CS5489
Lecture 1.2: K-Nearest Neighbors and Bayes Optimal Classifier

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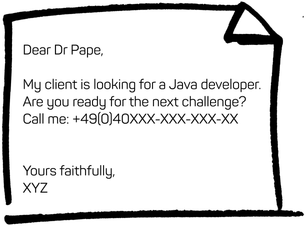
Example: Texts

- Given an email, predict whether it is spam or not spam

垃圾邮件



SPAM

vs.

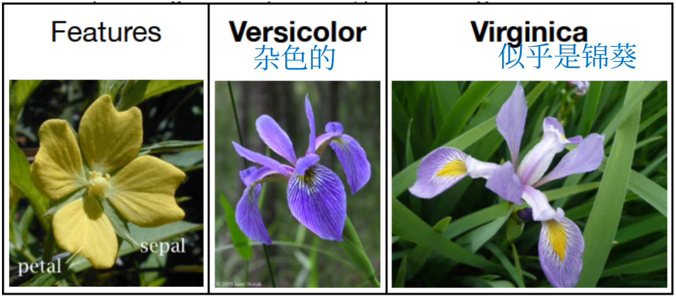
HAM

蹩脚演员？还是火腿

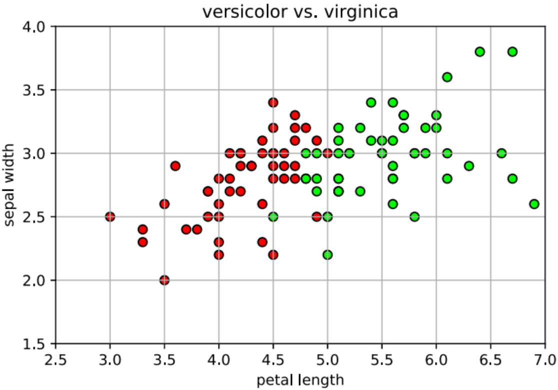
Example: Images

- Given the petal length and sepal width, predict the type of iris flower

花瓣 花萼 鸢尾花



Example: Images



The Classification Task

Definition: The Classification Task

Given a feature vector $\mathbf{x} \in \mathbb{R}^N$ that describes an object that belongs to one of C classes from the set $\mathcal{Y}$, predict which class the object belongs to

- In the previous example of iris classification
  - $\mathbf{x} = \begin{bmatrix} \text{petal length} \\ \text{sepal width} \end{bmatrix} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \in \mathbb{R}^2$, where $N = 2$
  - $\mathcal{Y} = \{\text{"versicolor"}, \text{"virginica"}\}$, where $|\mathcal{Y}| = C = 2$
  - Or equivalently as numbers $\mathcal{Y} = \{1, 2\}$

The Classifier Learning Problem

Definition: Classifier Learning

所以x(i) y(i)都是训练集

Given a data set of example pairs $\mathcal{D} = \{(\mathbf{x}^{(i)}, y^{(i)}), i = 1, \ldots, M\}$ where $\mathbf{x}^{(i)} \in \mathbb{R}^N$ is a feature vector and $y^{(i)} \in \mathcal{Y} = \{1, \ldots, C\}$ is a class label, learn a function $f : \mathbb{R}^N \mapsto \mathcal{Y}$ that accurately predicts the class label y for any feature vector $\mathbf{x}$

总共有C类的分类问题

Definition: Indicator Function

$$\mathbb{I}[A] = \begin{cases} 1, & \text{if event } A \text{ occurs} \\ 0, & \text{otherwise} \end{cases}$$

Classification Error and Accuracy

Definition: Classification Error Rate

Given a data set of example pairs $\mathcal{D} = \{(\mathbf{x}^{(i)}, y^{(i)}), i = 1, \ldots, M\}$ and a function $f : \mathbb{R}^N \mapsto \mathcal{Y}$, the classification error rate of f on $\mathcal{D}$ is

$$\mathrm{Err}(f, \mathcal{D}) = \frac{1}{M}\sum_{i=1}^{M}\mathbb{I}[y^{(i)} \neq f(\mathbf{x}^{(i)})]$$

fx是预测标签值

妈的，就是错误率和正确率，**非要用**sigma，I[]，这些破玩意儿来装神弄**鬼，傻逼数学**

Definition: Classification Accuracy Rate

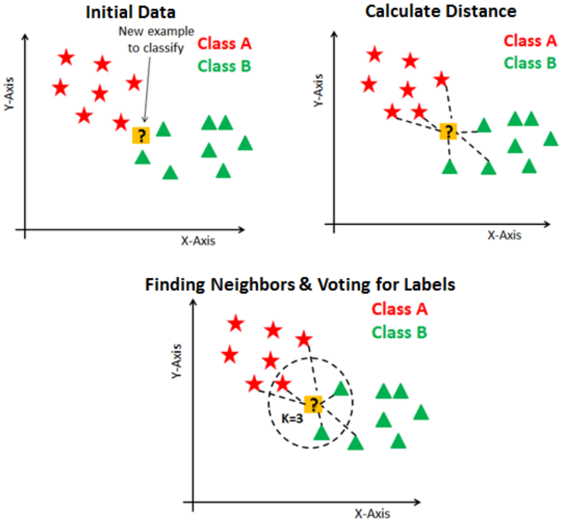
Given a data set of example pairs $\mathcal{D} = \{(\mathbf{x}^{(i)}, y^{(i)}), i = 1, \ldots, M\}$ and a function $f : \mathbb{R}^N \mapsto \mathcal{Y}$, the classification accuracy rate of f on $\mathcal{D}$ is

$$\mathrm{Acc}(f, \mathcal{D}) = \frac{1}{M}\sum_{i=1}^{M}\mathbb{I}[y^{(i)} = f(\mathbf{x}^{(i)})]$$

K-Nearest Neighbors (KNN) Classification

- The KNN classifier is one of the most basic yet essential classifier in machine learning
- It stores the training set $\mathcal{D}$, and classifies each **new** instance $\mathbf{x}$ using a majority vote over its K nearest neighbors $\mathcal{N}_K(\mathbf{x}) \subset \{1, \ldots, M\}$ Nk(x)**是**K个节点的索引的集合
- Use of KNN requires choosing the distance function $d : \mathbb{R}^N \times \mathbb{R}^N \mapsto \mathbb{R}$ and the number of neighbors K

Example: KNN


Initial Data
New example
to classify
Class A
Class B
Y-Axis
X-Axis
?
Calculate Distance
Class A
Class B
Y-Axis
X-Axis
?
Finding Neighbors & Voting for Labels
Class A
Class B
Y-Axis
X-Axis
?
K=3

Max vs. Arg Max

Max Operator

The max operator of a function $f(\mathbf{x})$ defined over $\mathbf{x} \in \mathcal{D}$ returns the maximum value of the function:

$$\max_{\mathbf{x}} f(\mathbf{x}) = \{f(\mathbf{x}) | \mathbf{x} \in \mathcal{D} \land \forall \mathbf{y} \in \mathcal{D}, f(\mathbf{y}) \leq f(\mathbf{x})\}$$

如果D是训练集（点和标签队），这里的x和y都是单独的某组点和标签而不是点/标签了，傻逼数学同符号换意思了。但这里应该D知识单纯的值一个值域，D属于R这种，傻逼数学同符号换意思了。

Arg Max Operator

The arg max operator of a function $f(\mathbf{x})$ defined over $\mathbf{x} \in \mathcal{D}$ gives the set of points for which $f(\mathbf{x})$ reaches the maximum value:

$$\arg\max_{\mathbf{x}} f(\mathbf{x}) = \{\mathbf{x} | \mathbf{x} \in \mathcal{D} \land \forall \mathbf{y} \in \mathcal{D}, f(\mathbf{y}) \leq f(\mathbf{x})\}$$

例子很好，f(x)=(x-2)2+5,，maxf(x)=5,argmaxf(x)=2,而argmax可以是一个区间

KNN Classification

KNN Classification Function

$$f_{\text{KNN}}(\mathbf{x}) = \arg\max_{c\in\{1,\ldots,C\}} \sum_{i\in\mathcal{N}_K(\mathbf{x})} \mathbb{I}[y^{(i)} = c]$$

y(i)的值就是C**类中的第几类**

i就是最邻近的那k**个点的索引号**

C放在这里就是函数output的值是c也就是0或者1（当然也可能是0和1）

I**出来**=1说明预测正确

argmax意味着我要选择能够让y(i)训练集标签值=c**正确率达到最高。**

但是这个x是啥破玩意儿，c**属于**{1,,,C}**放在**argmax下面是啥意思？？

Distance Function

- In general, KNN can work with any distance function d satisfying non-negativity $d(\mathbf{x}, \mathbf{x}') \geq 0$ and identity of indiscernibles $d(\mathbf{x}, \mathbf{x}) = 0$
  难以察觉的
- Generally, the more structure the distance function has (symmetry, triangle inequality), the more structure you can exploit when designing algorithms
  开发

Distance Metrics

norm本来就是求||的意思——**范数**

Definition: Minkowski Distance (ℓ_p-norm)

Given two data vectors $\mathbf{x}, \mathbf{x}' \in \mathbb{R}^N$, the Minkowski distance with parameter p (the ℓ_p-norm) is a proper metric defined as follows:

$$d_p(\mathbf{x}, \mathbf{x}') = \|\mathbf{x} - \mathbf{x}'\|_p = \left(\sum_{j=1}^{N} |x_j - x'_j|^p \right)^{1/p}$$

这似乎是要点对一一对应，**像是求**align时的MSE一样哈哈哈

欧几里得

曼哈顿

Special cases include Euclidean distance ($p = 2$), Manhattan distance ($p = 1$) and Chebyshev distance ($p = \infty$)

切比雪夫

Brute Force KNN

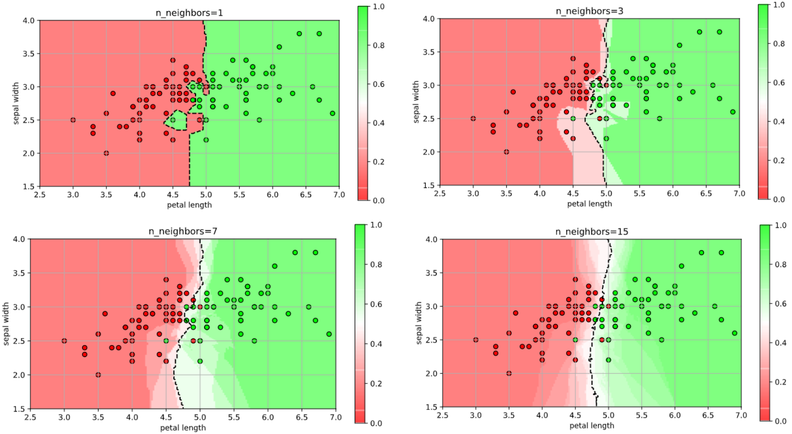
暴力算法

- Given any distance function d, brute force KNN works by computing the distance $d_i = d(\mathbf{x}^{(i)}, \mathbf{x})$ from a target point $\mathbf{x}$ to all of the training points $\mathbf{x}^{(i)}$

- Sort the distances $\{d_i, i = 1, \ldots, M\}$ and choose the data cases with the K smallest distances to form the neighbor **index** set $\mathcal{N}_K(\mathbf{x})$ Nk(x)是K个节点的索引的集合

- Once the K neighbors are selected, applying the classification rule is easy

KNN on Iris Dataset



KNN Variants

- Instead of giving all of the K neighbors equal weight in the majority vote, a distance-weighted majority can be used:

$$f_{\mathrm{KNN}}(\mathbf{x}) = \underset{c\in\{1,\ldots,C\}}{\arg\max} \frac{\sum_{i\in\mathcal{N}_K(\mathbf{x})} w_i \mathbb{I}[y^{(i)} = c]}{\sum_{i\in\mathcal{N}_K(\mathbf{x})} w_i},$$

$$w_i = \exp(-\alpha d_i)$$

- Instead of a brute force nearest neighbor search, data structures like K-d trees can be constructed over the training data that support nearest neighbor search with lower computational complexity

简单来说，AB距离很远，BC距离很近，那就没必要再计算AC距离了

KNN Trade-Offs

- **Advantages**:
  - No training period is involved (i.e., lazy learning), and new data can be added seamlessly without re-training the model
    无缝地
  - Converges to the correct decision surface as data goes to infinity
    集中于
- **Disadvantages**:
  - Does not work well with large datasets. Since KNN needs to store all training data, performing neighbor search requires a lot of memory and takes a lot of time
  - Does not work well with high dimensions. It becomes difficult for KNN to calculate the distance in each dimension. Moreover, everything is far from everything else in high dimensions (the so-called "curse of dimensionality") 不过我当时只用了四维还行
    诅咒，**不是**curve

Probabilistic Classifiers

- One type of classifier to model the data
- Model how the data is generated using probability distributions (i.e., **generative** models)
  生成式model
- Defining generative models:
  - The world has objects /patterns of various classes
  - The observer measures features/observations from the objects/patterns
  - Each class of objects/patterns has a particular (and possibly different) distribution of features

Class Model

- Possible classes are $\mathcal{Y}$
  - For example, in the iris dataset, $\mathcal{Y} = \{$"versicolor", "virginica"$\}$, or more generally, $\mathcal{Y} = \{1, 2\}$
- In the real world, the frequency that Class y occurs is given by the probability distribution $p(y)$
  - $p(y)$ is called the **prior distribution**

先验分布

- Example:
  - $p(y = 1) = 0.4$ and $p(y = 2) = 0.6$
  - This means in the world of iris flowers, there are 40% that are Class 1 (versicolor) and 60% that are Class 2 (virginica)
- Learn from our data:

$$p(y = c) = \frac{\sum_{i=1}^{M} \mathbb{I}[y^{(i)} = c]}{M}, \quad c \in \{1, 2\}$$

Observation Model

- We measure/observe feature vector $\mathbf{x}$
  - The values of the features **depend** on the class

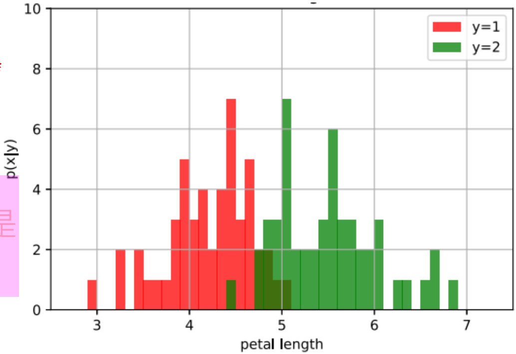
P of x given the y

- The observation is drawn according to the distribution $p(\mathbf{x}|y)$
  - $p(\mathbf{x}|y)$ is called the **class conditional distribution**
  - It indicates the probability of observing a particular feature vector $\mathbf{x}$ given the object is Class y
- Learn from our data:
  - In the iris dataset, we draw histograms of feature "petal length" for each class

直方图

Feature Histogram

这纵坐标单位是啥
？？%？？



纵坐标是count
P(x|y)可以理解是标题

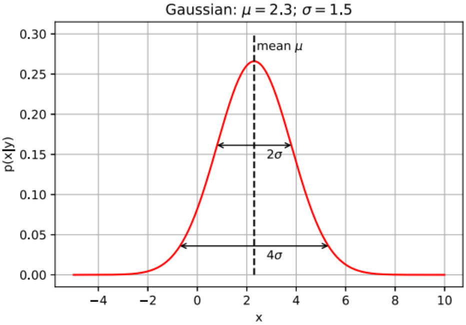
- Problem: looks a little bit noisy
- Solution: assume a probability model for the class conditional $p(\mathbf{x}|y)$

Gaussian Distribution

他妈的，高斯分布就是正态分布嘛，何必另外再用高斯分布这个说法，**以后我把01分布叫OX分布得了**

- Each class is modeled as a separate Gaussian distribution of the feature value
  - $p(x|y=c;\mu_c,\sigma_c^2)=\frac{1}{\sqrt{2\pi\sigma_c^2}}e^{-\frac{1}{2\sigma_c^2}(x-\mu_c)^2}$
  - Each class has its own mean and variance parameters (μ_c,σ_c^2)

不过为什么我们**可以假定所有的class都是高斯分布呢？**



每个class都有俩参数，所以这里有4个参数其实

Learn the Parameters from Data

- Maximum likelihood estimation (MLE)
  - Set the parameters (μ_c, σ_c^2) to maximize the likelihood (probability) of the samples for Class c
  - Let $\mathcal{D}_c = \{\mathbf{x}^{(i)}, y^{(i)}\}_{i=1}^{M_c}$ be the data for Class c (i.e., $y^{(i)} = c$):

这个Mc是什么鬼？？

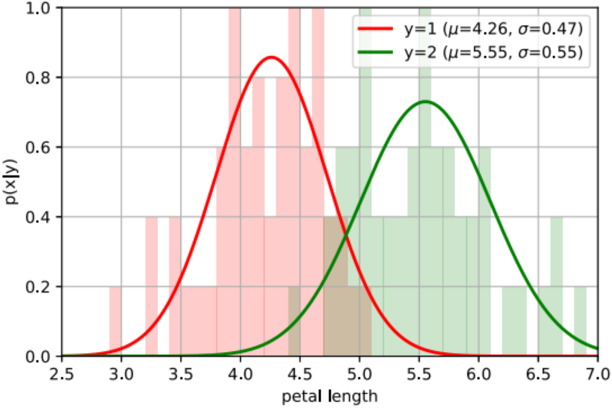
M-c是样本数
Dc是一个样本空间

$$(\hat{\mu}_c, \hat{\sigma}_c^2) = \arg\max_{\mu_c, \sigma_c^2} \sum_{i=1}^{M_c} \log p(x^{(i)} | y^{(i)}; \mu_c, \sigma_c^2)$$

  - When we view the above objective as a function of the parameters $\{\mu_c, \sigma_c^2\}$, we instead call it the likelihood function of the data

- Solution:
  - Sample mean: $\hat{\mu}_c = \frac{1}{M_c} \sum_{i=1}^{M_c} x^{(i)}$
  - Sample variance: $\hat{\sigma}_c^2 = \frac{1}{M_c} \sum_{i=1}^{M_c} (x^{(i)} - \hat{\mu}_c)^2$

Gaussian Class Conditionals



Bayesian Decision Rule

- The Bayesian decision rule (BDR) makes the **optimal** decisions on problems involving probability (uncertainty)
  - Minimizes the probability of making a prediction error
- Bayes optimal classifier
  - Given observation $\mathbf{x}$, pick the class c with the **largest posterior probability** $p(y=c|\mathbf{x})$:

（在时/序上）较后的

$$f_{\mathrm{B}}(\mathbf{x}) = \underset{c\in\{1,\ldots,C\}}{\arg\max}\, p(y=c|\mathbf{x})$$

贝叶斯法则：用后验知识修改先验判断

- Example:
  - If $p(y=1|\mathbf{x}) > p(y=2|\mathbf{x})$, then choose Class 1
  - If $p(y=1|\mathbf{x}) < p(y=2|\mathbf{x})$, then choose Class 2
- Problem: we don't have $p(y|\mathbf{x})$
  - We only have $p(y)$ and $p(\mathbf{x}|y)$

Bayes' Rule

- The posterior probability can be calculated using Bayes' rule:

$$p(y|\mathbf{x}) = \frac{p(\mathbf{x}|y)p(y)}{p(\mathbf{x})}$$

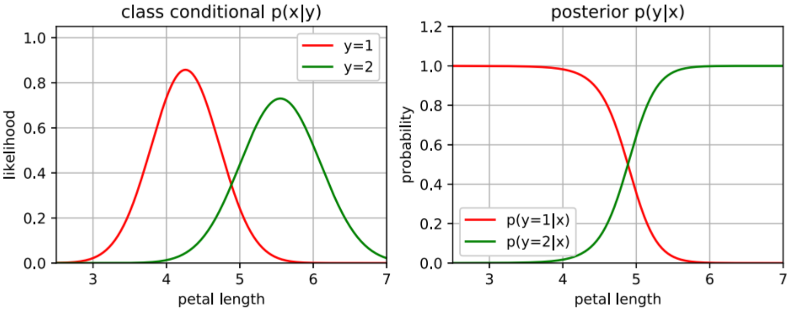
本来上面是P(x,y)

  - The denominator is the probability of $\mathbf{x}$:
    - $p(\mathbf{x}) = \sum_{y\in\mathcal{Y}} p(\mathbf{x}, y) = \sum_{y\in\mathcal{Y}} p(\mathbf{x}|y)p(y)$
  - The denominator makes $p(y|\mathbf{x})$ sum to 1

- Bayes' rule:

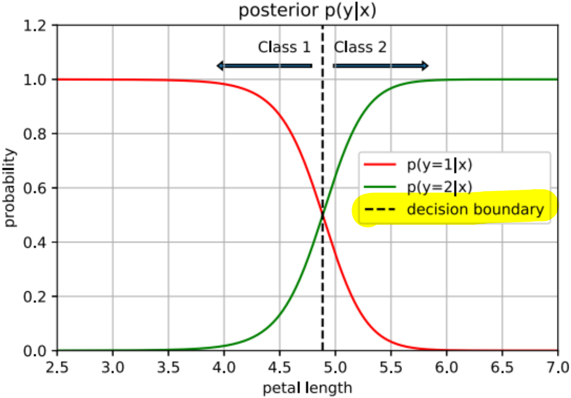
$$p(y|\mathbf{x}) = \frac{p(\mathbf{x}|y)p(y)}{p(\mathbf{x}|y=1)p(y=1) + p(\mathbf{x}|y=2)p(y=2)}$$

Posterior Probability



Decision Boundary

- The decision boundary is where the two posterior probabilities are equal
  - $p(y = 1|\mathbf{x}) = p(y = 2|\mathbf{x})$



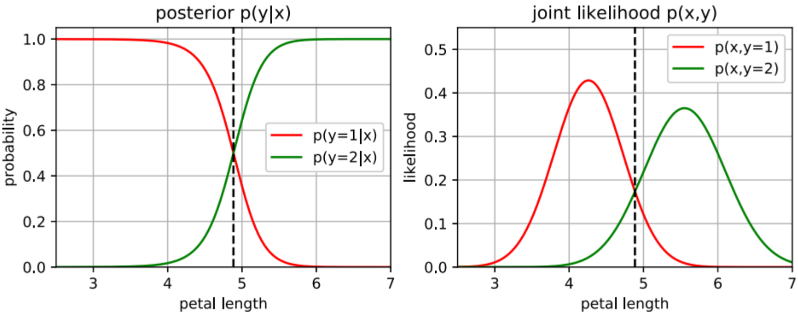
Bayes' Rule Revisited

- Bayes' rule:

$$p(y|\mathbf{x}) = \frac{p(\mathbf{x}|y)p(y)}{p(\mathbf{x})}$$

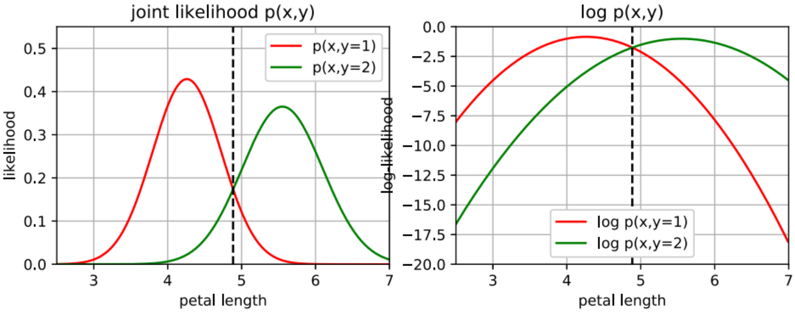
- Note that the denominator is the same for each class y
  - Hence, we can compare just the numerator $p(\mathbf{x}|y)p(y)$
  - This also called the **joint likelihood** of the observation and class
    - $p(\mathbf{x}, y) = p(\mathbf{x}|y)p(y)$
- Example:
  - BDR using joint likelihoods:
    - If $p(\mathbf{x}|y = 1)p(y = 1) > p(\mathbf{x}|y = 2)p(y = 2)$, then choose Class 1
    - Otherwise, choose Class 2

BDR Using Joint Likelihoods



Bayes' Rule Revisited

- Can also apply a monotonic increasing function (like log) and do the comparison
  单调的
  - Using log likelihoods:
    - $\log p(\mathbf{x}|y=1) + \log p(y=1) > \log p(\mathbf{x}|y=2) + \log p(y=2)$
  - This is more numerically stable when the likelihoods are small



Bayes Classifier Summary

- **Training**:
  1. Collect training data from each class
  2. For each class c, estimate the class conditional densities $p(\mathbf{x}|y = c)$:
     1. Select a form of the distribution (e.g., Gaussian)
     2. Estimate its parameters with MLE
  3. Estimate the class priors $p(y)$ using MLE
- **Classification**:
  1. Given a new sample $\mathbf{x}^*$, calculate the likelihood $p(\mathbf{x}^*|y = c)$ for each class c
  2. Pick the class c with the largest posterior probability $p(y = c|\mathbf{x}^*)$
     - Equivalently, use $p(\mathbf{x}^*|y = c)p(y = c)$ or $\log p(\mathbf{x}^*|y = c) + \log p(y = c)$