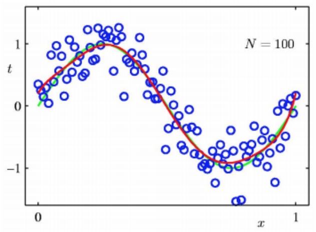
- If $\mathcal{H}$ powerful and $\mathcal{X}$ small, then learner can choose some $h \in \mathcal{H}$ that fits idiosyncrasies or noise in data
- Deep ANNs would like to have at least thousands or tens of thousands of data points
- In classification of high-dimensional data (e.g., image classification), want learned 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

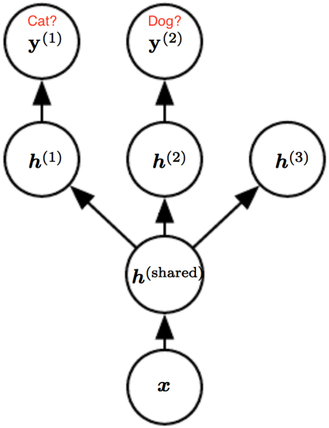
Regularization
Data Augmentation





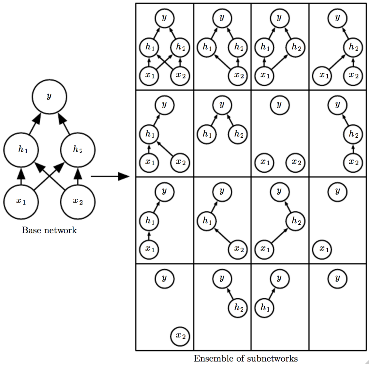
Regularization
Multitask Learning

- 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 μ, which determines which nodes are used (e.g., P$(\mu_i = 1) = 0.8$ for input unit, 0.5 for hidden unit)

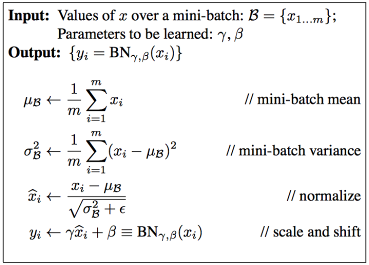


- When training done, re-scale by P$(\mu_i = 1)$

Regularization

Batch Normalization (Ioffe and Szegedy 2015)

- Addresses **internal covariate shift**, where changing parameters of layer i changes distribution of inputs to layer $i+1$
- Related to z-**normalization**, where one subtracts sample mean and scales with standard deviation



```
Input: Values of $x$ over a mini-batch: $\mathcal{B} = \{x_{1\ldots m}\}$;
       Parameters to be learned: $\gamma, \beta$
Output: $\{y_i = \mathrm{BN}_{\gamma,\beta}(x_i)\}$

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

Algorithm 1: Batch Normalizing Transform, applied to activation x over a mini-batch.

- γ, β learnable parameters
- Allows use of higher learning rates, possibly speeding convergence
- In some cases, reduces/eliminates need for dropout

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:

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

  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 generalization performance of a hypothesis
  - Tuning hyperparameters
  - 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 ANN$_1$ better than 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

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

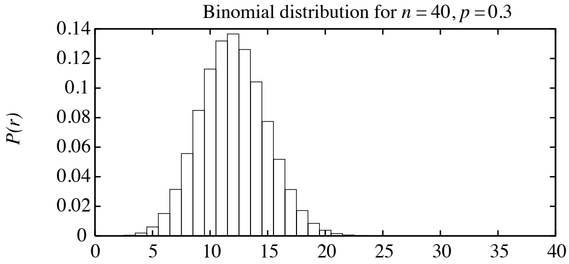
$N\%$:	50%	68%	80%	90%	95%	98%	99%
z_c:	0.67	1.00	1.28	1.64	1.96	2.33	2.58

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:



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

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, σ_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 $\mu_{error_{\mathcal{V}}(h)} = error_{\mathcal{D}}(h)$ (**unbiased estimator**)
- 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)

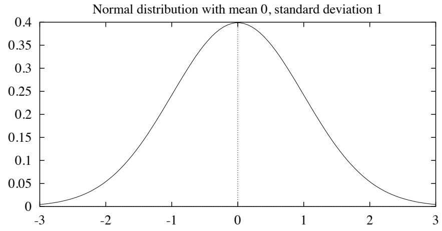
Want to compute confidence interval = interval centered at $error_{\mathcal{D}}(h)$ containing c% of the weight under the distribution

Approximate binomial by **normal** (Gaussian) dist:

- mean $\mu_{error_{\mathcal{V}}(h)} = error_{\mathcal{D}}(h)$
- standard deviation $\sigma_{error_{\mathcal{V}}(h)}$

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

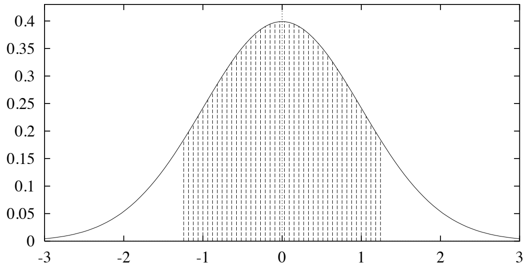
Normal Probability Distribution



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

- 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)



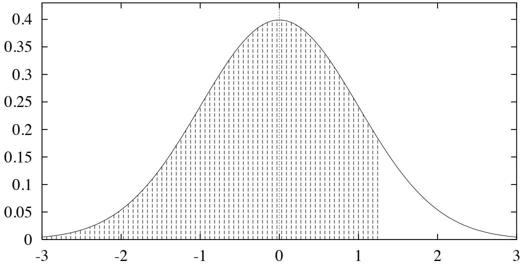
80% of area (probability) lies in $\mu \pm 1.28\sigma$

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 μ and finite variance σ^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., $error_{\mathcal{V}}(h) = r/N$)

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

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

(**Guideline:** $N \geq 30$ 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**
- Also helpful for **hyperparameter tuning**

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

$\Rightarrow$ Confidence that L^1 is better than L^2 on learning task

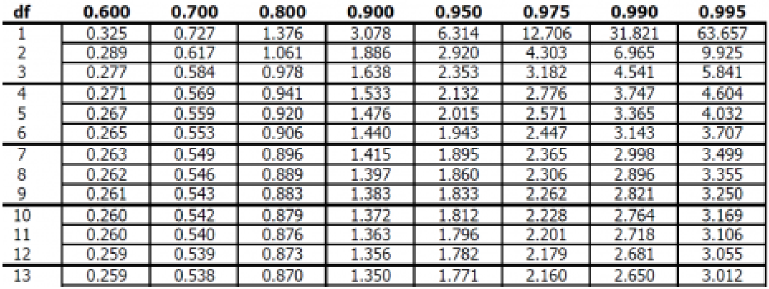
- Use **one-sided test**, with confidence derived from **student's t distribution** with $K-1$ **degrees of freedom**
- With approximately c% probability, true difference of expected error between L^1 and L^2 is at most

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

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

$\Rightarrow$ There's an over 18.5% chance that at least one is wrong

$\Rightarrow$ Our overall confidence is only just over 81%

- Need to account for this, or use more appropriate test

More Specific Performance Measures

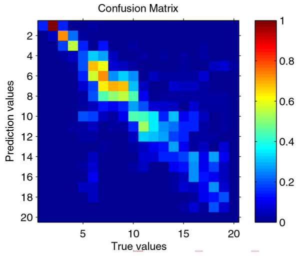
- So far, we've looked at a single error rate to compare hypotheses/learning algorithms/etc.
- This may not tell the whole story:
  - 1000 test examples: 20 positive, 980 negative
  - h^1 gets 2/20 pos correct, 965/980 neg correct, for accuracy of $(2+965)/(20+980) = 0.967$
  - Pretty impressive, except 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)

Confusion Matrices

Break down error into type: true positive, etc.

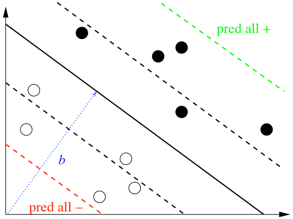
	Predicted Class		
True Class	Positive	Negative	Total
Positive	tp : true positive	fn : false negative	p
Negative	fp : false positive	tn : true negative	n
Total	p'	n'	N

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



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

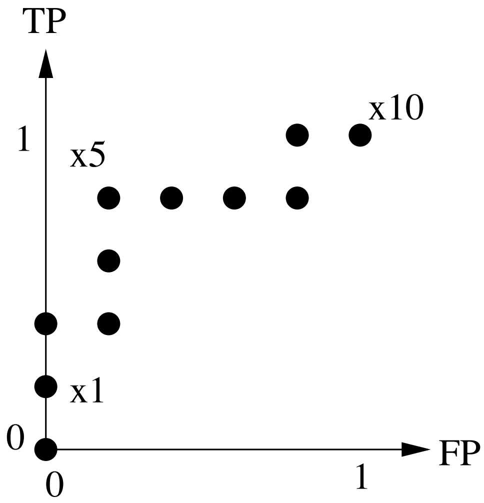
ROC Curves
Plotting *tp* versus *fp*

- 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

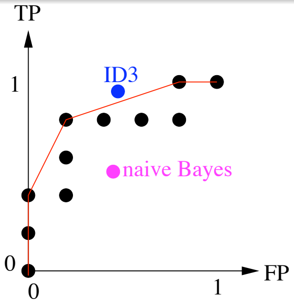
Ex	Confidence	label	Ex	Confidence	label
x_1	169.752	$+$	x_6	-12.640	$-$
x_2	109.200	$+$	x_7	-29.124	$-$
x_3	19.210	$-$	x_8	-83.222	$-$
x_4	1.905	$+$	x_9	-91.554	$+$
x_5	-2.75	$+$	x_{10}	-128.212	$-$

ROC Curves

Plotting *tp* versus *fp* (cont'd)



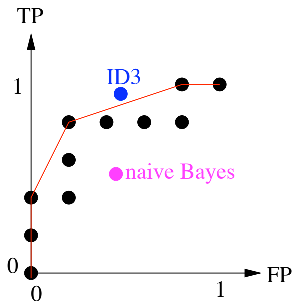
ROC Curves
Convex Hull



- 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

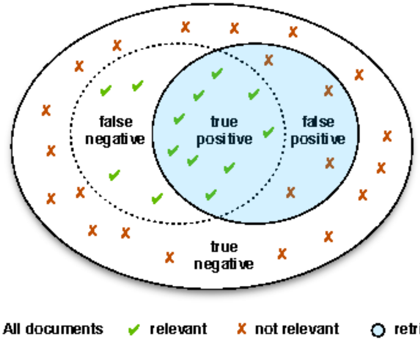
- What is the worst possible ROC curve?
- One metric for measuring a curve's goodness: **area under curve** (AUC):

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

  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

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

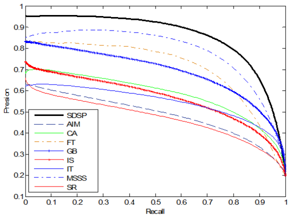


precision $= tp/p' =$ fraction of retrieved that are positive

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

Precision-Recall Curves (cont'd)

- 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_β-measure to combine at a specific point, where β weights precision vs recall:

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

Summary

- In machine learning, tend to search for a hypothesis that optimizes some **objective function**
- Often try to minimize **loss** on training set, but doing that too aggressively can cause **overfitting**
- Prevent overfitting via **regularization** (e.g., early stopping, complexity penalties, dropout, batch norm)
- Once hypothesis is trained, need to estimate its **generalization performance** by evaluating on an **independent test set**
- Statistical analyses on the test results yields **confidence intervals** and **paired t tests**
- Other ways of analyzing performance are **confusion matrices**, **ROC curves**, and **precision-recall curves**
- And remember: **Don't test on the training set!**