Machine Learning: ITCS 4156

Naïve Bayes

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Three Parametric Approaches to Classification

- 1) Discriminant Functions: construct $f: X \rightarrow T$ that directly assigns a vector **x** to a specific class C_k .
 - Inference and decision combined into a single learning problem.
 - *Linear Discriminant*: the decision surface is a hyperplane in X:
 - Fisher 's Linear Discriminant
 - Perceptron
 - Support Vector Machines

Three Parametric Approaches to Classification

- 2) Probabilistic Discriminative Models: directly model the posterior class probabilities $p(C_k | \mathbf{x})$.
 - Inference and decision are separate.
 - Less data needed to estimate $p(C_k | \mathbf{x})$ than $p(\mathbf{x} | C_k)$.
 - Can accommodate many overlapping features.
 - Logistic Regression
 - Conditional Random Fields

Three Parametric Approaches to Classification

- 3) Probabilistic Generative Models:
 - Model class-conditional $p(\mathbf{x} | C_k)$ as well as the priors $p(C_k)$, then use Bayes's theorem to find $p(C_k | \mathbf{x})$.
 - or model $p(\mathbf{x}, C_k)$ directly, then marginalize to obtain the posterior probabilities $p(C_k | \mathbf{x})$.
 - Inference and decision are separate.
 - Can use $p(\mathbf{x})$ for outlier or novelty detection.
 - Need to model dependencies between features.
 - Naïve Bayes.
 - Hidden Markov Models.

Unbiased Learning of Generative Models

- Let $\mathbf{x} = [x_1, x_2, ..., x_M]^T$ be a feature vector with M features.
- Assume Boolean features:

 \Rightarrow distribution $p(\mathbf{x} | C_k)$ is completely specified by a table of 2^M probabilities, of which 2^M -1 are independent.

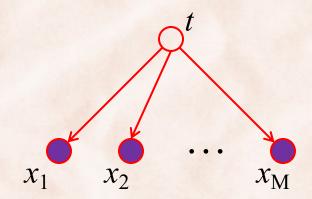
• Assume binary classification:

 \Rightarrow need to estimate 2^M -1 parameters for each class

- \Rightarrow total of 2(2^M-1) independent parameters to estimate.
- -30 features \Rightarrow more than 2 billion parameters to estimate!

The Naïve Bayes Model

• Assume features are conditionally independent given the target output:



$$\Rightarrow p(\mathbf{x} \mid C_k) = \prod_{i=1}^M p(x_i \mid C_k)$$

• Assume binary classification & features: \Rightarrow need to estimate only 2M parameters, a lot less than $2(2^{M}-1)$.

$$p(x_i = 0|C_k) + p(x_i = 1|C_k) = 1$$
, for all *i* between 1 and M.

The Naïve Bayes Model: Inference

• Posterior distribution:

$$p(C_k | \mathbf{x}) = \frac{p(\mathbf{x} | C_k) p(C_k)}{p(\mathbf{x})} \text{, where } p(\mathbf{x}) = \sum_j p(\mathbf{x} | C_j) p(C_j)$$
$$= \frac{p(C_k) \prod_j p(x_j | C_k)}{p(\mathbf{x})}$$

• Inference \equiv find C_* to minimize missclassification rate:

 $C_* = \arg \max_{C_k} p(C_k | \mathbf{x})$ $= \arg \max_{C_k} p(C_k) \prod_j p(x_j | C_k)$

The Naïve Bayes Model: Training

- Training = estimate parameters $p(x_i|C_k)$ and $p(C_k)$.
- Maximum Likelihood (ML) estimation:

$$\hat{p}(x_i = v \mid t = C_k) = \frac{\sum_{(\mathbf{x},t)\in D} \delta_{C_k}(t)}{\sum_{(\mathbf{x},t)\in D} \delta_{C_k}(t)} \qquad \text{# training examples in which } x_i = v \text{ and } t = C_k$$

$$\hat{p}(t = C_k) = \frac{\sum_{(\mathbf{x},t)\in D} \delta_{C_k}(t)}{\mid D \mid}$$

The Naïve Bayes Model: Training

- Maximum A-Posteriori (MAP) estimation:
 - assume a Dirichlet prior over the NB parameters, with equalvalued parameters.
 - assume x_i can take V values, label t can take K values.

$$\hat{p}(x_{i} = v \mid t = C_{k}) = \frac{\sum_{(\mathbf{x},t)\in D} \delta_{v}(x_{i}) \delta_{C_{k}}(t) + l}{\sum_{(\mathbf{x},t)\in D} \delta_{C_{k}}(t) + lV} \qquad \Leftrightarrow lV \text{ ``hallucinated''} examples spread evenly over all V values of } x_{i}.$$

$$\hat{p}(t = C_{k}) = \frac{\sum_{(\mathbf{x},t)\in D} \delta_{C_{k}}(t) + l}{|D| + lK}$$

Text Categorization with Naïve Bayes

- Text categorization problems:
 - Spam filtering.
 - Targeted advertisement in Gmail.
 - Classification in multiple categories on news websites.
- Representation as one feature per word:
 ⇒ each document is a very high dimensional feature vector.
- Most words are rare:
 - Zipf's law and heavy tail distribution.

 \Rightarrow feature vectors are sparse.

Text Categorization with Naïve Bayes

- Generative model of documents:
 - 1) Generate document category by sampling from $p(C_k)$.
 - 2) Generate a document as a bag of words by repeatedly sampling with replacement from a vocabulary $V = \{w_1, w_2, ..., w_{|V|}\}$ based on $p(w_i | C_k)$.
- Inference with Naïve Bayes:
 - Input :
 - Document **x** with *n* words v_1, v_2, \ldots, v_n .
 - Output:

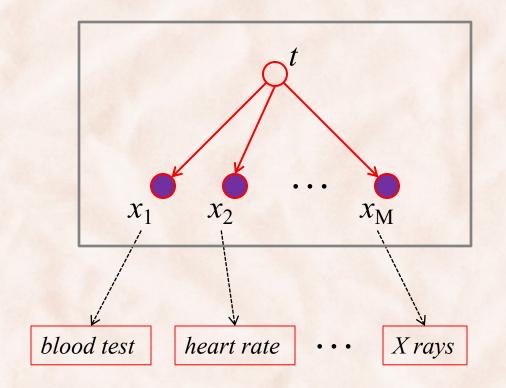
• Category
$$C_* = \arg \max_{C_k} p(C_k) \prod_{j=1}^n p(v_j | C_k)$$

Text Categorization with Naïve Bayes

- Training with Naïve Bayes:
 - Input:
 - Dataset of training documents D with vocabulary V.
 - Output:
 - Parameters $p(C_k)$ and $p(w_i | C_k)$.
 - 1. for each category C_k :
 - 2. let D_k be the subset of documents in category C_k
 - 3. set $p(C_k) = |D_k| / |D|$
 - 4. let n_k be the total number of words in D_k
 - 5. **for** each word $w_i \in V$:
 - 6. **let** n_{ki} be the number of occurrences of w_i in D_k
 - 7. **set** $p(w_i | C_k) = (n_{ki}+1) / (n_k + |V|)$

Medical Diagnosis with Naïve Bayes

• Diagnose a disease T={*Yes*, *No*}, using information from various medical tests.



$$p(\mathbf{x} \mid C_k) = \prod_{i=1}^M p(x_i \mid C_k)$$

Medical tests may result in continuous values \Rightarrow need Naïve Bayes to work with *continuous features*.

Naïve Bayes with Continuous Features

- Assume $p(x_i | C_k)$ are Gaussian distributions $N(\mu_{ik}, \sigma_{ik})$.
- Training: use ML or MAP criteria to estimate μ_{ik}, σ_{ik} :

$$\hat{\mu}_{ik} = \frac{\sum_{(\mathbf{x},t)\in D} x_i \delta_{C_k}(t)}{\sum_{(\mathbf{x},t)\in D} \delta_{C_k}(t)} \qquad \hat{\sigma}_{ik}^2 = \frac{\sum_{(\mathbf{x},t)\in D} (x_i - \hat{\mu}_{ik})^2 \delta_{C_k}(t)}{\sum_{(\mathbf{x},t)\in D} \delta_{C_k}(t)}$$

• Inference:

$$C_* = \arg \max_{C_k} p(C_k \mid \mathbf{x}) = \arg \max_{C_k} p(C_k) \prod_i p(x_i \mid C_k)$$

Numerical Issues

- Multiplying lots of probabilities may results in underflow:
 especially when many attributes (e.g. text categorization).
- Compute everything in *log space*:

$$p(\mathbf{x} | C_k) = \prod_{i=1}^M p(x_i | C_k) \iff \ln k$$

$$\ln p(\mathbf{x} \,|\, C_k) = \sum_{i=1}^M \ln p(x_i \,|\, C_k)$$

 $C_* = \arg \max_{C_k} p(C_k \mid \mathbf{x}) \iff C_* = \arg \max_{C_k} \ln p(C_k \mid \mathbf{x})$

 $= \arg \max_{C_k} \left\{ \ln p(C_k) + \ln p(\mathbf{x} \mid C_k) \right\}$

Naïve Bayes

- Often has good performance, despite strong independence assumptions:
 - quite competitive with other classification methods on UCI datasets.
- It does not produce accurate probability estimates when independence assumptions are violated:
 - the estimates are still useful for finding max-probability class.
- Does not focus on completely fitting the data ⇒ resilient to noise.



Probabilistic Generative Models: Binary Classification (K = 2)

• Model class-conditional $p(\mathbf{x} | C_1)$, $p(\mathbf{x} | C_2)$ as well as the priors $p(C_1)$, $p(C_2)$, then use Bayes's theorem to find $p(C_1 | \mathbf{x})$, $p(C_2 | \mathbf{x})$:

$$p(C_1 | \mathbf{x}) = \frac{p(\mathbf{x} | C_1) p(C_1)}{p(\mathbf{x} | C_1) p(C_1) + p(\mathbf{x} | C_2) p(C_2)}$$

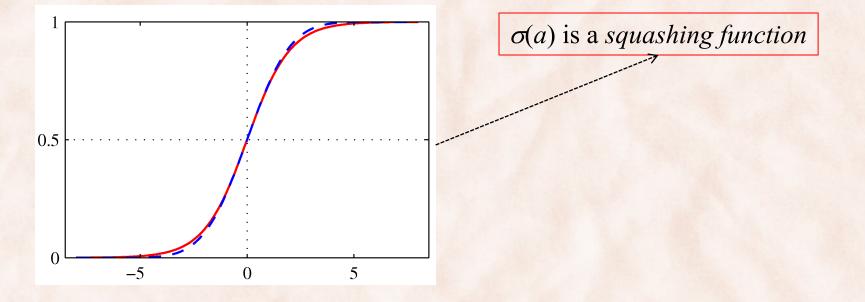
= $\sigma(a(\mathbf{x}))$ logistic sigmoid
where $\sigma(a) = \frac{1}{1 + \exp(-a)}$ log odds
 $a(\mathbf{x}) = \ln \frac{p(\mathbf{x} | C_1) p(C_1)}{p(\mathbf{x} | C_2) p(C_2)} = \ln \frac{p(C_1 | \mathbf{x})}{p(C_2 | \mathbf{x})}$

 $\left(\alpha \right)$

Probabilistic Generative Models: Binary Classification (K = 2)

• If $a(\mathbf{x})$ is a linear function of $\mathbf{x} \Rightarrow p(C_1 | \mathbf{x})$ is a generalized linear *model*:

$$p(C_1 | \mathbf{x}) = \frac{1}{1 + \exp(-a(\mathbf{x}))} = \sigma(a(\mathbf{x})) = \sigma(\lambda^T \mathbf{x})$$



The Naïve Bayes Model

• Assume binary features $x_i \in \{0,1\}$:

$$\Rightarrow p(\mathbf{x} | C_k) = \prod_{i=1}^{M} p(x_i | C_k)$$
$$= \prod_{i=1}^{M} \mu_{ki}^{x_i} (1 - \mu_{ki})^{1 - x_i} \text{, where } \mu_{ki} = p(x_i = 1 | C_k)$$

$$\Rightarrow p(C_k \mid \mathbf{x}) = \frac{\exp(a_k(\mathbf{x}))}{\sum_j \exp(a_j(\mathbf{x}))}$$

, where $a_k(\mathbf{x}) = \sum_{i=1}^M \{x_i \ln \mu_{ki} + (1 - x_i) \ln(1 - \mu_{ki})\} + \ln p(C_k)$
 $= \lambda_k^T \mathbf{x} \Rightarrow \text{NB is a generalized linear model.}$

Probabilistic Generative Models: Multiple Classes ($K \ge 2$)

 Model class-conditional p(x |C_k) as well as the priors p(C_k), then use Bayes's theorem to find p(C_k | x):

$$p(C_{k} | \mathbf{x}) = \frac{p(\mathbf{x} | C_{k})p(C_{k})}{\sum_{j} p(\mathbf{x} | C_{j})p(C_{j})}$$

$$= \frac{\exp(a_{k}(\mathbf{x}))}{\sum_{j} \exp(a_{j}(\mathbf{x}))}$$
normalized exponential i.e. softmax function

where $a_k(\mathbf{x}) = \ln p(\mathbf{x} | C_k) p(C_k)$

• If $a_k(\mathbf{x}) = \boldsymbol{\lambda}_k^T \mathbf{x} \Rightarrow p(C_k \mid \mathbf{x})$ is a generalized linear model.