CHAPTER 19:

DESIGN AND ANALYSIS OF MACHINE LEARNING EXPERIMENTS

Introduction

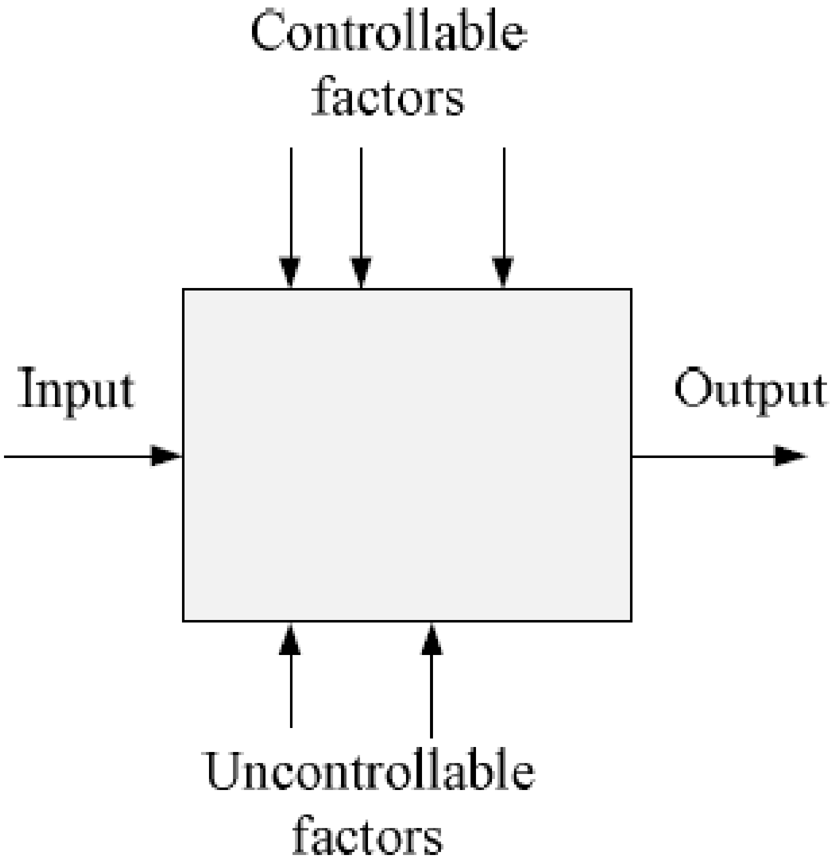
- Questions:
  - Assessment of the expected error of a learning algorithm: Is the error rate of 1-NN less than 2%?
  - Comparing the expected errors of two algorithms: Is k-NN more accurate than MLP ?
- Training/validation/test sets
- Resampling methods: K-fold cross-validation

Algorithm Preference

- Criteria (Application-dependent):
  - Misclassification error, or risk (loss functions)
  - Training time/space complexity
  - Testing time/space complexity
  - Interpretability
  - Easy programmability
- Cost-sensitive learning

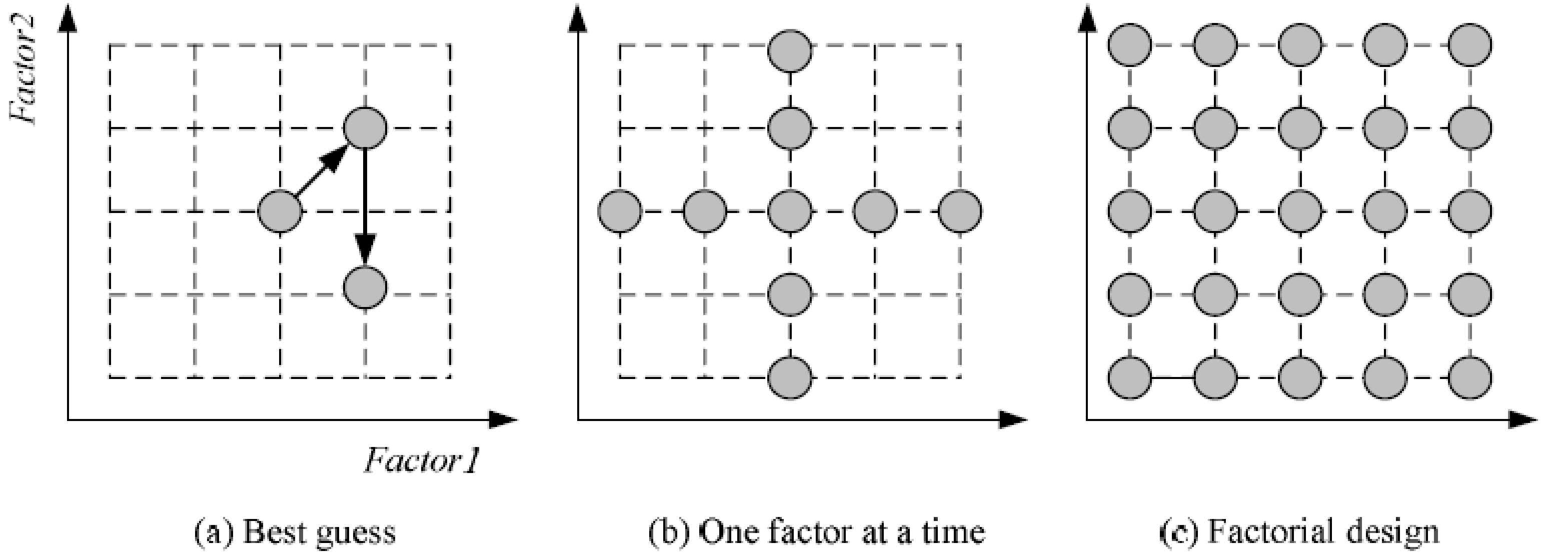
Factors and Response

- Response function based on output to be maximized
- Depends on controllable factors
- Uncontrollable factors introduce randomness
- Find the configuration of controllable factors that maximizes response and *minimally affected by uncontrollable factors*



Strategies of Experimentation

How to search the factor space?



Response surface design for approximating and maximizing the response function in terms of the controllable factors

Guidelines for ML experiments

A. Aim of the study
B. Selection of the response variable
C. Choice of factors and levels
D. Choice of experimental design
E. Performing the experiment
F. Statistical Analysis of the Data
G. Conclusions and Recommendations

Resampling and *K*-Fold Cross-Validation

- The need for multiple training/validation sets

  $\{X_i, V_i\}_i$: Training/validation sets of fold i
- K-fold cross-validation: Divide X into k, $X_i, i=1,\ldots,K$

$$
\begin{aligned}
V_1 &= X_1 & T_1 &= X_2 \cup X_3 \cup \cdots \cup X_K \\
V_2 &= X_2 & T_2 &= X_1 \cup X_3 \cup \cdots \cup X_K \\
&\vdots \\
V_K &= X_K & T_K &= X_1 \cup X_2 \cup \cdots \cup X_{K-1}
\end{aligned}
$$

- T_i share K-2 parts

5×2 Cross-Validation

- 5 times 2 fold cross-validation (Dietterich, 1998)

$$
\boxed{\begin{array}{ll} T_1 = X_1^{(1)} & V_1 = X_1^{(2)} \\ T_2 = X_1^{(2)} & V_2 = X_1^{(1)} \end{array}}
$$

$$
\boxed{\begin{array}{ll} T_3 = X_2^{(1)} & V_3 = X_2^{(2)} \\ T_4 = X_2^{(2)} & V_4 = X_2^{(1)} \end{array}}
$$

$$\vdots$$

$$
\boxed{\begin{array}{ll} T_9 = X_5^{(1)} & V_9 = X_5^{(2)} \\ T_{10} = X_5^{(2)} & V_{10} = X_5^{(1)} \end{array}}
$$

Bootstrapping

- Draw instances from a dataset *with replacement*
- Prob that we do not pick an instance after N draws

$$\left(1-\frac{1}{N}\right)^{N} \approx e^{-1} = 0.368$$

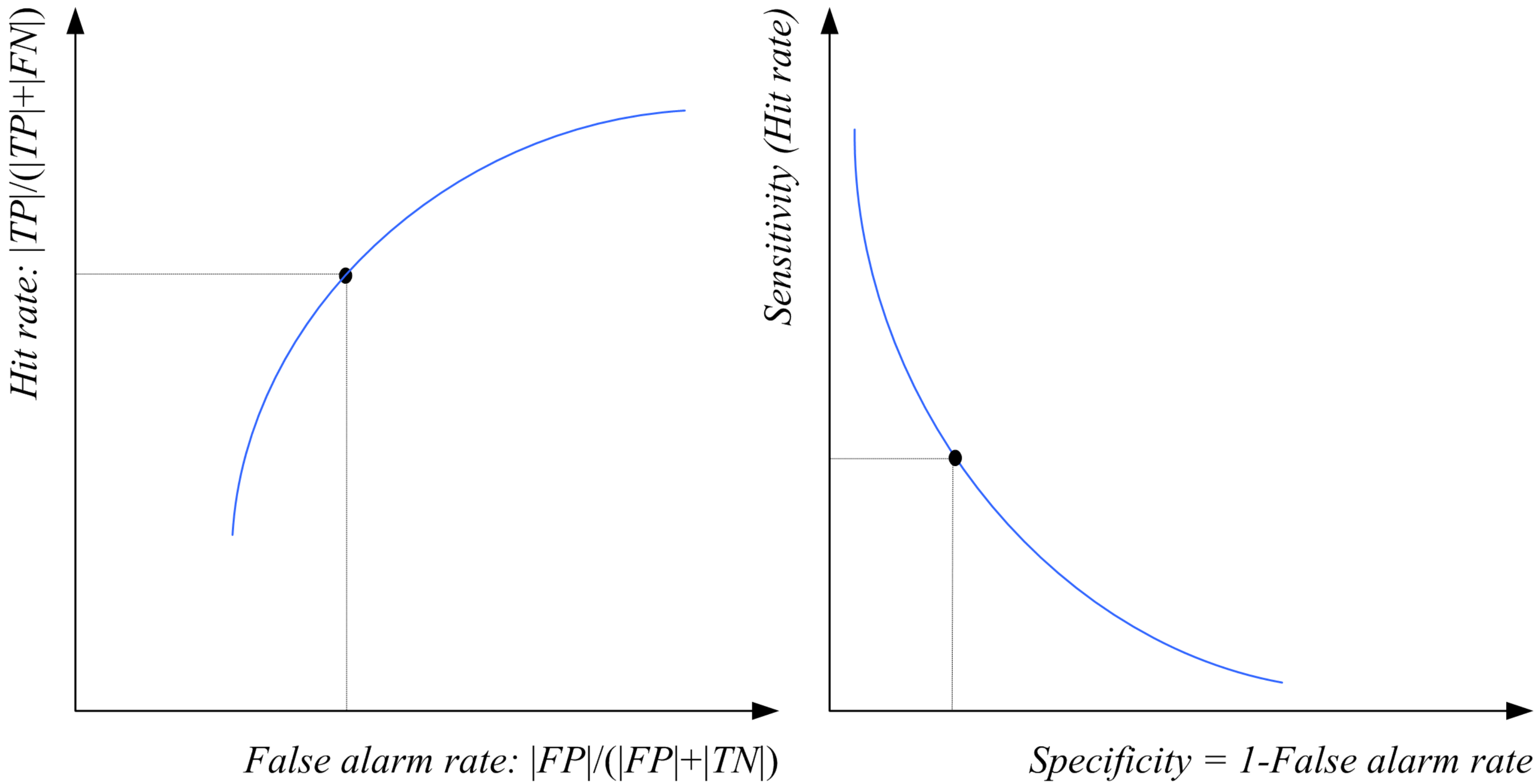
that is, only 36.8% is new!

Performance Measures

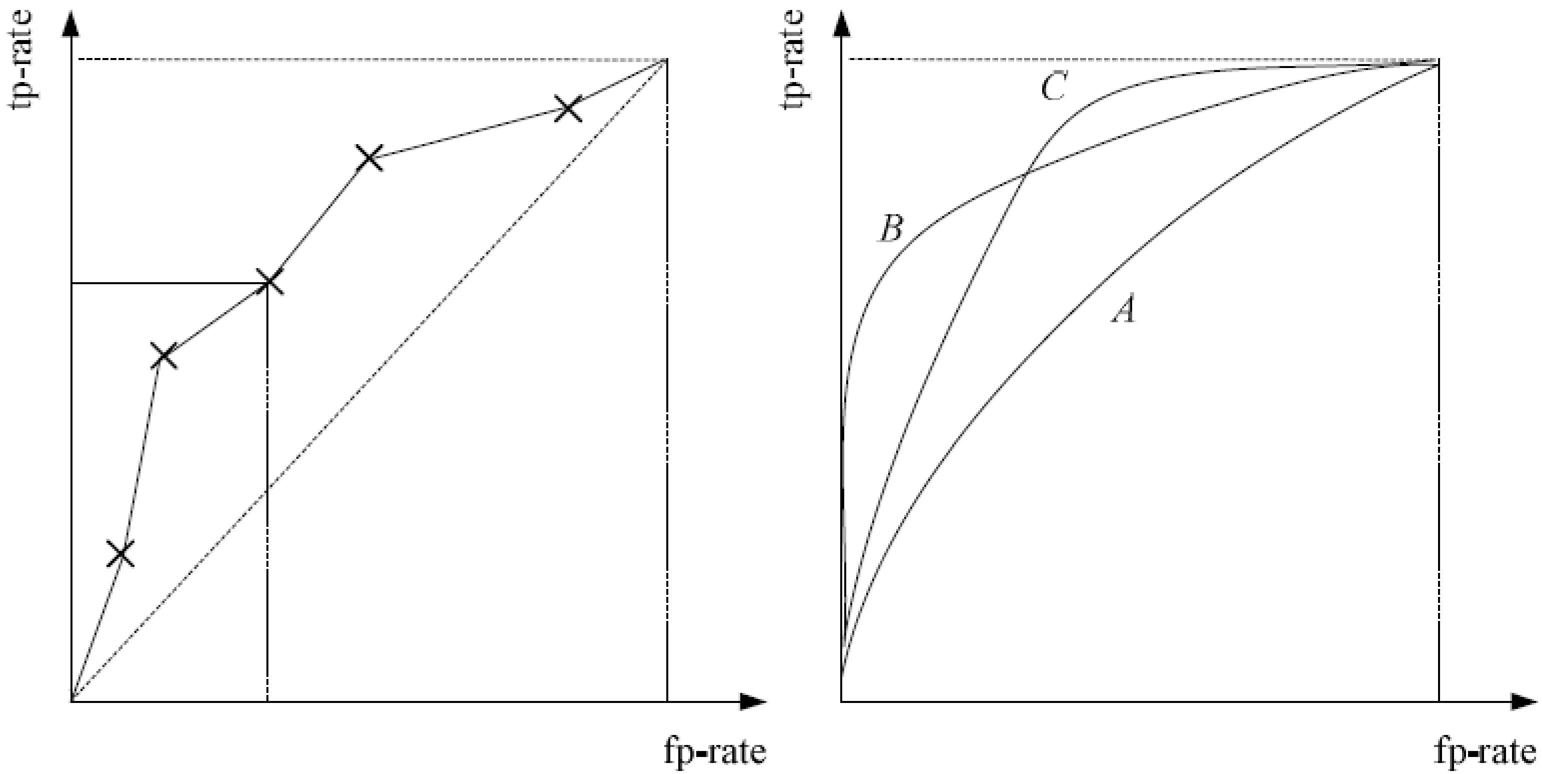
	Predicted class	
True Class	Yes	No
Yes	TP: True Positive	FN: False Negative
No	FP: False Positive	TN: True Negative

- Error rate = # of errors / # of instances = (FN+FP) / N
- Recall = # of found positives / # of positives
  = TP / (TP+FN) = sensitivity = hit rate
- Precision = # of found positives / # of found
  = TP / (TP+FP)
- Specificity = TN / (TN+FP)
- False alarm rate = FP / (FP+TN) = 1 - Specificity

ROC Curve



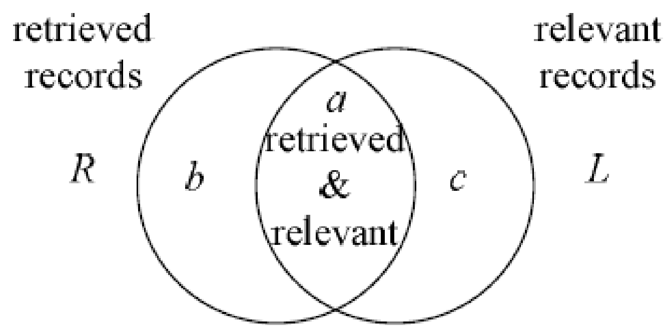
Hit rate: |TP|/(|TP|+|FN|)
False alarm rate: |FP|/(|FP|+|TN|)
Sensitivity (Hit rate)
Specificity = 1-False alarm rate



(a) Example ROC curve

(b) Different ROC curves for different classifiers

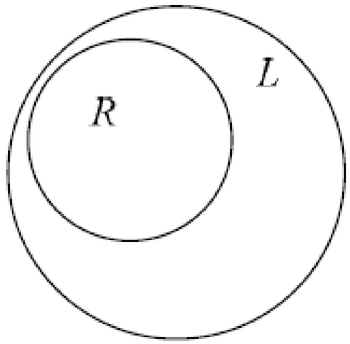
Precision and Recall



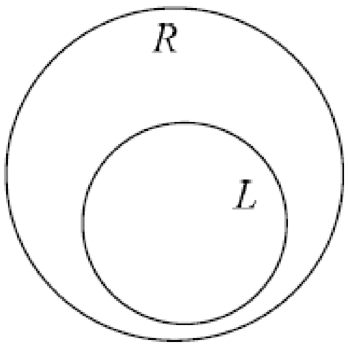
$$\text{Precision: } \frac{a}{a+b}$$

$$\text{Recall: } \frac{a}{a+c}$$

(a) Precision and recall



(b) Precision = 1



(c) Recall = 1

Interval Estimation

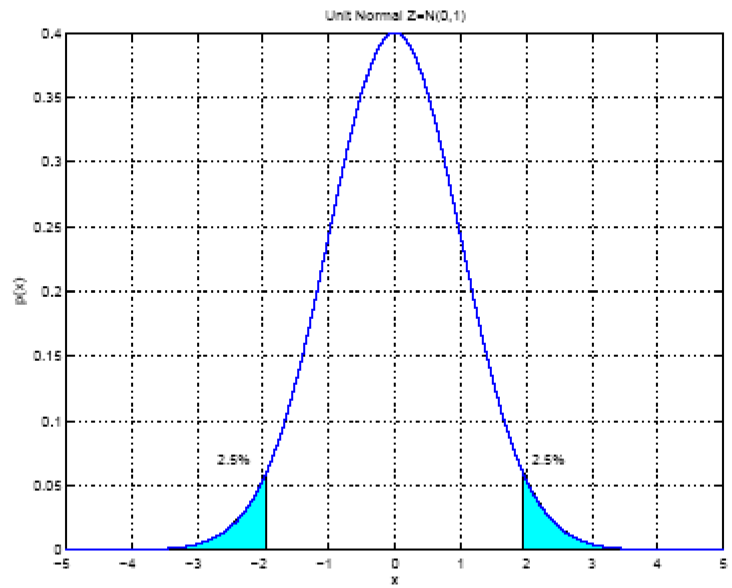
- $X = \{ x^t \}_t$ where $x^t \sim N(\mu, \sigma^2)$
- $m \sim N(\mu, \sigma^2/N)$

$$\sqrt{N}\frac{(m-\mu)}{\sigma} \sim Z$$

$$P\left\{-1.96 < \sqrt{N}\frac{(m-\mu)}{\sigma} < 1.96\right\} = 0.95$$

$$P\left\{m - 1.96\frac{\sigma}{\sqrt{N}} < \mu < m + 1.96\frac{\sigma}{\sqrt{N}}\right\} = 0.95$$

$$P\left\{m - z_{\alpha/2}\frac{\sigma}{\sqrt{N}} < \mu < m + z_{\alpha/2}\frac{\sigma}{\sqrt{N}}\right\} = 1 - \alpha$$



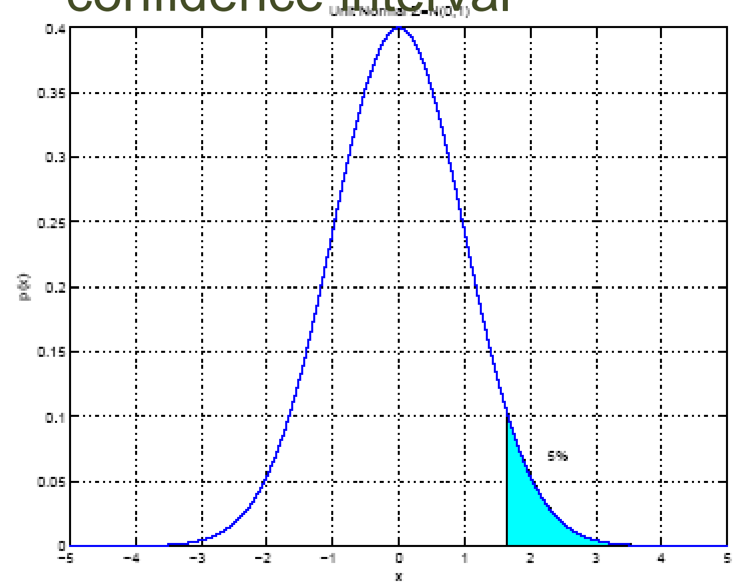
$100(1-\alpha)$ percent confidence interval

$$P\left\{\sqrt{N}\frac{(m-\mu)}{\sigma}<1.64\right\}=0.95$$

$$P\left\{m-1.64\frac{\sigma}{\sqrt{N}}<\mu\right\}=0.95$$

$$P\left\{m-z_{\alpha}\frac{\sigma}{\sqrt{N}}<\mu\right\}=1-\alpha$$

100(1- α) percent one-sided
confidence interval



When σ^2 is not known:

$$S^2=\sum_t\left(x^t-m\right)^2/(N-1) \qquad \frac{\sqrt{N}(m-\mu)}{S}\sim t_{N-1}$$

$$P\left\{m-t_{\alpha/2,N-1}\frac{S}{\sqrt{N}}<\mu<m+t_{\alpha/2,N-1}\frac{S}{\sqrt{N}}\right\}=1-\alpha$$

Hypothesis Testing

- Reject a null hypothesis if not supported by the sample with enough confidence

  $X = \{ x^t \}_t$ where $x^t \sim N(\mu, \sigma^2)$

  $H_0: \mu = \mu_0$ vs. $H_1: \mu \neq \mu_0$

  Accept H_0 with level of significance α if μ_0 is in the $100(1-\alpha)$ confidence interval

$$\frac{\sqrt{N}(m-\mu_0)}{\sigma} \in \left(-z_{\alpha/2}, z_{\alpha/2}\right)$$

  Two-sided test

	Decision	
Truth	Accept	Reject
True	Correct	Type I error
False	Type II error	Correct (Power)

- One-sided test: H_0: $\mu \leq \mu_0$ vs. H_1: $\mu > \mu_0$

  Accept if $$\frac{\sqrt{N}(m-\mu_0)}{\sigma} \in (-\infty, z_\alpha)$$

- Variance unknown: Use t, instead of z

  Accept H_0: $\mu = \mu_0$ if

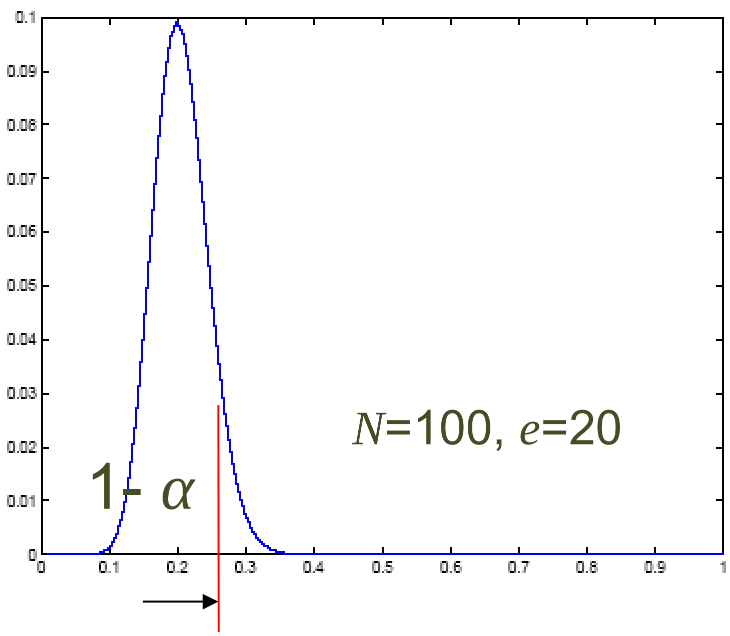
$$\frac{\sqrt{N}(m-\mu_0)}{S} \in \left(-t_{\alpha/2,N-1}, t_{\alpha/2,N-1}\right)$$

Assessing Error: $H_0: p \leq p_0$ vs. $H_1: p > p_0$

- Single training/validation set: Binomial Test

  If error prob is p_0, prob that there are e errors or less in N validation trials is

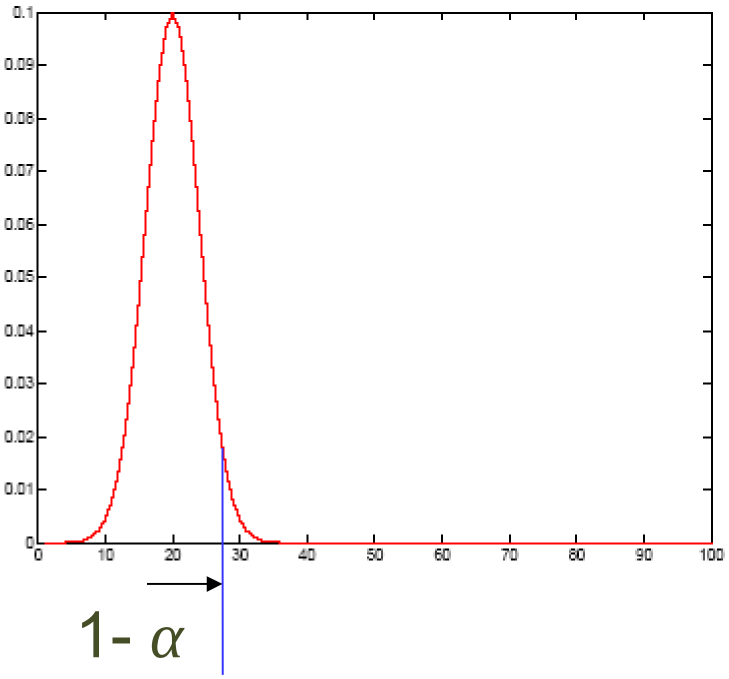
$$P\{X \leq e\} = \sum_{j=1}^{e} \binom{N}{j} p_0^{\,j} \left(1 - p_0^{\,j}\right)^{N-j}$$



Accept if this prob is less than 1- α

Normal Approximation to the Binomial

- Number of errors X is approx N with mean Np_0 and var $Np_0(1\text{-}p_0)$



$$\frac{X - Np_0}{\sqrt{Np_0(1-p_0)}} \sim Z$$

Accept if this prob for $X = e$ is less than $z_{1\text{-}\alpha}$

Paired t Test

- Multiple training/validation sets
- x^t_i = 1 if instance t misclassified on fold i
- Error rate of fold i:

$$p_i = \frac{\sum_{t=1}^{N} x_i^t}{N}$$

- With m and s^2 average and var of p_i , we accept p_0 or less error if

$$\frac{\sqrt{K}\left(m - p_0\right)}{S} \sim t_{K-1}$$

is less than $t_{\alpha,K\text{-}1}$

Comparing Classifiers: $H_0: \mu_0 = \mu_1$ vs. $H_1: \mu_0 \neq \mu_1$

- Single training/validation set: McNemar's Test

e_{00}: Number of examples misclassified by both	e_{01}: Number of examples misclassified by 1 but not 2
e_{10}: Number of examples misclassified by 2 but not 1	e_{11}: Number of examples correctly classified by both

- Under H_0, we expect $e_{01} = e_{10} = (e_{01} + e_{10})/2$

$$\frac{\left(\left|e_{01} - e_{10}\right| - 1\right)^2}{e_{01} + e_{10}} \sim X_1^2$$

Accept if $< X^2_{\alpha,1}$

K-Fold CV Paired t Test

- Use K-fold cv to get K training/validation folds
- p_i^1, p_i^2: Errors of classifiers 1 and 2 on fold i

  $p_i = p_i^1 - p_i^2$: Paired difference on fold i
- The null hypothesis is whether p_i has mean 0

$H_0 : \mu = 0$ vs. $H_0 : \mu \neq 0$

$$m = \frac{\sum_{i=1}^{K} p_i}{K} \qquad s^2 = \frac{\sum_{i=1}^{K} (p_i - m)^2}{K-1}$$

$$\frac{\sqrt{K}(m-0)}{s} = \frac{\sqrt{K} \cdot m}{s} \sim t_{K-1} \text{ Accept if in } \left(-t_{\alpha/2,K-1}, t_{\alpha/2,K-1}\right)$$

5×2 cv Paired t Test

- Use 5×2 cv to get 2 folds of 5 tra/val replications (Dietterich, 1998)
- $p_i^{(j)}$: difference btw errors of 1 and 2 on fold j=1, 2 of replication i=1,...,5

$$\overline{p}_i = \left(p_i^{(1)} + p_i^{(2)}\right)/2 \qquad s_i^2 = \left(p_i^{(1)} - \overline{p}_i\right)^2 + \left(p_i^{(2)} - \overline{p}_i\right)^2$$

$$\frac{p_1^{(1)}}{\sqrt{\sum_{i=1}^{5} s_i^2 / 5}} \sim t_5$$

Two-sided test: Accept H_0: $\mu_0 = \mu_1$ if in $(-t_{\alpha/2,5}, t_{\alpha/2,5})$

One-sided test: Accept H_0: $\mu_0 \leq \mu_1$ if $< t_{\alpha,5}$

5×2 cv Paired F Test

$$\frac{\sum_{i=1}^{5}\sum_{j=1}^{2}\left(p_i^{(j)}\right)^2}{2\sum_{i=1}^{5} s_i^2} \sim F_{10,5}$$

Two-sided test: Accept H_0: $\mu_0 = \mu_1$ if $< F_{\alpha,10,5}$

Comparing L>2 Algorithms: Analysis of Variance (Anova)

$$H_0 : \mu_1 = \mu_2 = \cdots = \mu_L$$

- Errors of L algorithms on K folds

$$X_{ij} \sim \mathcal{N}\left(\mu_j, \sigma^2\right), j = 1,\ldots,L,\ i = 1,\ldots,K$$

- We construct two estimators to σ^2 .

  One is valid if H_0 is true, the other is always valid.

  We reject H_0 if the two estimators disagree.

If H_0 is true:

$$m_j = \sum_{i=1}^{K} \frac{X_{ij}}{K} \sim N \left(\mu, \sigma^2 / K\right)$$

$$m = \frac{\sum_{j=1}^{L} m_j}{L} \qquad S^2 = \frac{\sum_j \left(m_j - m\right)^2}{L-1}$$

Thus an estimator of σ^2 is $K \cdot S^2$, namely,

$$\hat{\sigma}^2 = K \sum_{j=1}^{L} \frac{\left(m_j - m\right)^2}{L-1}$$

$$\sum_j \frac{\left(m_j - m\right)^2}{\sigma^2 / K} \sim X_{L-1}^2 \quad SSb \equiv K \sum_j \left(m_j - m\right)^2$$

So when H_0 is true, we have

$$\frac{SSb}{\sigma^2} \sim X_{L-1}^2$$

Regardless of H_0 our second estimator to σ^2 is the average of group variances S_j^2 :

$$S_j^2 = \frac{\sum_{i=1}^{K} \left(X_{ij} - m_j\right)^2}{K-1} \qquad \hat{\sigma}^2 = \sum_{j=1}^{L} \frac{S_j^2}{L} = \sum_j \sum_i \frac{\left(X_{ij} - m_j\right)^2}{L\left(K-1\right)}$$

$$SSw \equiv \sum_j \sum_i \left(X_{ij} - m_j\right)^2$$

$$\left(K-1\right)\frac{S_j^2}{\sigma^2} \sim \mathrm{X}_{K-1}^2 \qquad \frac{SSw}{\sigma^2} \sim \mathrm{X}_{L(K-1)}^2$$

$$\left(\frac{SSb/\sigma^2}{L-1}\right) \Bigg/ \left(\frac{SSw/\sigma^2}{L\left(K-1\right)}\right) = \frac{SSb/\left(L-1\right)}{SSw/\left(L\left(K-1\right)\right)} \sim F_{L-1,L(K-1)}$$

$$H_0 : \mu_1 = \mu_2 = \cdots = \mu_L \text{ if } < F_{\alpha,L-1,L(K-1)}$$

ANOVA table

Source of variation	Sum of squares	Degrees of freedom	Mean square	F_0
Between groups	$SS_b \equiv K\sum_j (m_j - m)^2$	$L-1$	$MS_b = \frac{SS_b}{L-1}$	$\frac{MS_b}{MS_w}$
Within groups	$SS_w \equiv \sum_j \sum_i (X_{ij} - m_j)^2$	$L(K-1)$	$MS_w = \frac{SS_w}{L(K-1)}$	
Total	$SS_T \equiv \sum_j \sum_i (X_{ij} - m)^2$	$L \cdot K - 1$		

If ANOVA rejects, we do pairwise posthoc tests

$$H_0 : \mu_i = \mu_j \text{ vs } H_1 : \mu_i \neq \mu_j$$

$$t = \frac{m_i - m_j}{\sqrt{2}\sigma_w} \sim t_{L(K-1)}$$

Comparison over Multiple Datasets

- Comparing two algorithms:

  Sign test: Count how many times A beats B over N datasets, and check if this could have been by chance if A and B did have the same error rate

- Comparing multiple algorithms

  Kruskal-Wallis test: Calculate the average rank of all algorithms on N datasets, and check if these could have been by chance if they all had equal error

  If KW rejects, we do pairwise posthoc tests to find which ones have significant rank difference

Multivariate Tests

- Instead of testing using a single performance measure, e.g., error, use multiple measures for better discrimination, e.g., [fp-rate,fn-rate]
- Compare p-dimensional distributions
- Parametric case: Assume p-variate Gaussians

$$H_0 : \boldsymbol{\mu}_1 = \boldsymbol{\mu}_2 \text{ vs. } H_1 : \boldsymbol{\mu}_1 \neq \boldsymbol{\mu}_2$$

Multivariate Pairwise Comparison

- Paired differences $\boldsymbol{d}_i = \boldsymbol{x}_{1i} - \boldsymbol{x}_{2i}$

$$H_0 : \boldsymbol{\mu}_d = \mathbf{0} \text{ vs. } H_1 : \boldsymbol{\mu}_d \neq \mathbf{0}$$

- Hotelling's multivariate T^2 test

$$T'^2 = K\boldsymbol{m}^T\mathbf{S}^{-1}\boldsymbol{m}$$

- For p=1, reduces to paired t test

Multivariate ANOVA

- Comparsion of L>2 algorithms

$$
\begin{aligned}
H_0 &: \boldsymbol{\mu}_1 = \boldsymbol{\mu}_2 = \cdots = \boldsymbol{\mu}_L \text{ vs.} \\
H_1 &: \boldsymbol{\mu}_r \neq \boldsymbol{\mu}_s \text{ for at least one pair } r, s
\end{aligned}
$$

$$
\begin{aligned}
\mathbf{H} &= K \sum_{j=1}^{L} (\boldsymbol{m}_j - \boldsymbol{m})(\boldsymbol{m}_j - \boldsymbol{m})^T \\
\mathbf{E} &= \sum_{j=1}^{L} \sum_{i=1}^{K} (\boldsymbol{x}_{ij} - \boldsymbol{m}_j)(\boldsymbol{x}_{ij} - \boldsymbol{m}_j)^T
\end{aligned}
$$

$$
\Lambda' = \frac{|\mathbf{E}|}{|\mathbf{E} + \mathbf{H}|}
$$

is Wilks's Λ distributed with $p, L(K-1), L-1$ degrees of freedom