Nearest Neighbors and Naive Bayes

Baseline algorithms

- Simple algorithms but effective
- Two different methods:
  - ***Nearest Neighbor.*** Non parametric method: In this case a lazy Instance Based Learning method that does not build any model.
  - ***Naïve Bayes.*** Parametric: It builds a probabilistic model of your data following some assumptions.

Nearest Neighbor classifier

Instance Based Learning / Lazy Methods

Instance Based Learning

- Lazy learning methods: they don't build a model of the data
- Assign the label to an observation depending on the labels of "closest" examples
- Only requirements:
  - A training set
  - A similarity measure

Instance Based Learning Algorithms

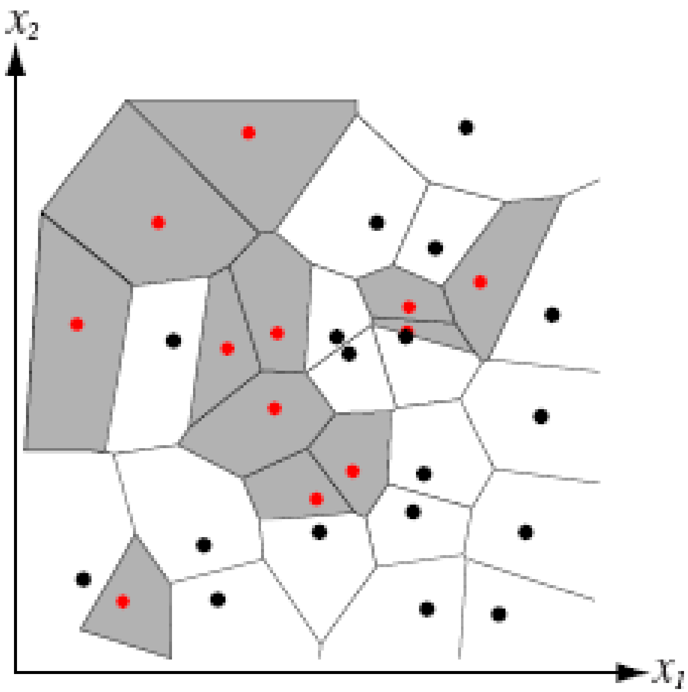
- K-NN
- Distance Weighted kNN
- How to select K??
- How to solve some problems

K-NN

- K-Nearest neighbor algorithm
- It interprets each example as a point in a space defined by the features describing the data
- In that space a similarity measure allows as to classify new examples.
- Class is assigned depending on the *K* closest examples

1-NN example

- Two real features (x1, x2) define the space.
- Each red point is a positive example. Black points are negative examples



Equivalen to to draw the Voronoi space of your data.

1-NN example

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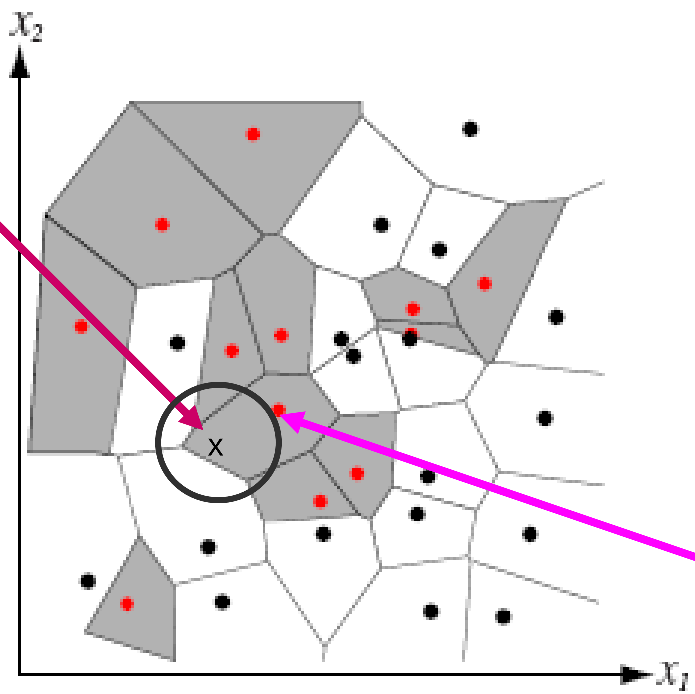
query point q_f



Equivalen to to draw the Voronoi space of your data.

X new data is classified as positive

nearest neighbor q_i

Distance measures

- Distance is a parameter of the algorithm
- When dataset is numeric, usually Euclidean:

$$d(x_i, x_j) = \sqrt{\sum_{k=1}^{m} (x_i(k) - x_j(k))^2}$$

- In mixed data sets, Gower or any other appropriate distance measure
- **CAVEAT**: Data should be normalized or standardized in order to ensure same relevance to each feature in the computation of distance.

Some comments

Advantages:

- Fast training
- Ability to learn very complex functions

Problems:

- Very slow in testing. Needed some smart structure representation of data in trees
- Fooled by noise
- Fooled when irrelevant features

Some comments:

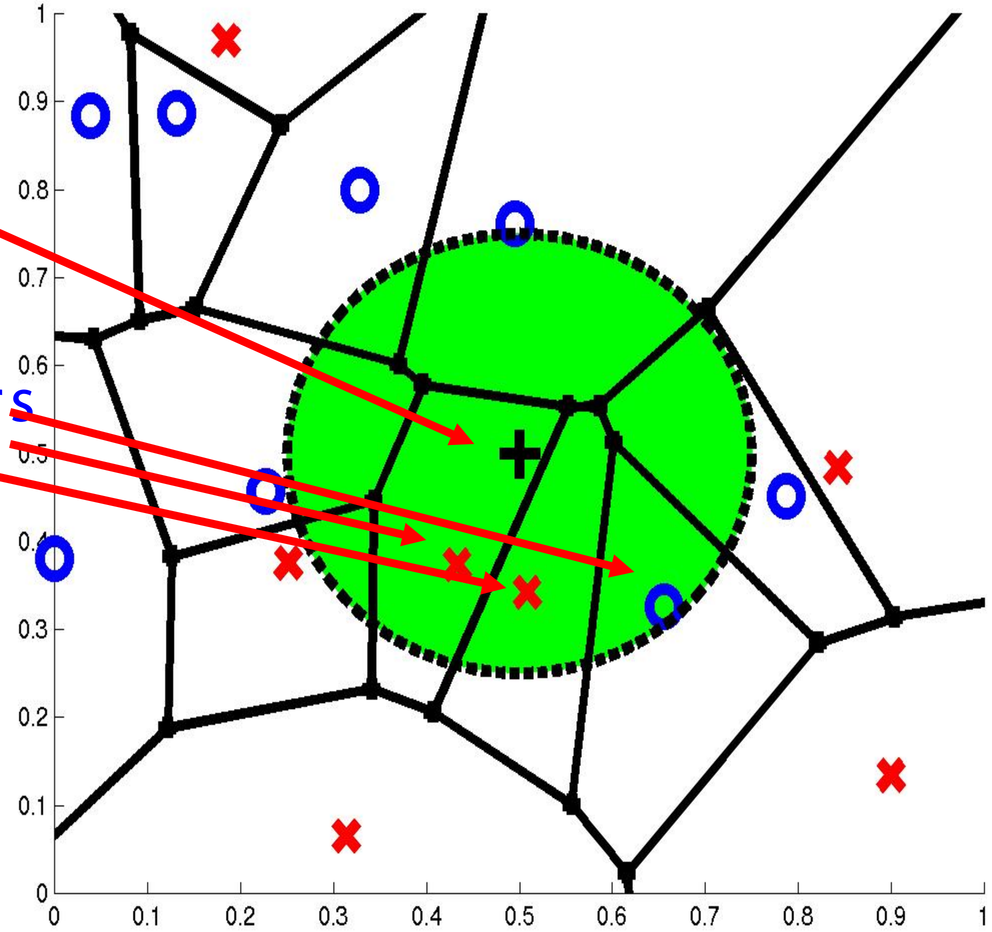
- Building more robust classifiers
  - Results do not depend on the closest example but on the k clossest examples (so *k-nearest neighbours* (kNN) name)

3-Nearest Neighbors

query point q_f

3 nearest neighbors

2x,1o

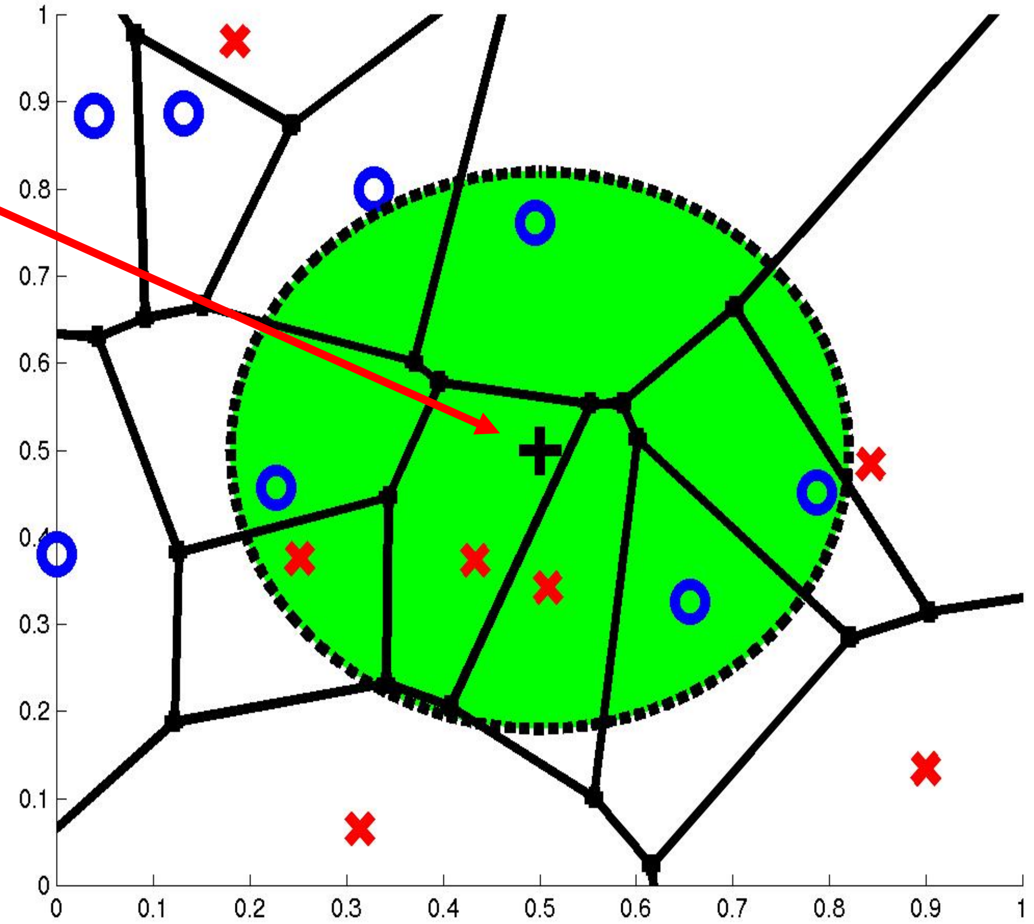


7-Nearest Neighbors

query point qf

7 nearest neighbors

3x,4o



K-NN algorithm

- **Parameters**:
  - Natural number *k (odd number)*
  - Training set
  - Distance measure
- Algorithm:
  1. Store all training set <x_i, label(x_i)>
  2. Given new observation, x_q, compute the nearest k neighbors
  3. Let vote the nearest k neighbors to assign the label to the new data.

How to select k?

- High number of k show two advantages:
  - Smother frontiers
  - Reduces sensibility to noise
- But too large values are bad because
  - We loose locality in the decision because very distant points can interfere in assigning labels
  - Computation time is increased
- K-value usually is chosen by cross-validation.

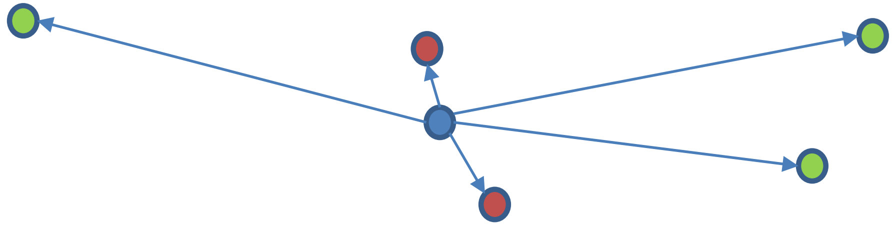
Distance Weighted kNN

- A smart variation of KNN.
- When voting, all k neighbors have the same influence, but some of them are more distant than the others (so the should influence less in decisions)

k=5

2 votes

3 votes



- Solution: **Given more weight to closest examples**

Distance Weighted kNN

Lets define a weigth for each of the k-closest examples:

$$w_i = K(d(x_i, x_q))$$

where x_q is the *query point*, x_i is the *i-closest example*, d is the distance function and *K* is the kernel (a decreasing function with respect to distance function)

Predicted label for x_q is computed according to:

$$\text{sign}\left(\sum_{i=1}^{k} w_i l(x_i)\right)$$

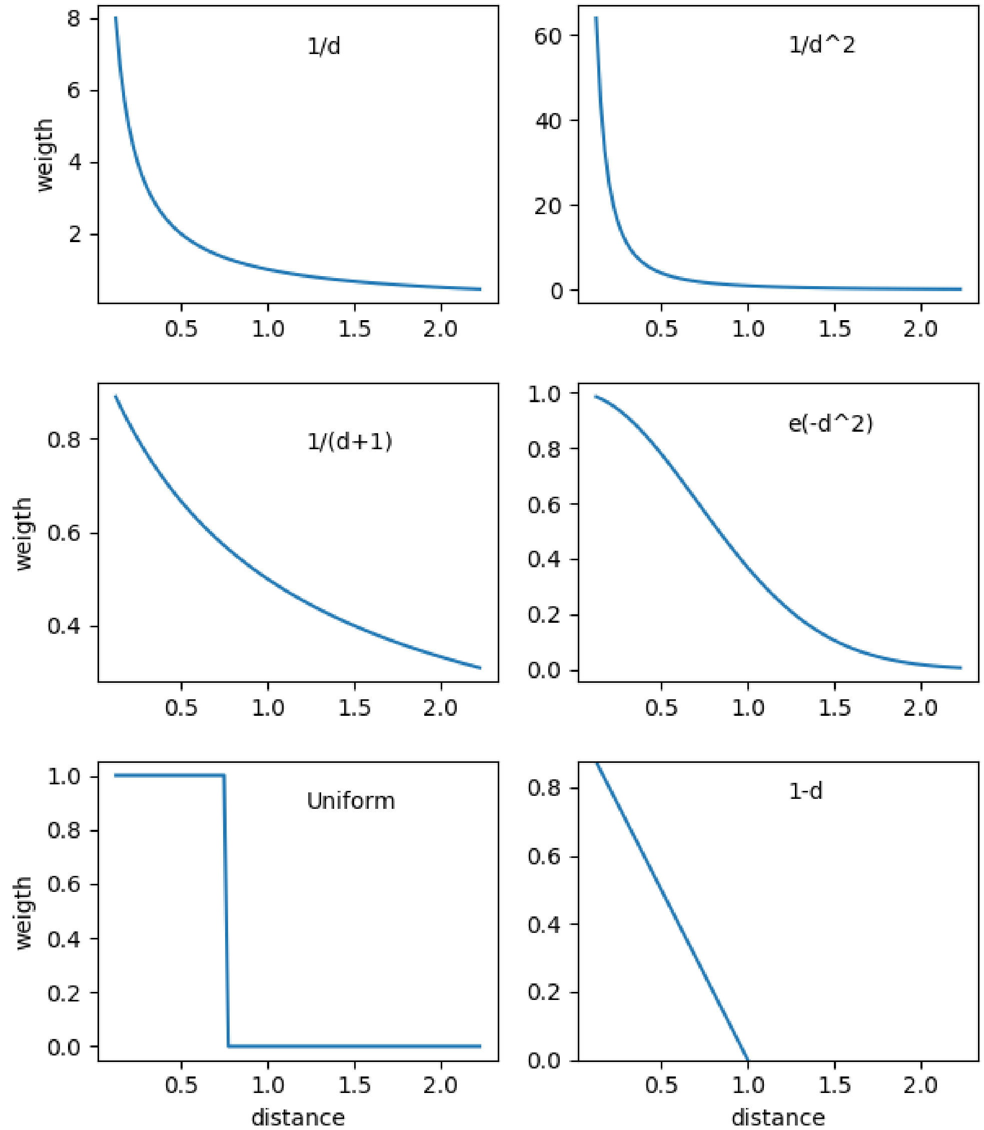
where $l(x_i)$ is {-1,1} the label of exemple x_i, and w_i is the weight of example x_i

In previous example, it could be something like:

$$\text{sign}\left(0.9 * 1 + 0.8 * * 1 + 0.4 * (-1) + 0.35 * (-1) + 0.3 * (-1)\right) = \text{sign}(0.65) = +1$$

Kernel functions

Examples of kernel functions



Problems with irrelevant features

- K-NN is fooled when irrelevant features are widely present in the data set
  - For instance, examples are described using 20 attributes, but only 2 of them are relevant to the classification…
- Solution consists in **feature selection**. For instance:
  - Use weighted distance:

$$d_z(x_i, x_j) = \sum_{k=1}^{n} z_l (x_i(k) - x_j(k))^2$$

  - Limit weights to 0 and 1. Notice that setting $z_j = 0$ means removing the feature
  - Find weights $z_1,\ldots,z_n$ (one for each feature), that minimize error in a validation data set using cross-validation

Naïve Bayes

Probabilistic model

Naive Bayes basics

- From examples in the dataset, we can estimate the likelihood of our data:

$$p(x_1, x_2, \ldots x_n | c_i)$$

read as probability to observe example with features $(x_1, x_2 \ldots x_n)$ [x_i, represents **feature** *i* of observation *x*] in class c_i

- But, for classifying an observation $(x_1, x_2 \ldots x_n)$, we should look for the class that maximizes the probability of the observation belonging to the class:

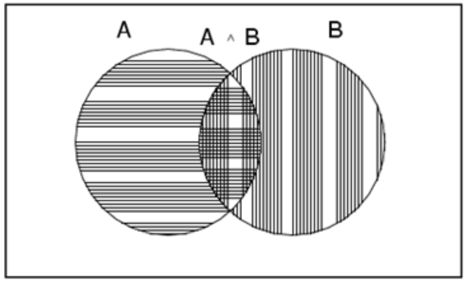
$$c_{MAP} = \underset{c_j \in C}{\operatorname{argmax}}\, P(c_j \mid x_1, x_2, \ldots, x_n)$$

Naïve Bayes classifiers

We will use the Bayes' theorem:

$$c_{MAP} = \underset{c_j \in C}{\operatorname{argmax}} P(c_j \mid x_1, x_2, \ldots, x_n) = \underset{c_j \in C}{\operatorname{argmax}} \frac{P(x_1, x_2, \ldots, x_n \mid c_j) P(c_j)}{P(x_1, x_2, \ldots, x_n)}$$

Bayes' theorem :



$$\begin{cases} P(A|B) = P(A \wedge B) / P(B) \\ P(B|A) = P(A \wedge B) / P(A) \end{cases}$$

$$\Rightarrow P(A \wedge B) = P(A|B)\,P(B) = P(B|A)\,P(A)$$

$$\Rightarrow \boxed{P(A|B) = \frac{P(B|A)\,P(A)}{P(B)}}$$

Computing probabilities

- $P(c_j)$ - Simply proportion of elements in class j
- $P(x_1,x_2,\ldots,x_n|c_j)$
  - Problem $|X|^n.|C|$ parameters!
  - It can only be estimated from a very huge dataset. Impractical
- **Solution: <u>Independence assumption</u>** (very *Naïve*) **: attribute values are independent**. So in this case, we can easily compute

$$P(x_1, x_2, \ldots, x_n \mid c_j) = \prod_i P(x_i \mid c_j)$$

Computing probabilities

- $P(x_k|c_j)$
  - Now we only need $n.|C|$ probability estimations
  - Very easy. Number of values with property x_k in class c_j over the complet number of cases in class c_j
- Solving now, $P(x_1, x_2, \ldots, x_n \mid c_j) = \prod_i P(x_i \mid c_j)$

  the class assigned to a new observation is:

$$\boxed{c_{NB} = \underset{c_j \in C}{\operatorname{argmax}} \frac{P(x_1, x_2, \ldots, x_n \mid c_j) P(c_j)}{P(x_1, x_2, \ldots, x_n)} = \underbrace{\underset{c_j \in C}{\arg\max}\, P(c_j) \prod_i P(x_i \mid c_j)}_{\text{Equation to be used}}}$$

Practical issues

- Being probabilities in range 0..1, products quickly lead to *floating-point underflow* errors
- Knowing that *log(xy) = log(x) + log(y),* it is better to work with log(p) than with probabilities.

- Now:

$$c_{NB} = \operatorname*{argmax}_{c_j \in C} \left(\log P(c_j) + \sum_{i \in positions} \log P(x_i \mid c_j) \right)$$

Example: Learning to classify texts

- Training set: X document corpus
- Each document is labeled with f(x)=*like/dislike*
- Goal: Learn function that permits given new document if you like it or not.
- Questions:
  - How do we represent documents?
  - How to compute probabilities?

Example: Learning to classify texts

- **How do we represent documents?**
  - Each document is represented as a *Bag of Words*
  - <u>Attributes</u>: All words that appear in the document
  - So each document is represented as a boolean vector with length N: 0 – word does not appear ; 1 – word appear

- Practical problem: A very huge table.
- Solution : Use sparse representation of matrixes

Example: Learning to classify texts

- Some numbers
  - 10.000 documents
  - 500 words per document
  - Maximum theoretical number of words: 50.000 (much less because of word repetitions)

- Reducing the number of attributes
  - Removing the number (sing/plural) and verbal forms (*stemming*)
  - Remove conjunctions, propositions and articles (*stop words*)
  - Now we have about. 10.000 attributes

Example: Learning to classify texts

$$v_{NB} = \underset{v \in \{like, dislike\}}{\operatorname{argmax}} P(v) \prod_i P(x_i = word_i \mid v)$$

- **How to compute probabilities?**
  - First compute $P(v_i)$ for each class [“a priori” probability for like and dislike classes]

$$P(v_{like}) = \frac{\#\text{documents like}}{\text{total number of documents}}$$

$$P(v_{dislike}) = \frac{\#\text{documents dislike}}{\text{total number of documents}}$$

Example: Learning to classify texts

$$v_{NB} = \underset{v \in \{like, dislike\}}{\operatorname{argmax}} P(v) \prod_i P(x_i = word_i \mid v)$$

- **How to compute probabilities?**
  - Second, compute $P(x_i = word_i \mid v)$ for each word:

$$P(word_k \mid v) = \frac{\#(\text{docs. } v \text{ in training where } word_k \text{ apears})}{\#(\text{documents } v)} = \frac{n_k}{n}$$

  - Number of parameters to estimate is not too large: 10.000 words and two classes (so about 20.000)

Example: Learning to classify texts

- Problem:

$$\mathbf{P(word_k \mid v)} = \frac{\mathbf{\#\,(docs.\ \ v\ \ del\ training\ on\ word_k\ \ apareix)}}{\mathbf{\#(documents\ v)}} = \frac{\mathbf{n_k}}{\mathbf{n}}$$

  - When n_k is low, not an accurate probability
  - when n_k is 0 for $word_k$ for one class v, then any document with that word will never be assigned to v (independent of other appearing words)

Example: Learning to classify texts

- Solution: More robust computation of probabilities (Laplace *smoothing*)

$$\mathbf{P(word_k \mid v) = \frac{n_k + mp}{n + m}}$$

- Where:
  - n_k is # of documents of class v in which word *k* appear
  - n is # of documents with label *v*
  - *p* it's a likelihood estimation of "a priori" $P(x_k|v)$ (f.i., uniform distribution)
  - m is the number of labels

Example: Learning to classify texts

Smoothing: $$\mathbf{P(x_k \mid v)} = \frac{\mathbf{n_k + mp}}{\mathbf{n + m}}$$

More common “a priori” uniform distribution:

1. When two classes: p=1/2, m=2 (Laplace Rule)

$$\mathbf{P(x_k \mid v)} = \frac{\mathbf{n_k + 1}}{\mathbf{n + 2}}$$

2. Generic case (*c* classes): p = 1/*c*, m=*c*

$$\mathbf{P(x_k \mid v)} = \frac{\mathbf{n_k + 1}}{\mathbf{n} + c}$$

Example: Learning to classify texts

- Naïve Bayes return good accuracy results even when independence assumption is not fulfilled
  - In fact, Spam/not Spam implementation of Thunderbird work in this way
  - Applied to document filtering (fi. *Newsgroups* or *incoming mails*)
- Learning and testing time are linear with the number of attributes!

Extension to continuous attributes

- Assume each class follows a normal distribution for each variable

$$f(x) = \frac{1}{\sqrt{2\pi\sigma}} e^{\frac{(x-\mu)^2}{2\sigma^2}}$$

- For instance 73 is average of feature temp. for class x, and std=26.2, we compute conditional prob in the following way:

$$p(temperature = 66 \mid x) = \frac{1}{\sqrt{2\pi 6.2}} e^{\frac{(66-73)^2}{26.2^2}} = 0.034$$