CS 4900/5900: Machine Learning

Feature Selection

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Feature Selection

- Datasets with thousands of features are common:
  - text documents
  - gene expression data
- Processing thousands of features during training & testing can be computationally infeasible.
- Many irrelevant features can lead to overfitting.

=> select most relevant features in order to obtain *faster*, *better* and *easier* to understand learning models.

Feature Selection: Methods

- **Wrapper method:**
  - uses a classifier to assess features or feature subsets.
- **Filter method:**
  - ranks features or feature subsets independently of the classifier.
- **Univariate method**:
  - considers one feature at a time.
- **Multivariate method:**
  - considers subsets of features together.

The Wrapper Method

Greedy Forward Selection:

- F is the set of all features.
- $S \subseteq F$ is the subset of selected features.

1. Start with no features in $S = \{\}$
2. For each feature f in $F - S$, train model with $S + \{f\}$
3. Add to S the best performing feature(s).
4. Repeat from 2 until:
   (a) performance does not improve, or
   (b) performance good enough.

The Wrapper Method

Greedy Backward Elimination:

- F is the set of all features.
- $S \subseteq F$ is the subset of selected features.

1. Start with all features in $S = F$
2. For each feature in S, train model without that feature.
3. Remove from S feature corresponding to best model.
4. Repeat from 2 until:
   (a) performance does not improve, or
   (b) performance good enough.

The Wrapper Method

- **Forward**: Greedily add features one (more) at a time.

  Efficiently Inducing Features of Conditional Random Fields"
  [McCallum, UAI'03]
- **Backward**: Greedily remove features one (more) at a time.

  Multiclass cancer diagnosis using tumor gene expression signatures"
  [Ramaswamy et al., PNAS'01]
- **Combined**: Two steps forward, one step back.

- Train multiple times ⇒ can be very time consuming!
  - Alternative: use external criteria to decide feature relevance ⇒ the Filter Method.

Recursive Feature Elimination with SVM

[Guyon et al., ML'03]

- An instance of Greedy Backward Elimination.

1. Let F = {1, 2, ..., K} be the set of features.
2. Let S = [] be the ranked set of features.
3. Repeat until F – S is empty:
   I. Train weight vector **w** using a linear SVM and F – S.
   II. Find feature f in F – S with minimum $|\mathbf{w}_f|$.
   III. Append f to S.
4. Return S.

The Filter Method

1. Rank all features using a measure of correlation with the label.
2. Select top *k* features to use in the model.

- Measures of correlation between feature X and label Y:
  - Mutual Information
  - Chi-square Statistic

    } *nominal features & label*
  - Pearson Correlation Coefficient
  - Signal-to-Noise Ratio
  - T-test

Mutual Information

- Independence:

$$P(X,Y) = P(X)P(Y)$$

- Measure of dependence:

$$MI(X,Y) = \sum_{X \in \mathcal{X}} \sum_{Y \in \mathcal{Y}} p(X,Y) \log \frac{p(X,Y)}{p(X)p(Y)}$$

$$= KL(p(X,Y) \,\|\, p(X)p(Y))$$

  - It is 0 when X and Y are independent.
  - It is maximum when X=Y.

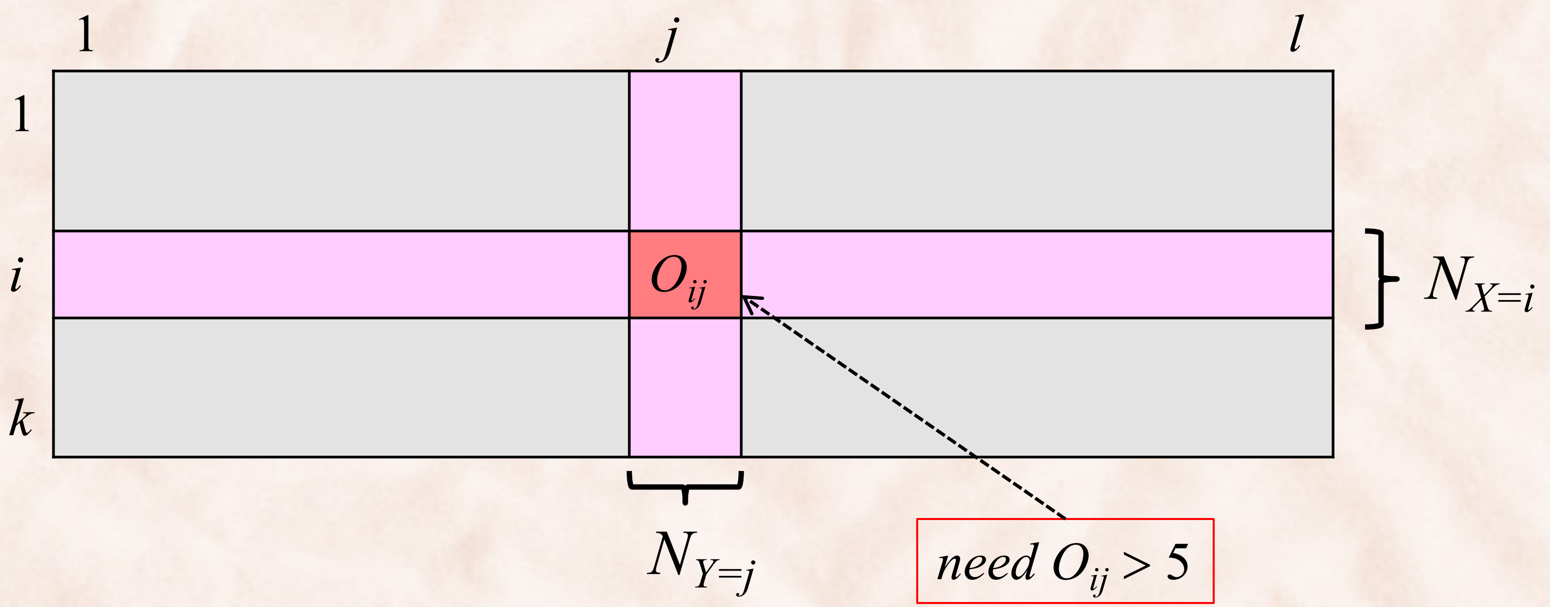
Mutual Information

- Problems:
  - Works only with nominal features & labels $\Rightarrow$ discretization.
  - Biased toward high arity features $\Rightarrow$ normalization.
  - May choose redundant features.
  - Features may become relevant in the context of other $\Rightarrow$ use conditional MI [Fleuret, JMLR '04].
- Other measures:
  - Chi square (χ^2).
  - Log-likelihood Ratio (LLR).
- Comparison between MI, χ^2, and LLR in [Dunning, CL'98]

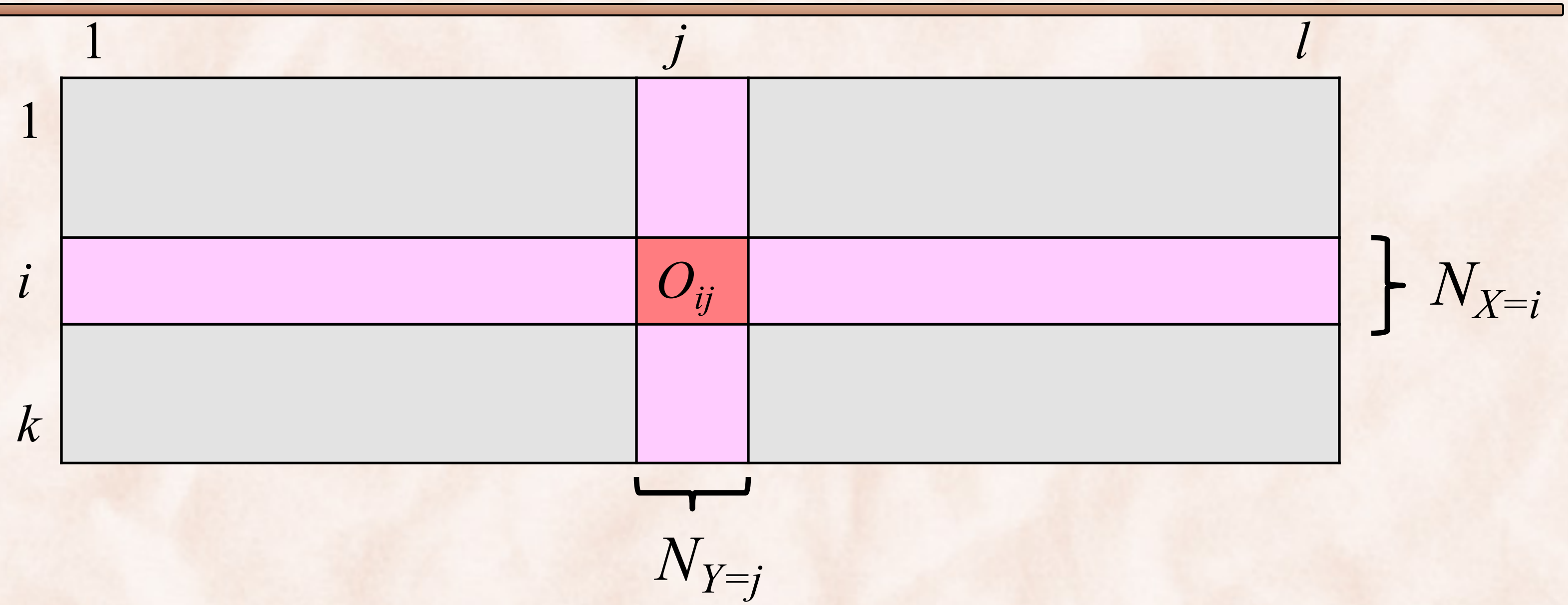
  "Accurate methods for the statistics of surprise and coincidence"

Chi Square (χ^2) Test of Independence

- N training examples (observations).
- X is a discrete feature with k possible values.
- Y is a label with l possible values.
- Create k-by-l contingency table with cells for every feature-label combination.



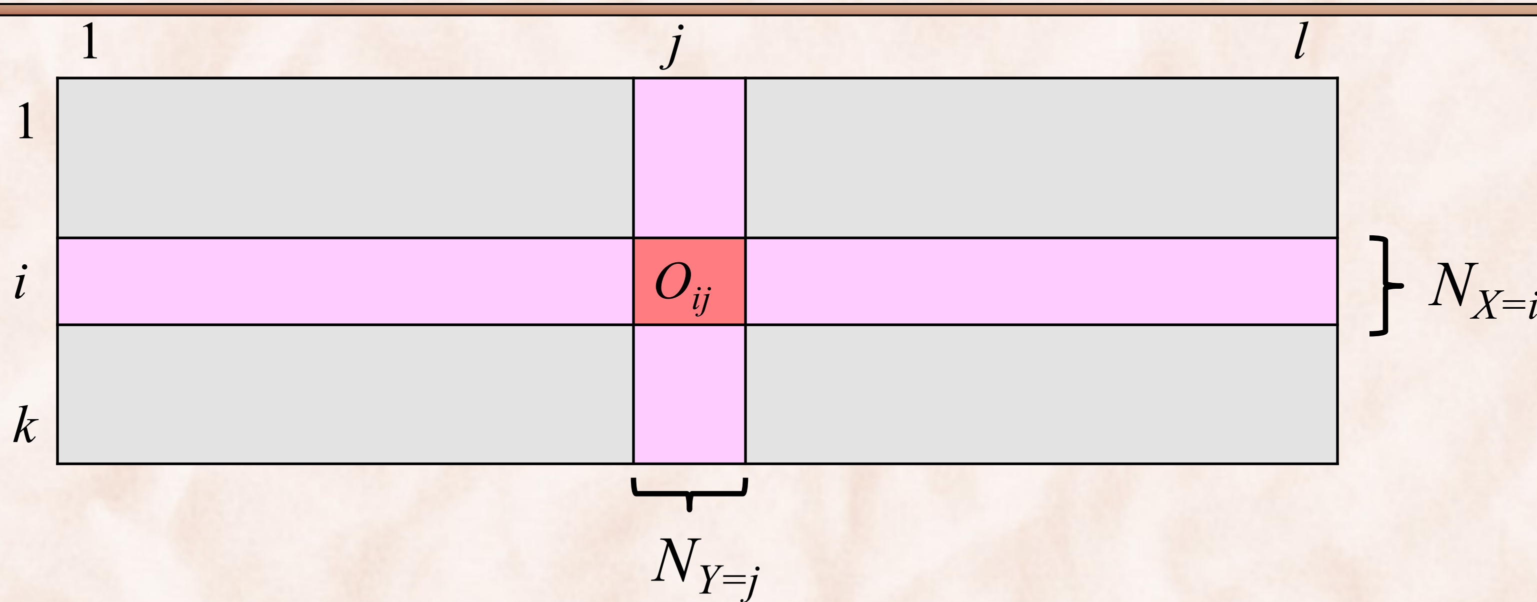
Chi Square (χ^2) Test of Independence



- O_{ij} is the observed count for $X=i$ & $Y=j$.
- E_{ij} is the expected value for $X=i$ & $Y=j$, assuming X,Y are independent.

$$E_{ij} = \frac{N_{X=i} \times N_{Y=j}}{N} = \frac{\left(\sum_{c=1}^{l} O_{ic}\right) \times \left(\sum_{r=1}^{k} O_{rj}\right)}{N}$$

Chi Square (χ^2) Test of Independence



$$X^2 = \sum_{i=1}^{k}\sum_{j=1}^{l}\frac{\left(O_{ij} - E_{ij}\right)^2}{E_{ij}}$$

asymptotically distributed as χ^2 with $(k\text{-}1)(l\text{-}1)$ degrees of freedom if X,Y are independent.

Use X^2 test value to rank features X with respect to label Y.

Pearson Correlation Coefficient

- Feature X and label Y are two random variables.
- Population correlation coefficient (*linear dependence*):

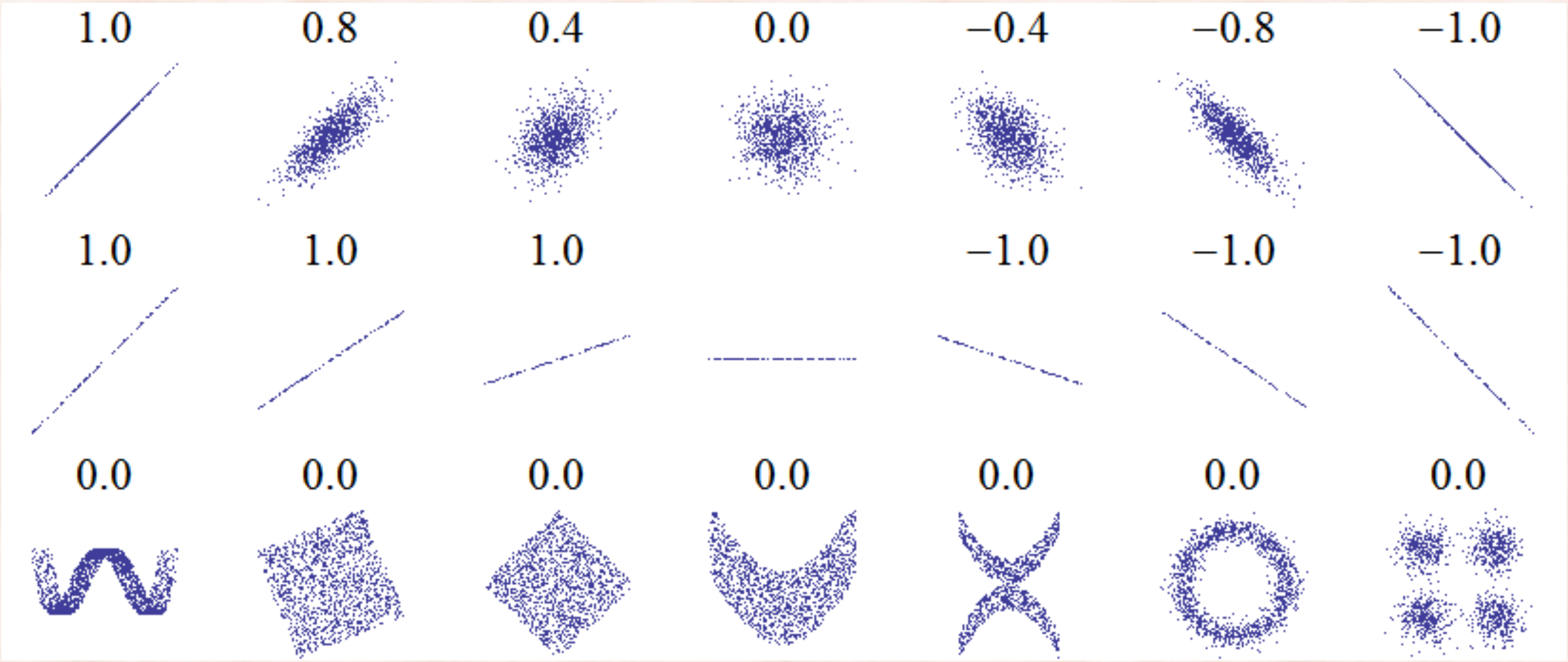
$$\rho(X,Y) = \frac{E[(X-\mu_X)(Y-\mu_Y)]}{\sigma_X \sigma_Y}$$

- Sample correlation coefficient:

$$\rho(X,Y) = \frac{\sum_{i=1}^{n}(X_i-\bar{X})(Y_i-\bar{Y})}{\sqrt{\sum_{i=1}^{n}(X_i-\bar{X})^2}\sqrt{\sum_{i=1}^{n}(Y_i-\bar{Y})^2}}$$

- Values always between [–1,+1]
  - when linearly dependent +1, –1, when independent 0.

Pearson Correlation Coefficient

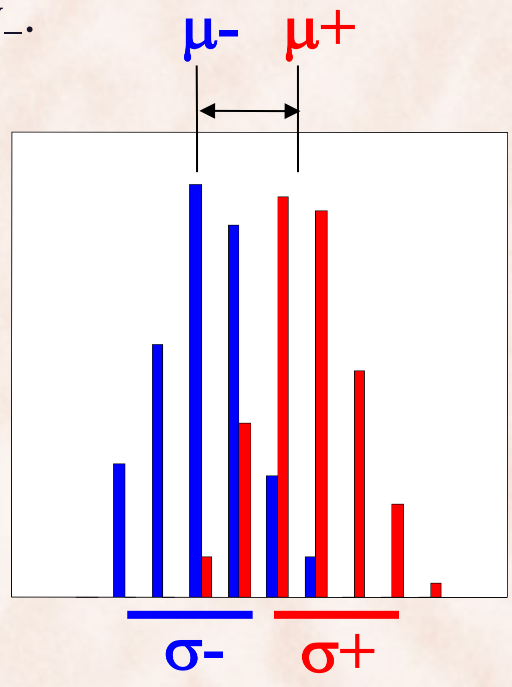


Signal-to-Noise Ratio (S2N)

- Feature X and label Y are two random variables:
  - Y is binary, $Y \in \{y_+, y_-\}$
- Let μ_+, σ_+ be the sample μ, σ of X for which $Y = y_+$.
- Let μ_-, σ_- be the sample μ, σ of X for which $Y = y_-$.

$$\mu(X,Y) = \frac{|\mu_+ - \mu_-|}{\sigma_+ + \sigma_-}$$

related to Fisher's criterion



Ranking Features with the T-test

- Let m_+ be the number of samples in class y_+.
- Let m_- be the number of sample in class y_- .

$$T(X,Y) = \frac{|\mu_+ - \mu_-|}{\sqrt{\sigma_+^2/m_+ + \sigma_-^2/m_-}}$$