k-NN, Naive Bayes

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November 18, 2024

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Course Objectives: Where are we now?

After this course you should...

- Be able to reason about task/problems **suitable for ML**
  - Know when to use classification, regression and clustering
  - Be able to choose from this method Linear and Logistic Regression, Multilayer Perceptron, Nearest Neighbors, Naive Bayes, Gradient Boosted Decision Trees, k-means clustering
- Think about learning as (mostly probabilistic) **optimization on training data**
  - Know how the ML methods learn including theoretical explanation
- Know how to properly **evaluate** ML
  - Think about generalization (and avoiding overfitting)
  - Be able to choose a suitable evaluation metric
  - Responsibly decide what model is better
- Be able to **implement ML algorithms** on a conceptual level
- Be able to **use Scikit-learn** to solve ML problems in Python

Today's Lecture Objectives

After this lecture you should be able to

- Implement and use k-nearest neighbors for classification and regression
- Explain the very basic principles of Bayesian thinking
- Implement and use Naive Bayes Classifier

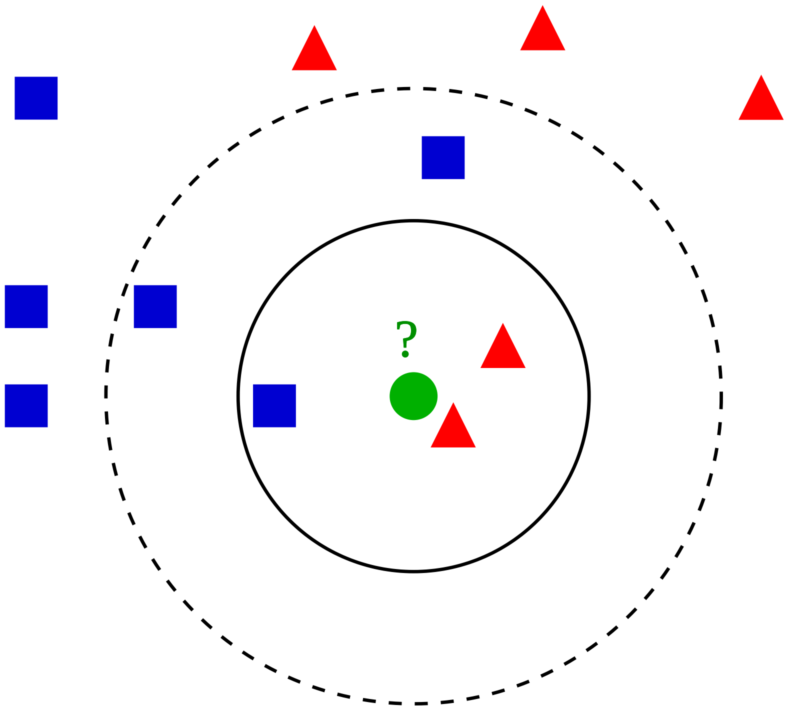
k-Nearest Neighbors

k-Nearest Neighbors

A simple but sometimes effective nonparametric method for both classification and regression is **k-nearest neighbors** algorithm.

The training phase of the k-nearest neighbors algorithm is trivial: only storing the whole train set (the so-called **lazy learning**).

For a given test example, the main idea is to use the targets of the most similar training data to perform the prediction.

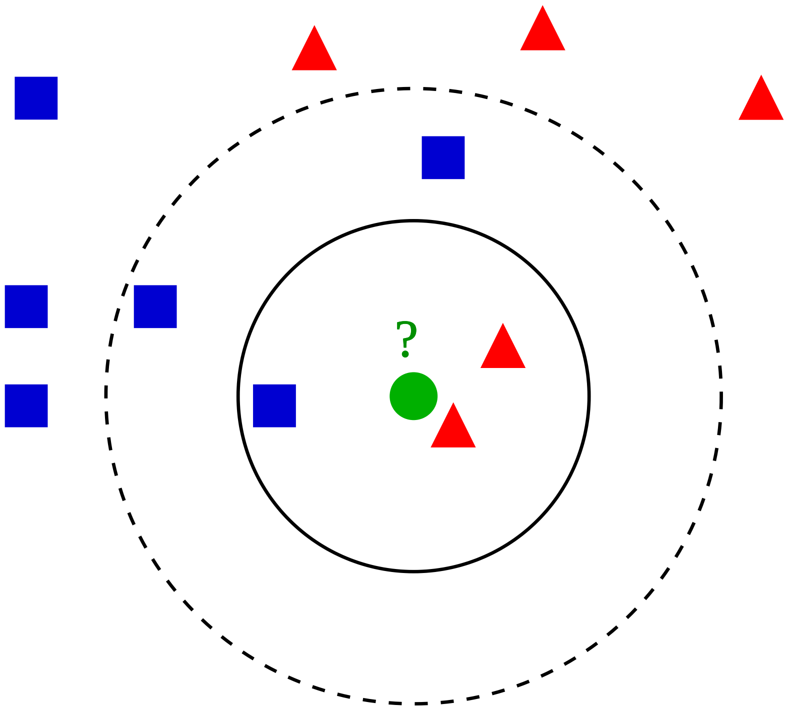


https://upload.wikimedia.org/wikipedia/commons/e/e7/KnnClassification.svg

Several hyperparameters influence the behavior of the prediction phase:

- **k**: consider k most similar training examples (higher k usually decreases variance, but increases bias);
- **metric**: a function used to find the nearest neighbors; common choices are metrics based on L^p norms (usual values of p: 1, 2, 3, ∞). For $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^D$, the distance is measured as $\|\boldsymbol{x} - \boldsymbol{y}\|_p$, where

$$\|\boldsymbol{x}\|_p = \Big(\sum\nolimits_i |x_i|^p\Big)^{1/p};$$



https://upload.wikimedia.org/wikipedia/commons/e/e7/KnnClassification.svg

- **weights**: optionally, more similar examples get higher weights:
  - *uniform*: all k nearest neighbors weighted equally;
  - *inverse*: the weights are proportional to the inverse of distance;
  - *softmax*: the weights are proportional to the $\operatorname{softmax}$ of negative distances.

Regression

To perform regression when k nearest neighbors have values t_i and weights w_i, we predict

$$t = \sum_i \frac{w_i}{\sum_j w_j} \cdot t_i.$$

Classification

For uniform weights, we can use **voting** during prediction – the most frequent class is predicted (with ties broken arbitrarily).

Otherwise, we weight the categorical distributions $\boldsymbol{t}_i \in \mathbb{R}^K$ (classification into K target classes represented using one-hot encoding), predicting a distribution

$$\boldsymbol{t} = \sum_i \frac{w_i}{\sum_j w_j} \cdot \boldsymbol{t}_i.$$

The predicted class is the one with the largest probability, i.e., $\arg\max_k \sum_i w_i t_{i,k}$.

k-Nearest Neighbors

A trivial implementation of the k-nearest neighbors algorithm is extremely demanding during the inference, requiring to measure distances of a given example to all training instances.

However, there exist several data structures that can speed up the k-nearest neighbor search, such as

- k-d trees, which allow both a static or dynamic construction and can perform nearest neighbor queries of uniformly random points in logarithmic time on average, but which become inefficient for high-dimensional data;
- ball trees, R-trees, …

Applications of Nearest Neighbors

- Typically in combination with representation learning
- Recommendation systems (e.g., for similar videos)
- Anonymous face recognition in photo collections

Bayesian Probability

Bayesian Probability

Until now, we considered the so-called *frequentist probability*, where the probability of an event is considered a limit of its frequency.

In *Bayesian probability* interpretation, probability is a quantification of **uncertainty**. Bayesian probability is the so-called *evidential* probability, where hypotheses have some initial **prior probability**, which is then updated in light of *new data* into **posterior probability**.

This update of prior probability into posterior probability is performed using the Bayes theorem

$$P(A|B) = \frac{P(B|A)P(A)}{P(B)}.$$

Textbook Example

1 of 10,000 products has a rare defect. We can detect it with both sensitivity and specificity of 99%. What is $P(\text{defect}|\text{positive})$?

$$P(\text{def}|\text{pos}) = \frac{\overbrace{P(\text{pos}|\text{def})}^{\text{sensitivity}} P(\text{def})}{P(\text{pos})}$$

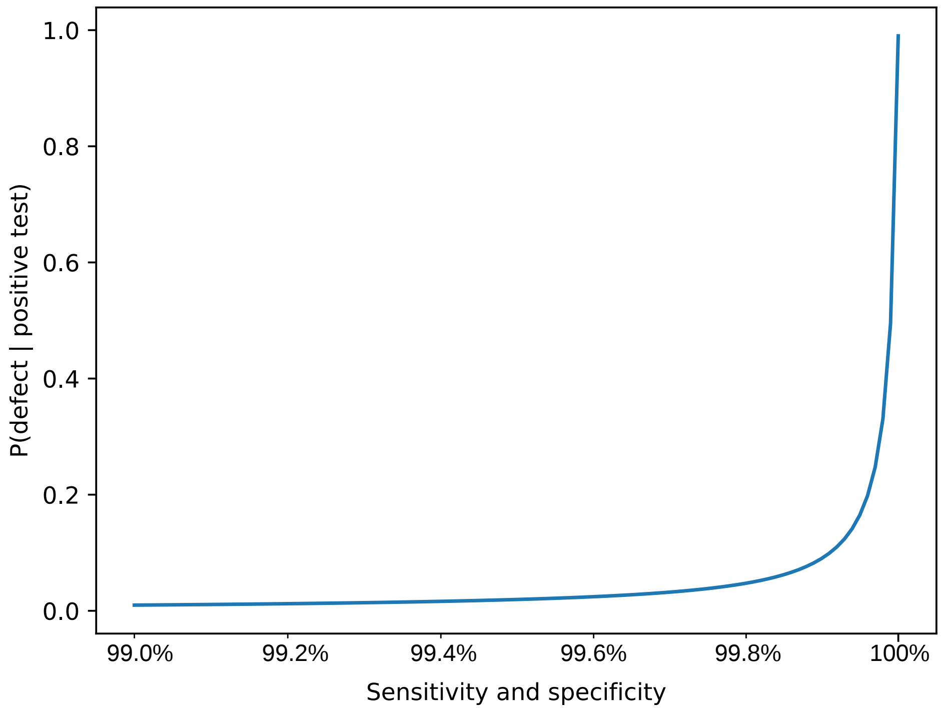
Now, we need to compute the denomniator $P(\text{pos})$ by splitting into joint probabilities:

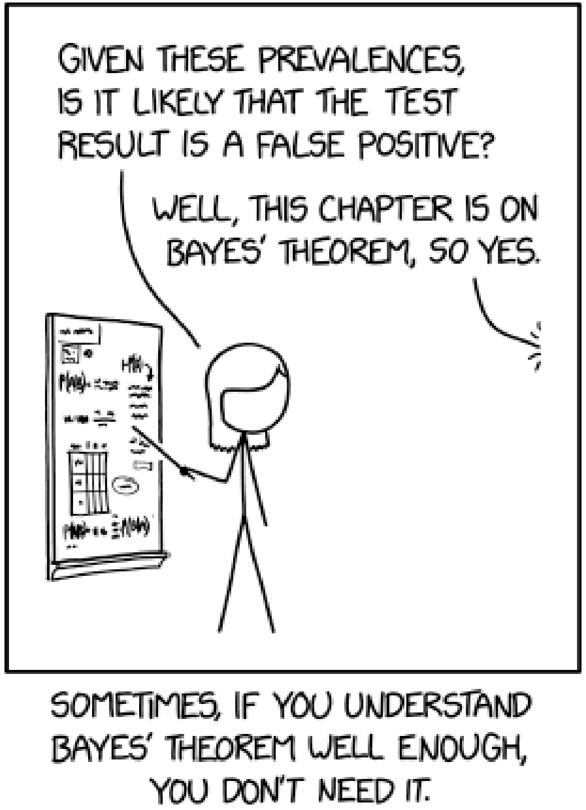
$$P(\text{pos}, \text{def}) + P(\text{pos}, \neg\text{def}) = P(\text{pos}|\text{def})P(\text{def}) + (1 - \underbrace{P(\neg\text{pos}|\neg\text{def})}_{\text{specificity}})(1 - P(\text{def}))$$

Together

$$P(\text{def}|\text{pos}) = \frac{.99 \cdot 10^{-4}}{.99 \cdot 10^{-4} + (1 - .99)(1 - 10^{-4})} \approx 0.98\%$$

Textbook Example: How accurate do we need to be?





https://www.explainxkcd.com/wiki/index.php/2545:_Bayes%27_Theorem

Moral: seemingly high-performing classifier might not be that high-performing.

Librarian or Farmer

As you consider the next question, please assume that Steve was selected at random from a representative sample. An individual has been described by a neighbor as follows: "Steve is very shy and withdrawn, invariably helpful but with little interest in people or in the world of reality. A meek and tidy soul, he has a need for order and structure, and a passion for detail." Is Steve more likely to be a librarian or a farmer?

The given description corresponds more to a librarian than to a farmer.

However, there are many more farmers than librarians (for example, in 2016 there were 4.33k librarians and 130.3k regular agricultural workers in the Czech Republic, a 30:1 ratio).

The description being more fitting for a librarian is in fact a *likelihood*, while the base rates of librarians and farmers play the role of a *prior*, and the whole question asks about the *posterior*:

$$P(librarian|description) \propto P(description|librarian) \cdot P(librarian).$$

The example is taken from the Thinking, Fast and Slow by D. Kahneman

Maximum A Posteriori Estimation

Maximum A Posteriori Estimation

We demonstrate the Bayesian probability on model fitting.

Recall the maximum likelihood estimation

$$\boldsymbol{w}_{\mathrm{MLE}} = \arg\max_{\boldsymbol{w}} p(\boldsymbol{X}; \boldsymbol{w}) = \arg\max_{\boldsymbol{w}} p(\boldsymbol{X}|\boldsymbol{w}).$$

In the Bayesian interpretation, we capture our initial assumptions about $\boldsymbol{w}$ using a prior probability $p(\boldsymbol{w})$. The effect of observing the data $\boldsymbol{X}$ can be then expressed as

$$p(\boldsymbol{w}|\boldsymbol{X}) = \frac{p(\boldsymbol{X}|\boldsymbol{w})p(\boldsymbol{w})}{p(\boldsymbol{X})}.$$

The quantity $p(\boldsymbol{X}|\boldsymbol{w})$ is evaluated using fixed data $\boldsymbol{X}$ and quantifies how probable the observed data is with respect to various values of the parameter $\boldsymbol{w}$. It is therefore a **likelihood**, because it is a function of $\boldsymbol{w}$.

Maximum A Posteriori Estimation

Therefore, we get that

$$\underbrace{p(\boldsymbol w|\boldsymbol X)}_{\text{posterior}} \propto \underbrace{p(\boldsymbol X|\boldsymbol w)}_{\text{likelihood}} \cdot \underbrace{p(\boldsymbol w)}_{\text{prior}},$$

where the symbol $\propto$ means "up to a multiplicative factor".

Using the above Bayesian inference formula, we can define **maximum a posteriori (MAP)** estimate as

$$\boldsymbol w_\mathrm{MAP} = \arg\max_{\boldsymbol w} p(\boldsymbol w|\boldsymbol X) = \arg\max_{\boldsymbol w} p(\boldsymbol X|\boldsymbol w)p(\boldsymbol w).$$

To utilize the MAP estimate for model training, we need to specify the parameter prior $p(\boldsymbol w)$, our *preference* among models.

Bayesian view on overfitting: it is just a problem of not using priors and that suitable priors would avoid it.

L2 Regularization as MAP

Frequently, the mean is assumed to be zero, and the variance is assumed to be σ^2. Given that we have no further information, we employ the maximum entropy principle, which provides us with $p(w_i) = \mathcal{N}(w_i; 0, \sigma^2)$, so that $p(\boldsymbol w) = \prod_{i=1}^D \mathcal{N}(w_i; 0, \sigma^2) = \mathcal{N}(\boldsymbol w; \boldsymbol 0, \sigma^2 \boldsymbol I)$. Then

$$\begin{aligned}\boldsymbol w_\mathrm{MAP} &= \arg\max_{\boldsymbol w} p(\boldsymbol X | \boldsymbol w) p(\boldsymbol w) \\ &= \arg\max_{\boldsymbol w} \prod\nolimits_{i=1}^N p(\boldsymbol x_i | \boldsymbol w) p(\boldsymbol w) \\ &= \arg\min_{\boldsymbol w} \sum\nolimits_{i=1}^N \Big(-\log p(\boldsymbol x_i | \boldsymbol w) - \log p(\boldsymbol w)\Big).\end{aligned}$$

By substituting the probability of the Gaussian prior, we get

$$\boldsymbol w_\mathrm{MAP} = \arg\min_{\boldsymbol w} \sum\nolimits_{i=1}^N \Big(-\log p(\boldsymbol x_i | \boldsymbol w) + \frac{D}{2}\log(2\pi\sigma^2) + \frac{\|\boldsymbol w\|^2}{2\sigma^2}\Big),$$

which is in fact the L^2-regularization.

Conjugate Distributions

- In Bayesian thinking, we typically think about distribution over parameters.
- After one coin toss (Bernoulli distribution), we do not believe there is a 100% probability of what happened because we had a prior belief of how a coin behaves.
- We believed the parameter p was distributed somehow and after the observation we believe in something else (by applying the Bayes theorem).
- Conjugate distribution: prior and posterior are of the same family.
- Instead of confidence intervals, credibility intervals over the parameters.

Naive Bayes Classifier

Naive Bayes Classifier: Overview

So far, our classifiers were so-called **discriminative** and had a form

$$p(C_k|\boldsymbol{x}) = p(C_k|x_1, x_2, \ldots, x_D).$$

Instead, we might use the Bayes' theorem, and rewrite the conditional probability to

$$p(C_k|\boldsymbol{x}) = \frac{p(\boldsymbol{x}|C_k)p(C_k)}{p(\boldsymbol{x})}.$$

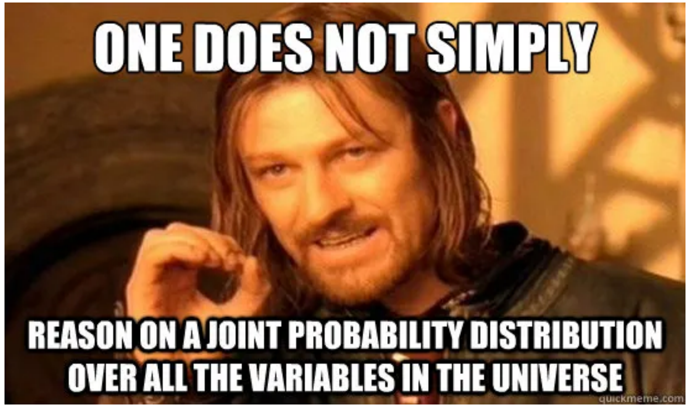
Then, classification could be performed as

$$\arg\max_k p(C_k|\boldsymbol{x}) = \arg\max_k \frac{p(\boldsymbol{x}|C_k)p(C_k)}{p(\boldsymbol{x})} = \arg\max_k p(\boldsymbol{x}|C_k)p(C_k).$$

Therefore, instead of modeling $p(C_k|\boldsymbol{x})$, we model

- the prior $p(C_k)$ according to the distribution of classes in the data, and
- the distribution $p(\boldsymbol{x}|C_k)$.

Modeling the distribution $p(\boldsymbol{x}|C_k)$ is difficult – $\boldsymbol{x}$ can be high-dimensional structured data.



https://medium.datadriveninvestor.com/naive-bayes-d36e57d80652

Therefore, the so-called **Naive Bayes classifier** assumes that

> *all x_d are independent given C_k,*

so we can rewrite

$$p(\boldsymbol{x}|C_k) = p(x_1|C_k)p(x_2|C_k, x_1)p(x_3|C_k, x_1, x_2)\cdots p(x_D|C_k, x_1, x_2, \ldots)$$

to

$$p(\boldsymbol{x}|C_k) = \prod\nolimits_{d=1}^{D} p(x_d|C_k).$$

Modeling $p(x_d|C_k)$ is substantially easier because it is a distribution over a single-dimensional quantity.

There are in fact several naive Bayes classifiers, depending on the distribution $p(x_d|C_k)$.

Gaussian Naive Bayes

In Gaussian naive Bayes, we expect a continuous feature to have normal distribution for a given C_k, and model $p(x_d|C_k)$ as a normal distribution $\mathcal{N}(\mu_{d,k}, \sigma^2_{d,k})$.

Assuming we have the training data $\boldsymbol{X}$ together with K-class classification targets $\boldsymbol{t}$, the "training" phase consists of estimating the parameters $\mu_{d,k}$ and $\sigma^2_{d,k}$ of the distributions $\mathcal{N}(\mu_{d,k}, \sigma^2_{d,k})$ for $1 \leq d \leq D$, $1 \leq k \leq K$, employing the maximum likelihood estimation.

Now let feature d and class k be fixed and let $\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_{N_k}$ be the training data *corresponding to the class* k. We already know that maximum likelihood estimation using N_k samples drawn from a Gaussian distribution $\mathcal{N}(\mu_{d,k}, \sigma^2_{d,k})$ amounts to

$$\operatorname*{arg\,min}_{\mu_{d,k}, \sigma_{d,k}} \frac{N_k}{2} \log(2\pi\sigma^2_{d,k}) + \sum_{i=1}^{N_k} \frac{(x_{i,d} - \mu_{d,k})^2}{2\sigma^2_{d,k}}.$$

Gaussian Naive Bayes

Setting the derivative with respect to $\mu_{d,k}$ to zero results in

$$0 = \sum\nolimits_{i=1}^{N_k} \frac{-2(x_{i,d} - \mu_{d,k})}{2\sigma_{d,k}^2},$$

which we can rewrite to $\mu_{d,k} = \frac{1}{N_k} \sum_{i=1}^{N_k} x_{i,d}$.

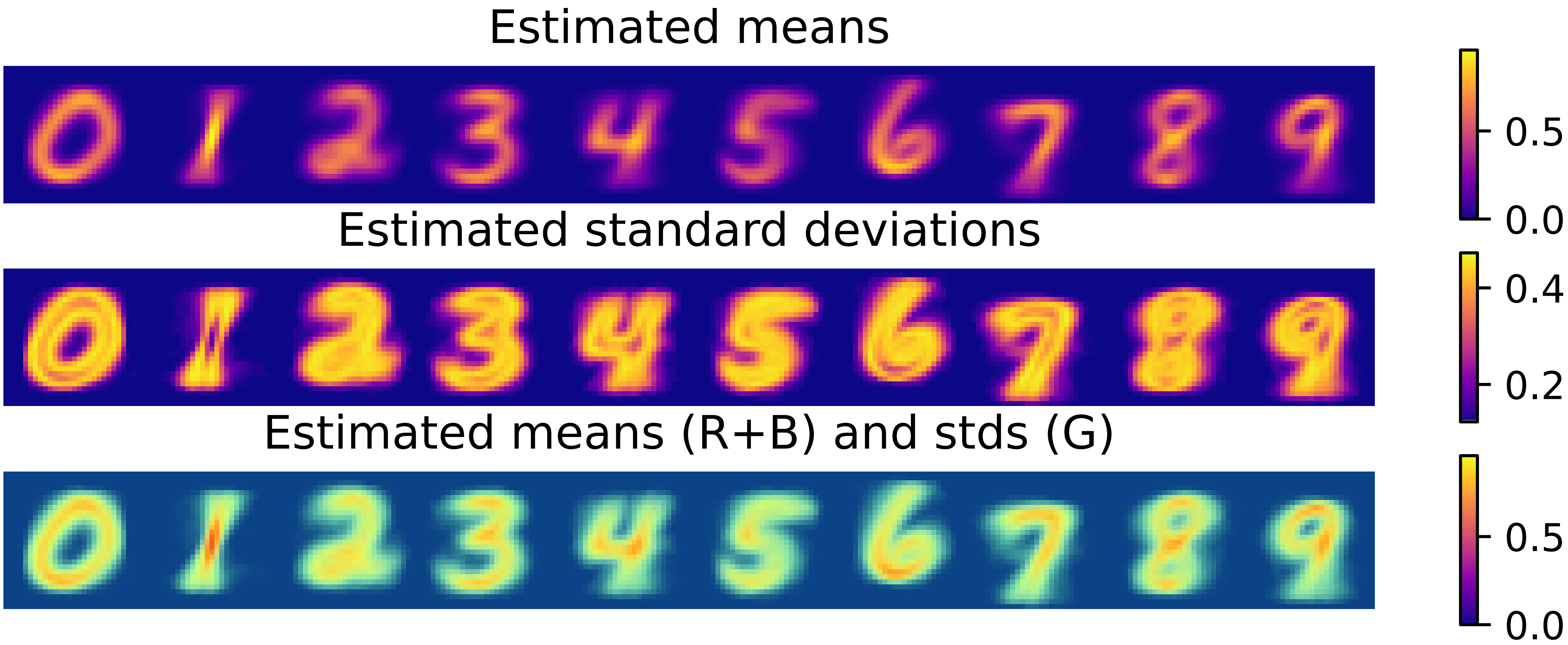
Similarly, zeroing out the derivative with respect to $\sigma_{d,k}^2$ gives

$$0 = \frac{N_k}{2\sigma_{d,k}^2} - \frac{1}{2(\sigma_{d,k}^2)^2} \sum\nolimits_{i=1}^{N_k} (x_{i,d} - \mu_{d,k})^2,$$

from which we obtain $\sigma_{d,k}^2 = \frac{1}{N_k} \sum_{i=1}^{N_k} (x_{i,d} - \mu_{d,k})^2$.

However, the variances are usually smoothed (increased) by a given constant α to avoid too sharp distributions (in Scikit-learn, the default value of α is 10^{-9} times the largest variance of all features).

Gaussian Naive Bayes Example



Means and standard deviations estimated by Gaussian NB on a subset of the MNIST dataset.

Bernoulli Naive Bayes

When the input features are binary, the $p(x_d|C_k)$ might be modeled using a Bernoulli distribution

$$p(x_d|C_k) = p_{d,k}^{x_d} \cdot (1 - p_{d,k})^{(1-x_d)}.$$

We can therefore write

$$p(C_k|\boldsymbol{x}) \propto \Big(\prod\nolimits_{d=1}^{D} p_{d,k}^{x_d} \cdot (1 - p_{d,k})^{(1-x_d)}\Big) p(C_k),$$

and by computing a logarithm we get

$$\log p(C_k|\boldsymbol{x}) + c = \log p(C_k) + \sum\nolimits_d \Big(x_d \log \tfrac{p_{d,k}}{1-p_{d,k}} + \log(1 - p_{d,k})\Big) = b_k + \boldsymbol{x}^T \boldsymbol{w}_k,$$

where the constant c does not depend on C_k and is therefore not needed for prediction

$$\arg\max_k \log p(C_k|\boldsymbol{x}) = \arg\max_k b_k + \boldsymbol{x}^T \boldsymbol{w}_k.$$

Bernoulli Naive Bayes Estimation: Derivation

To estimate the probabilities $p_{d,k}$, we turn again to the maximum likelihood estimation. The log-likelihood of N_k samples drawn from Bernoulli distribution with parameter $p_{d,k}$ is

$$\sum\nolimits_{i=1}^{N_k} \log \left(p_{d,k}^{x_{i,d}}(1 - p_{d,k})^{1-x_{i,d}}\right) = \sum\nolimits_{i=1}^{N_k} \left(x_{i,d} \log p_{d,k} + (1 - x_{i,d}) \log(1 - p_{d,k})\right).$$

Setting the derivative with respect to $p_{d,k}$ to zero, we obtain

$$0 = \sum\nolimits_{i=1}^{N_k} \left(\frac{x_{i,d}}{p_{d,k}} - \frac{1 - x_{i,d}}{1 - p_{d,k}}\right) = \frac{1}{p_{d,k}(1 - p_{d,k})} \sum\nolimits_{i=1}^{N_k} \Big((1 - p_{d,k})x_{i,d} - p_{d,k}(1 - x_{i,d})\Big),$$

giving us $p_{d,k} = \frac{1}{N_k} \sum_{i=1}^{N_k} x_{i,d}$.

Bernoulli Naive Bayes Estimation: Smoothing

We could therefore estimate the probabilities $p_{d,k}$ as

$$p_{d,k} = \frac{\text{number of documents of class } k \text{ with nonzero feature } d}{\text{number of documents of class } k}.$$

However, if a feature d is always set to one (or zero) for a given class k, then $p_{d,k} = 1$ (or 0). That is impractical because the resulting classifier would give probability zero to inputs with the opposite value of such a feature.

Therefore, **Laplace** or **additive smoothing** is used, and the probability $p_{d,k}$ estimated as

$$p_{d,k} = \frac{\text{number of documents of class } k \text{ with nonzero feature } d + \alpha}{\text{number of documents of class } k + 2\alpha}$$

for some pseudo-count $\alpha > 0$.

Note that even if this technique has a special name, it corresponds to using a *maximum a posteriori* estimate, using $\operatorname{Beta}(\alpha+1, \alpha+1)$ as a prior distribution.

Multinomial Naive Bayes

The last variant of naive Bayes we will describe is the **multinomial naive Bayes**, where $p(\boldsymbol{x}|C_k)$ is modeled to be multinomial distribution, $p(\boldsymbol{x}|C_k) \propto \prod_d p_{d,k}^{x_d}$.

Similarly to the Bernoulli NB case, we can write the log-likelihood as

$$\log p(C_k|\boldsymbol{x}) + c = \log p(C_k) + \sum\nolimits_d x_d \log p_{d,k} = b_k + \boldsymbol{x}^T \boldsymbol{w}_k.$$

Multinomial Naive Bayes Estimation

As in the previous cases, we turn to the maximum likelihood estimation in order to find out the values of $p_{d,k}$. We start with the log-likelihood

$$\sum_{i=1}^{N_k} \log\Big(\prod\nolimits_d p_{d,k}^{x_{i,d}}\Big) = \sum\nolimits_{i,d} x_{i,d} \log p_{d,k}.$$

To maximize this quantity with respect to a probability distribution $\sum_d p_{d,k} = 1$, we need to form a *Lagrangian*

$$\mathcal{L} = \sum\nolimits_{i,d} x_{i,d} \log p_{d,k} + \lambda\Big(1 - \sum\nolimits_d p_{d,k}\Big).$$

Setting the derivative with respect to $p_{d,k}$ to zero results in $0 = \sum_{i=1}^{N_k} \frac{x_{i,d}}{p_{d,k}} - \lambda$, so

$$p_{d,k} = \frac{1}{\lambda} \sum_{i=1}^{N_k} x_{i,d} = \frac{\sum_{i=1}^{N_k} x_{i,d}}{\sum_{i=1}^{N_k} \sum_{d'=1}^{D} x_{i,d'}}, \text{ where } \lambda \text{ is set to fulfill } \sum\nolimits_d p_{d,k} = 1.$$

Multinomial Naive Bayes Estimation: Smoothing

Denoting $n_{d,k}$ as the sum of features x_d for a class C_k, the probabilities $p_{d,k}$ could be therefore estimated as

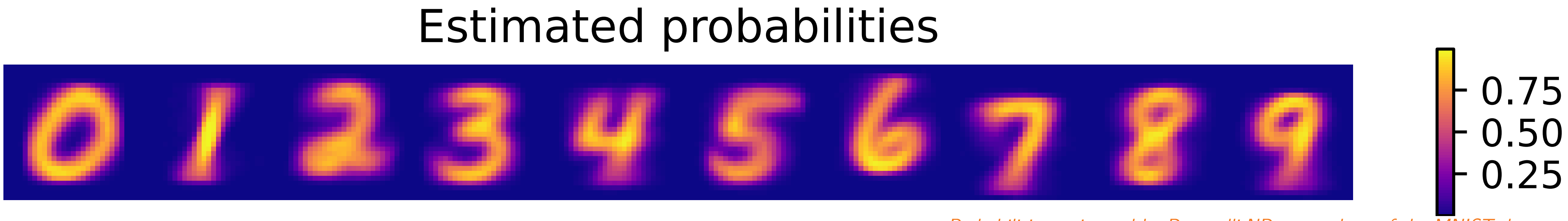
$$p_{d,k} = \frac{n_{d,k}}{\sum_{d'=1}^{D} n_{d',k}}.$$

However, for the same reasons as in the Bernoulli NB case, we also use the Laplace smoothing, i.e., utilize a Dirichlet prior $\operatorname{Dir}(\alpha + 1)$, and instead use

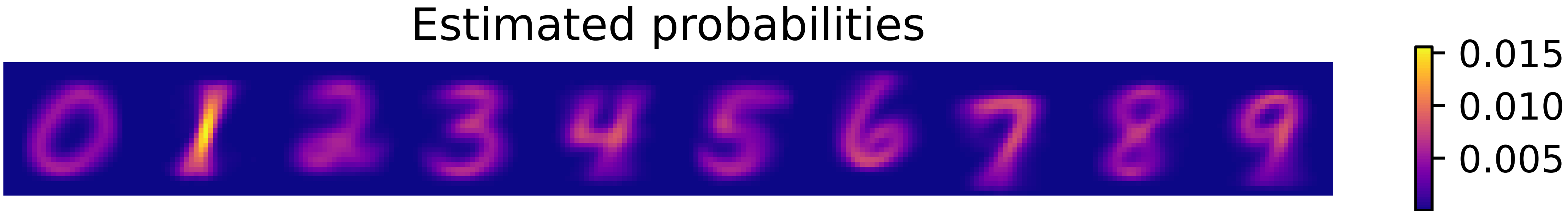
$$p_{d,k} = \frac{n_{d,k} + \alpha}{\sum_{d'=1}^{D}(n_{d',k} + \alpha)} = \frac{n_{d,k} + \alpha}{\left(\sum_{d'=1}^{D} n_{d',k}\right) + \alpha D}$$

with pseudo-count $\alpha > 0$.

Naive Bayes Example



Probabilities estimated by Bernoulli NB on a subset of the MNIST dataset.



Probabilities estimated by multinomial NB on a subset of the MNIST dataset.

Means estimated by Gaussian NB on a subset of the MNIST dataset.

Naive Bayes Conclusions

The choice among the Gaussian, Bernoulli and multinomial naive Bayes depends on the feature values.

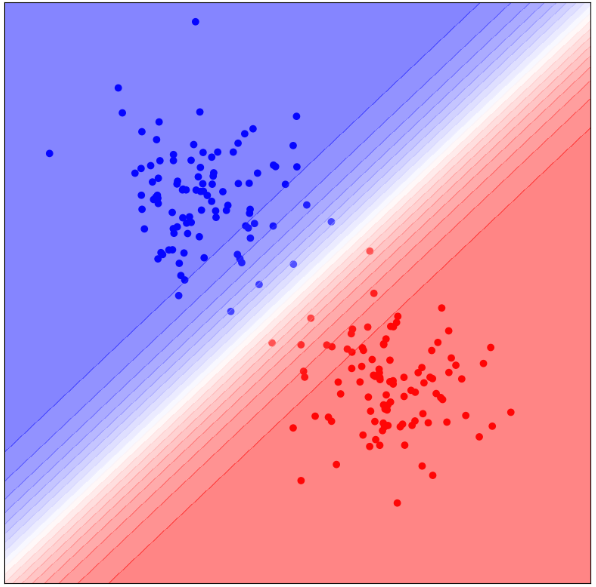
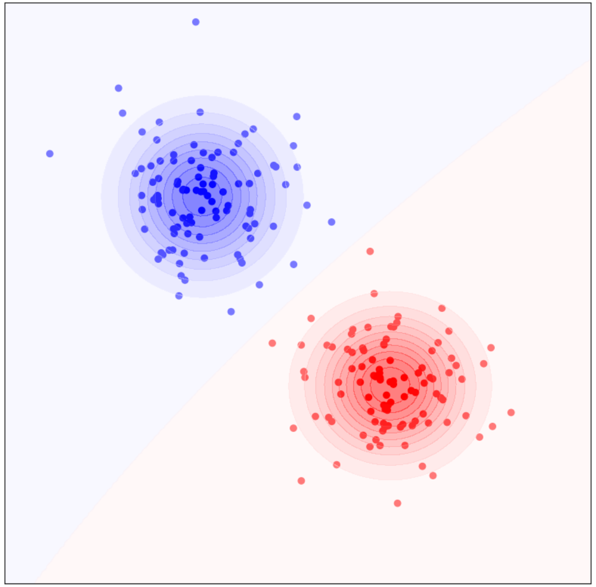
- If we expect the individual feature values to be roughly normally distributed, Gaussian NB is an obvious choice.
- To use multinomial NB, the features should roughly follow the multinomial distribution – they must be nonnegative, be interpretable as "counts", and "compete" with each other.
- In order to use Bernoulli NB, the features *must* be binary. However, an important difference is that contrary to the multinomial NB, the **absence of features** is also modeled by the $(1 - p_{d,k})$ term; the multinomial NB uses $p_{d,k}^0 = 1$ in such a case.

Generative and Discriminative Models

Generative and Discriminative Models

So far, all our classification models (except for the naive Bayes) have been **discriminative**, modeling a *conditional distribution* $p(t|\boldsymbol{x})$.

On the other hand, the **generative models** estimate *joint distribution* $p(t, \boldsymbol{x})$, often by employing Bayes' theorem and estimating $p(\boldsymbol{x}|t) \cdot p(t)$. They therefore model the probability of the data being generated by an outcome and only transform it to $p(t|\boldsymbol{x})$ during prediction.

	Discriminative Model	Generative Model
Goal	Estimate $P(t\|\boldsymbol{x})$	Estimate $P(t, \boldsymbol{x}) = P(\boldsymbol{x}\|t)P(t)$
What's learned	Decision boundary	Probability distribution of the data
Illustration		

Generative and Discriminative Models: Remarks

- Big topic in 2000's: Generative models are better with very little data, with enough data discriminative models are always better.
- What is now called generative (LLMs, Diffusion models) is disputable

Today's Lecture Objectives

After this lecture you should be able to

- Implement and use k-nearest neighbors for classification and regression
- Explain the very basic principles of Bayesian thinking
- Implement and use Naive Bayes Classifier