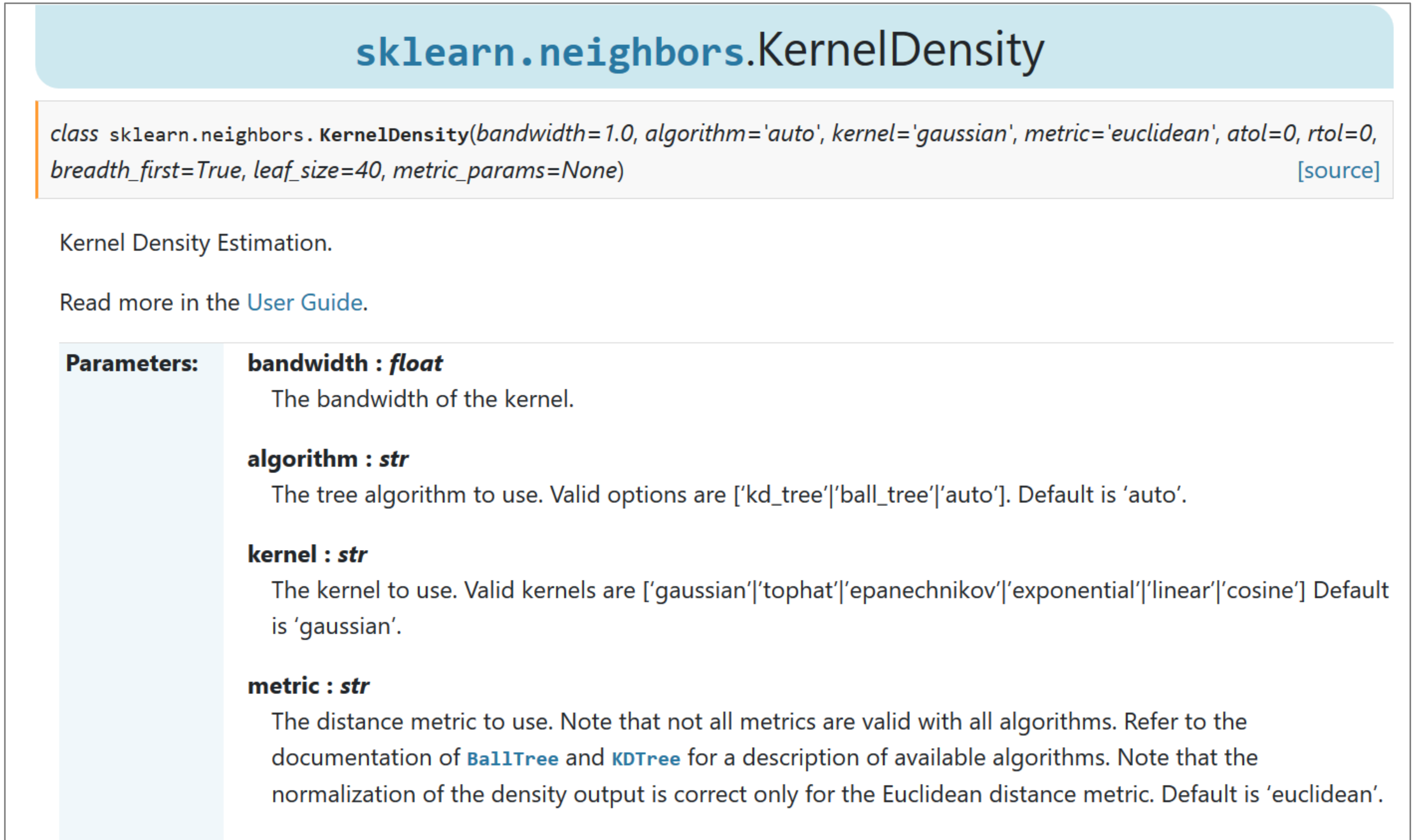
Bayesian Classifiers and Kernel Density Estimation

PHYS 453

Dr Daugherty

Neighbors???

Mystery for today: what is this thing? And what does it have to do with neighbors?



sklearn.neighbors.KernelDensity

class `sklearn.neighbors.`**`KernelDensity`**(*bandwidth=1.0, algorithm='auto', kernel='gaussian', metric='euclidean', atol=0, rtol=0, breadth_first=True, leaf_size=40, metric_params=None*) [source]

Kernel Density Estimation.

Read more in the User Guide.

Parameters:

bandwidth : *float*
The bandwidth of the kernel.

algorithm : *str*
The tree algorithm to use. Valid options are ['kd_tree'|'ball_tree'|'auto']. Default is 'auto'.

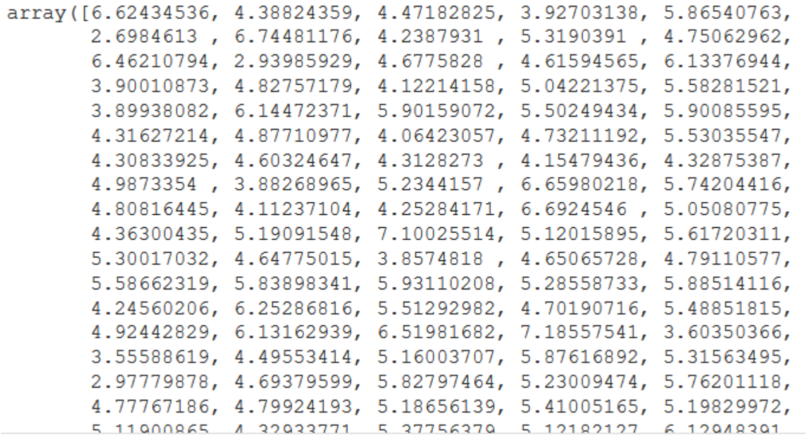
kernel : *str*
The kernel to use. Valid kernels are ['gaussian'|'tophat'|'epanechnikov'|'exponential'|'linear'|'cosine'] Default is 'gaussian'.

metric : *str*
The distance metric to use. Note that not all metrics are valid with all algorithms. Refer to the documentation of `BallTree` and `KDTree` for a description of available algorithms. Note that the normalization of the density output is correct only for the Euclidean distance metric. Default is 'euclidean'.

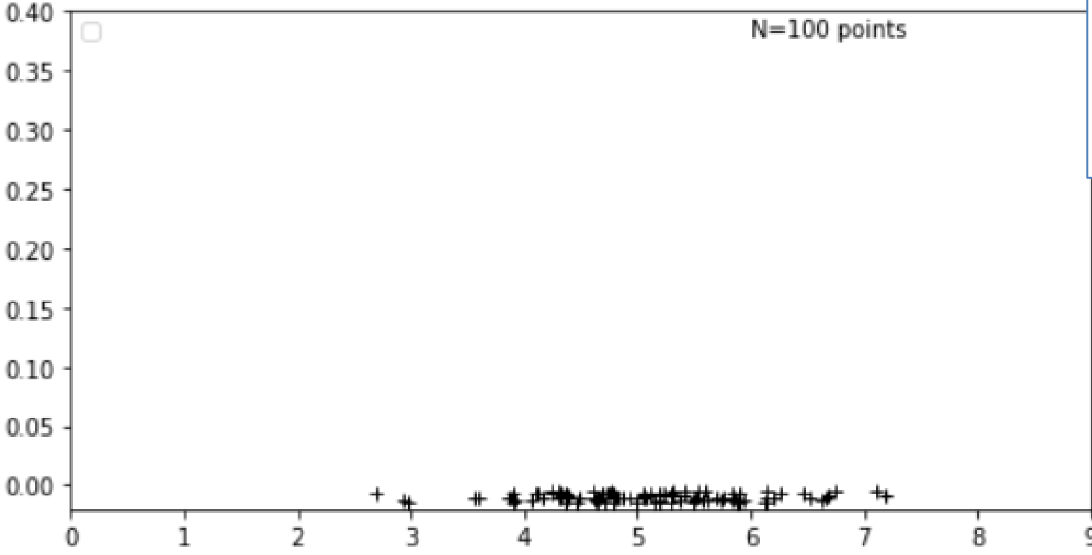
Kernel Density Estimation

The Problem

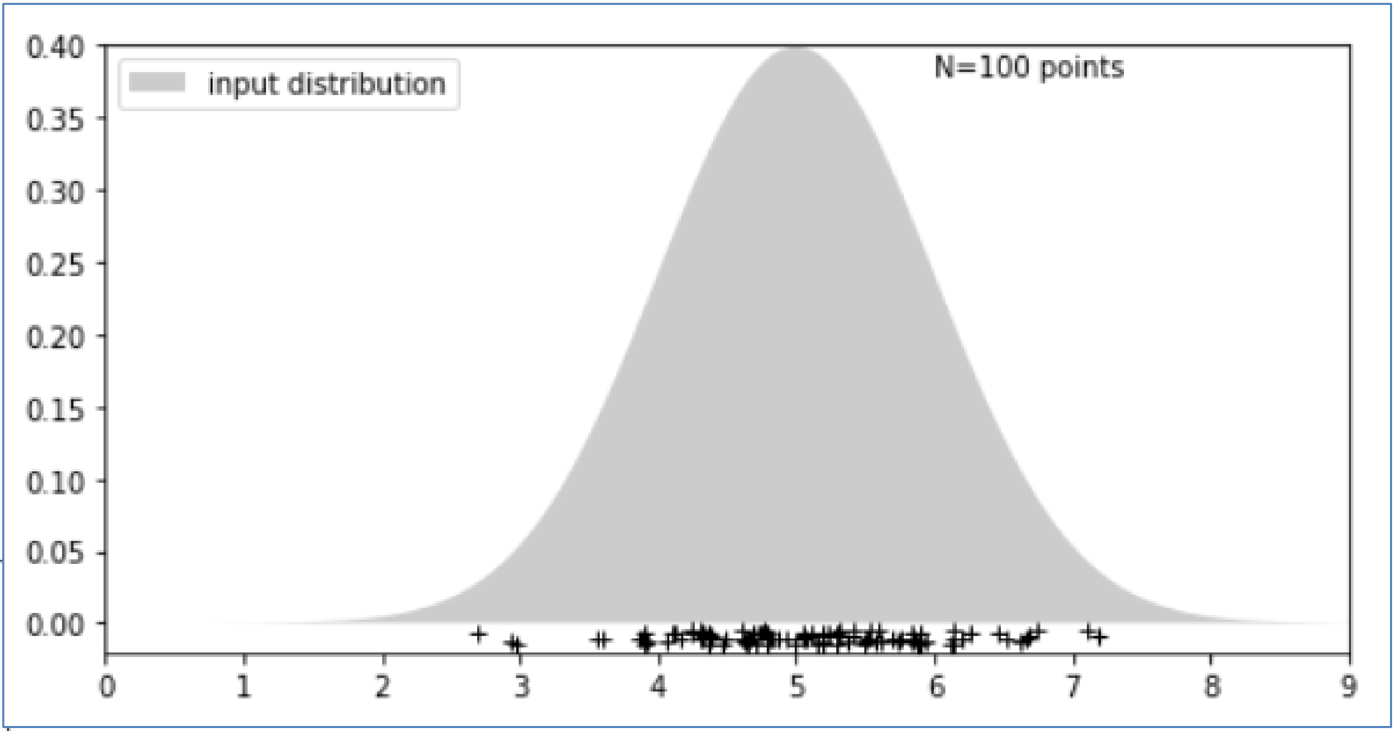
Given a list of training data points:

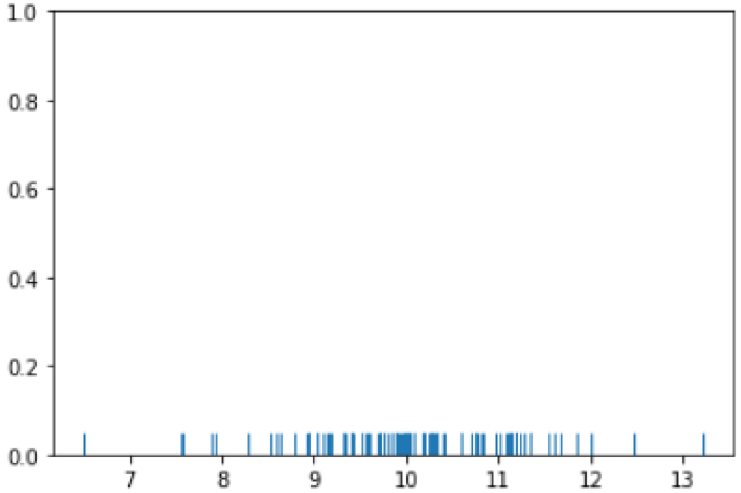


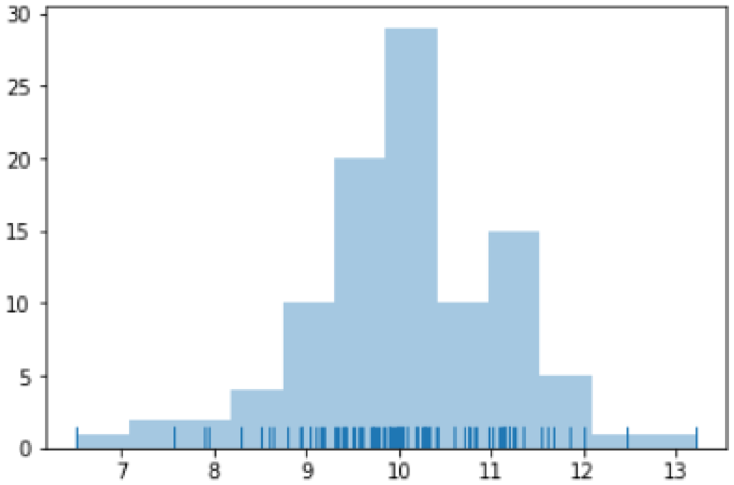
```
array([6.62434536, 4.38824359, 4.47182825, 3.92703138, 5.86540763,
       2.6984613 , 6.74481176, 4.2387931 , 5.3190391 , 4.75062962,
       6.46210794, 2.93985929, 4.6775828 , 4.61594565, 6.13376944,
       3.90010873, 4.82757179, 4.12214158, 5.04221375, 5.58281521,
       3.89938082, 6.14472371, 5.90159072, 5.50249434, 5.90085595,
       4.31627214, 4.87710977, 4.06423057, 4.73211192, 5.53035547,
       4.30833925, 4.60324647, 4.3128273 , 4.15479436, 4.32875387,
       4.9873354 , 3.88268965, 5.2344157 , 6.65980218, 5.74204416,
       4.80816445, 4.11237104, 4.25284171, 6.6924546 , 5.05080775,
       4.36300435, 5.19091548, 7.10025514, 5.12015895, 5.61720311,
       5.30017032, 4.64775015, 3.8574818 , 4.65065728, 4.79110577,
       5.58662319, 5.83898341, 5.93110208, 5.28558733, 5.88514116,
       4.24560206, 6.25286816, 5.51292982, 4.70190716, 5.48851815,
       4.92442829, 6.13162939, 6.51981682, 7.18557541, 3.60350366,
       3.55588619, 4.49553414, 5.16003707, 5.87616892, 5.31563495,
       2.97779878, 4.69379599, 5.82797464, 5.23009474, 5.76201118,
       4.77767186, 4.79924193, 5.18656139, 5.41005165, 5.19829972,
       5.11900865  4.32933771  5.37756379  5.12182127  6.12948391
```

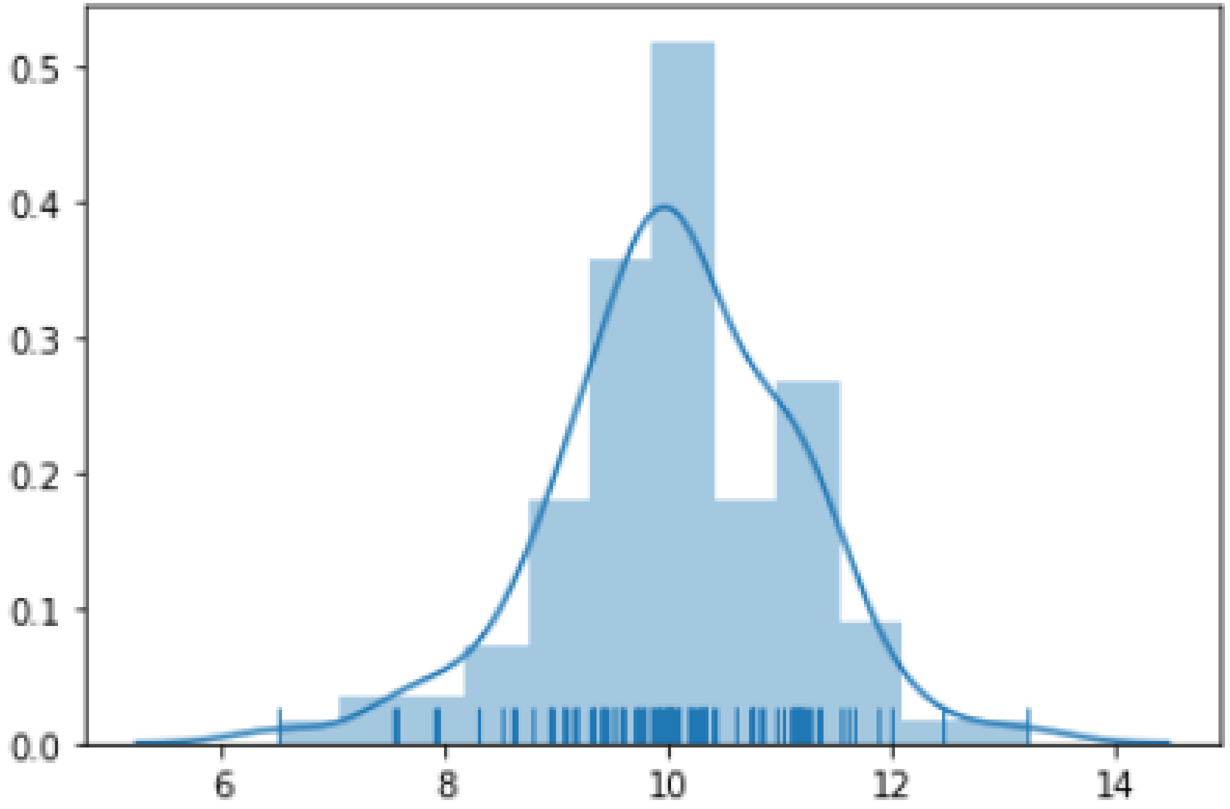


Estimate a probability distribution function




1.0
0.8
0.6
0.4
0.2
0.0
7
8
9
10
11
12
13


30
25
20
15
10
5
0
7
8
9
10
11
12
13


0.5
0.4
0.3
0.2
0.1
0.0
6
8
10
12
14

One approach:

To estimate the probability at a point, grow a circle until it contains k neighbors, then the probability is proportional to k / “Volume” of the region.

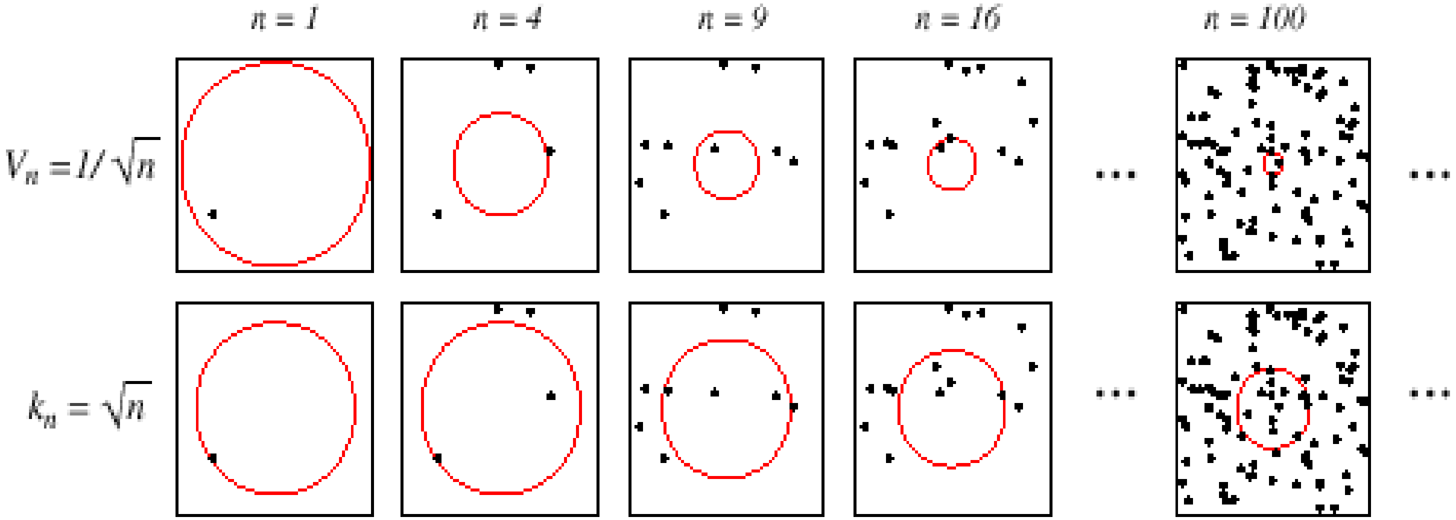
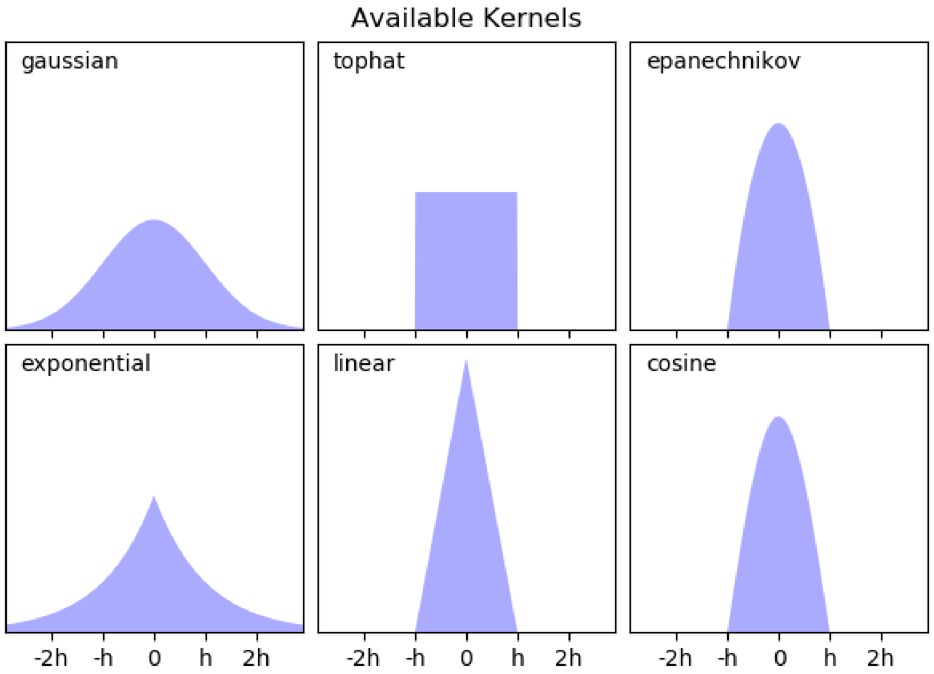


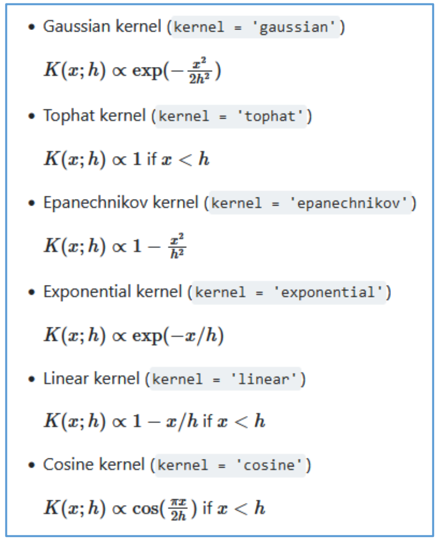
FIGURE 4.2. There are two leading methods for estimating the density at a point, here at the center of each square. The one shown in the top row is to start with a large volume centered on the test point and shrink it according to a function such as $V_n = 1/\sqrt{n}$. The other method, shown in the bottom row, is to decrease the volume in a data-dependent way, for instance letting the volume enclose some number $k_n = \sqrt{n}$ of sample points. The sequences in both cases represent random variables that generally converge and allow the true density at the test point to be calculated. From: Richard O. Duda, Peter E. Hart, and David G. Stork, *Pattern Classification*. Copyright © 2001 by John Wiley & Sons, Inc.

Reverse approach:

Draw a “kernel” (a shape with some set width) centered on every data point. The probability is proportional to the **sum** of all of these shapes.

https://scikit-learn.org/stable/auto_examples/neighbors/plot_kde_1d.html





- Gaussian kernel (`kernel = 'gaussian'`)

  $K(x;h) \propto \exp(-\frac{x^2}{2h^2})$

- Tophat kernel (`kernel = 'tophat'`)

  $K(x;h) \propto 1$ if $x < h$

- Epanechnikov kernel (`kernel = 'epanechnikov'`)

  $K(x;h) \propto 1 - \frac{x^2}{h^2}$

- Exponential kernel (`kernel = 'exponential'`)

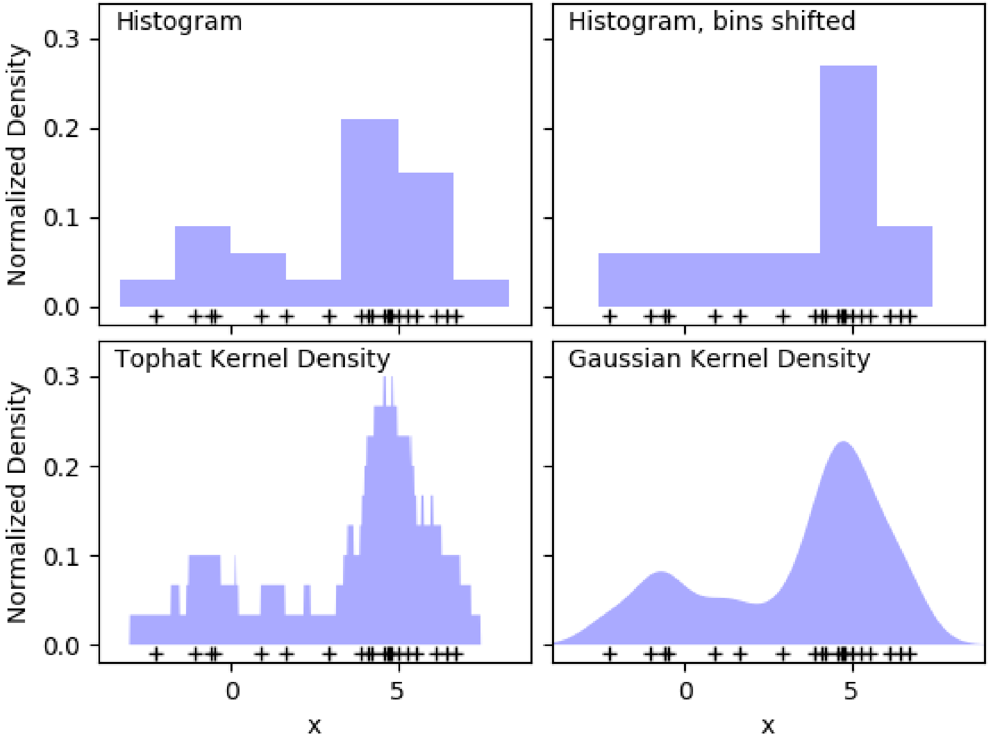
  $K(x;h) \propto \exp(-x/h)$

- Linear kernel (`kernel = 'linear'`)

  $K(x;h) \propto 1 - x/h$ if $x < h$

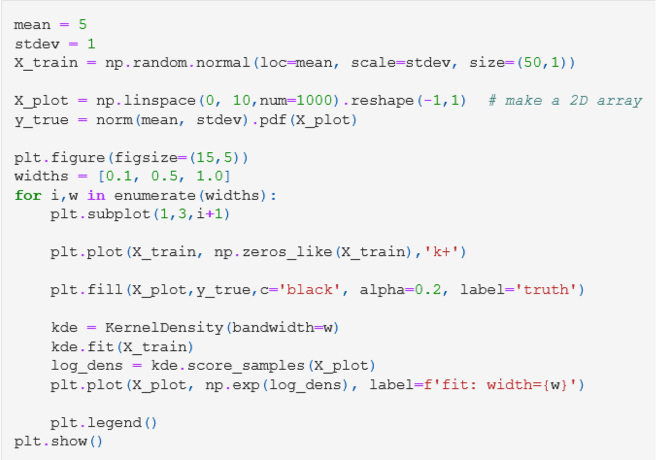
- Cosine kernel (`kernel = 'cosine'`)

  $K(x;h) \propto \cos(\frac{\pi x}{2h})$ if $x < h$

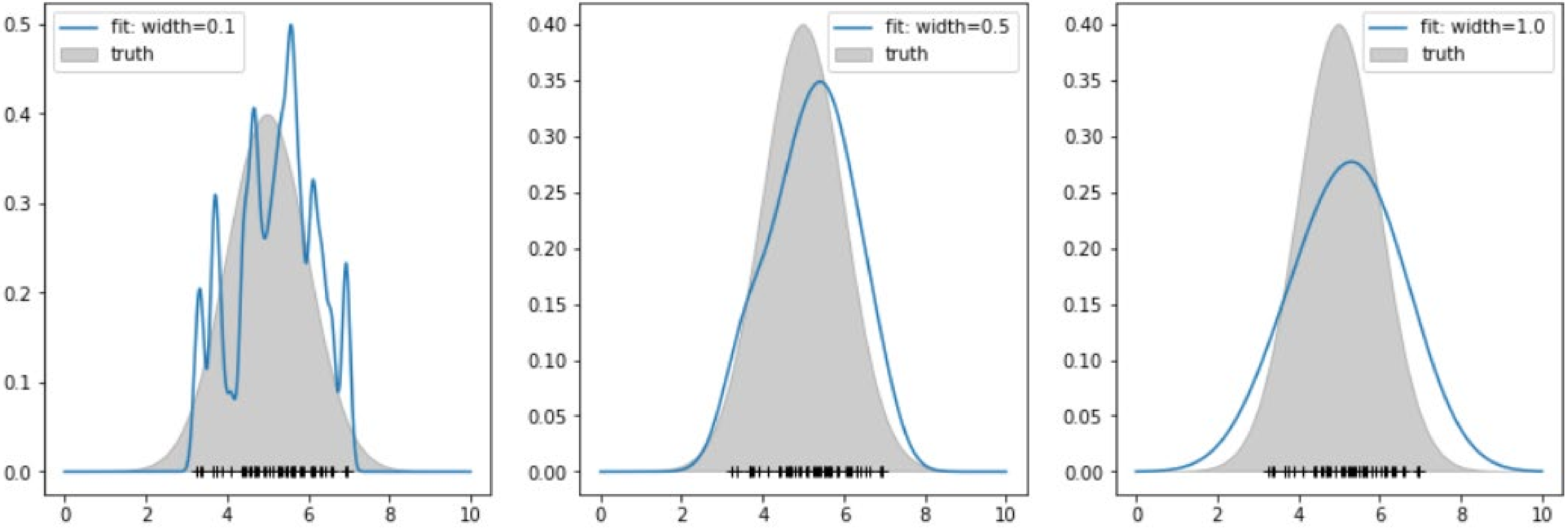


To estimate the probability at a point, find all “close” neighbors and add their kernels.

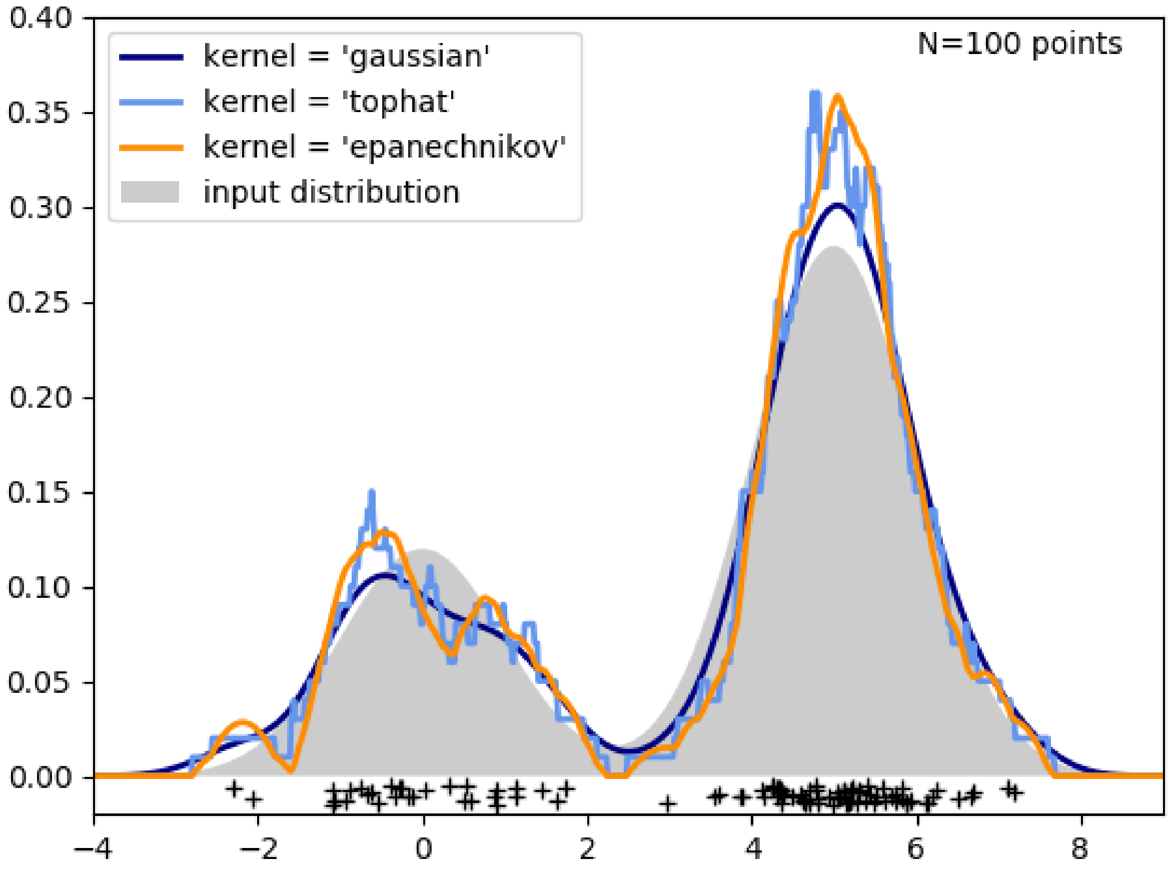
https://github.com/mdaugherity/PatternRecognition2020/blob/master/Class%20Work/Class%202-21%20KDE.ipynb



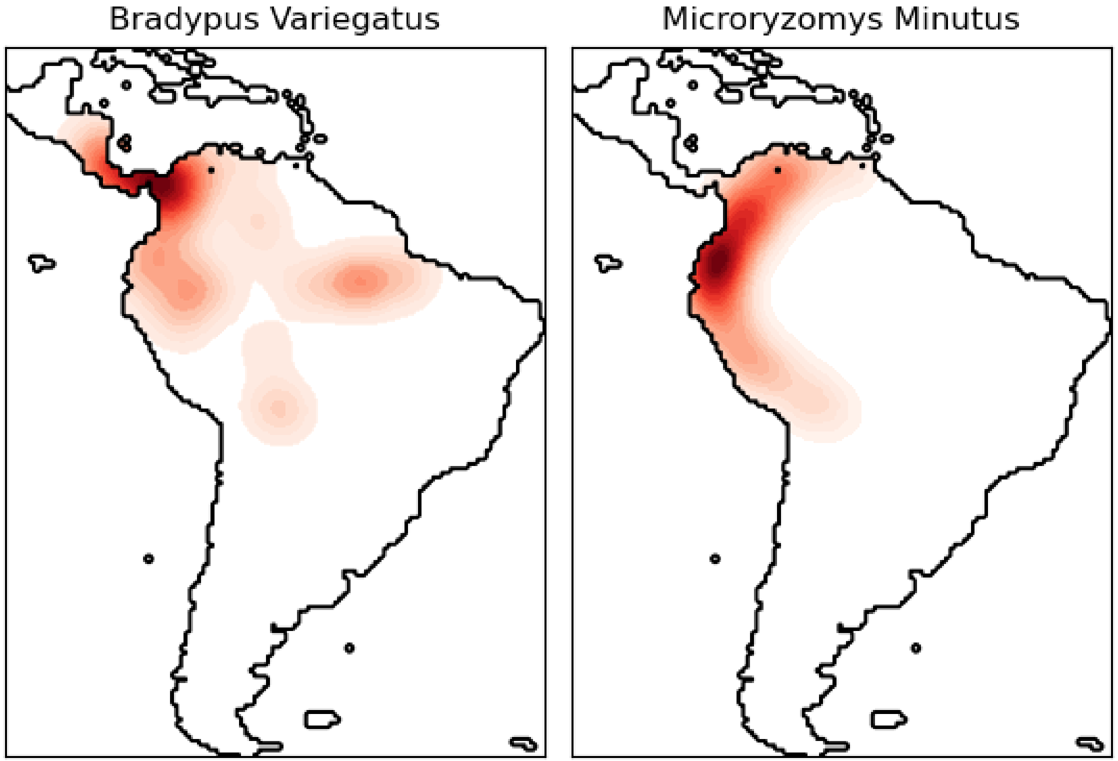
```
mean = 5
stdev = 1
X_train = np.random.normal(loc=mean, scale=stdev, size=(50,1))

X_plot = np.linspace(0, 10,num=1000).reshape(-1,1)  # make a 2D array
y_true = norm(mean, stdev).pdf(X_plot)

plt.figure(figsize=(15,5))
widths = [0.1, 0.5, 1.0]
for i,w in enumerate(widths):
    plt.subplot(1,3,i+1)

    plt.plot(X_train, np.zeros_like(X_train),'k+')

    plt.fill(X_plot,y_true,c='black', alpha=0.2, label='truth')

    kde = KernelDensity(bandwidth=w)
    kde.fit(X_train)
    log_dens = kde.score_samples(X_plot)
    plt.plot(X_plot, np.exp(log_dens), label=f'fit: width={w}')

    plt.legend()
plt.show()
```



https://scikit-learn.org/stable/auto_examples/neighbors/plot_kde_1d.html

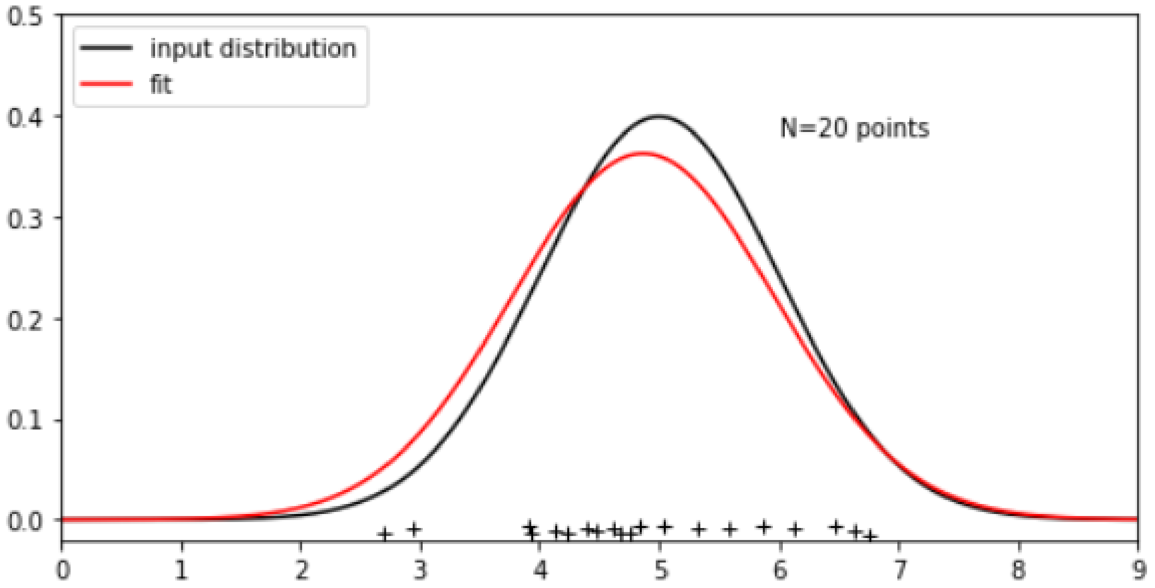


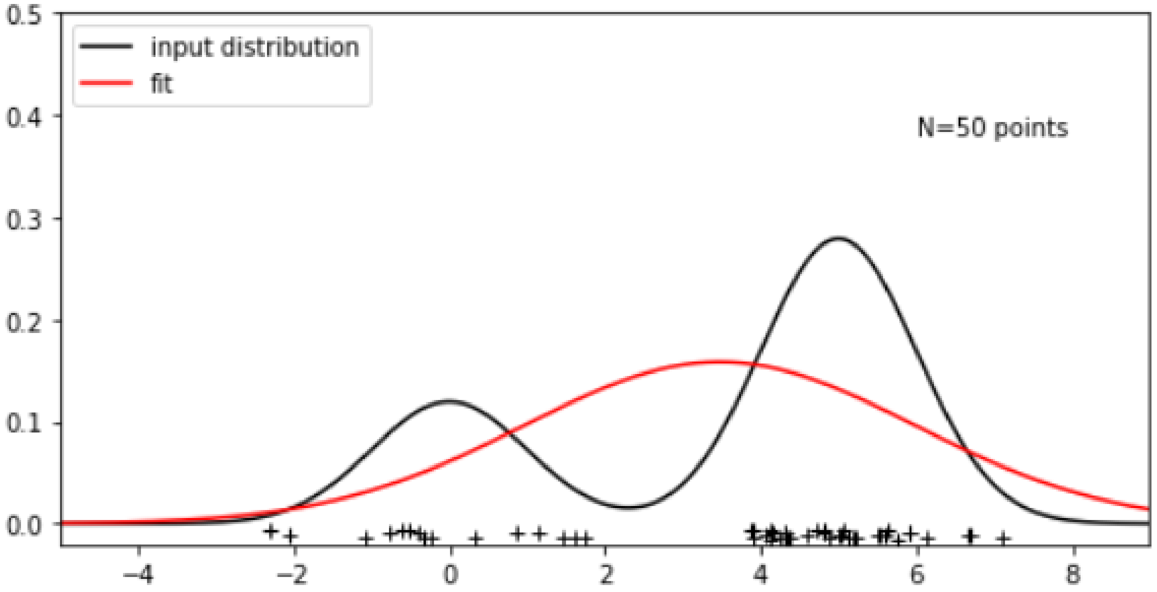
https://scikit-learn.org/stable/auto_examples/neighbors/plot_species_kde.html



Third approach:

Fit the entire distribution to some function and hope for the best.



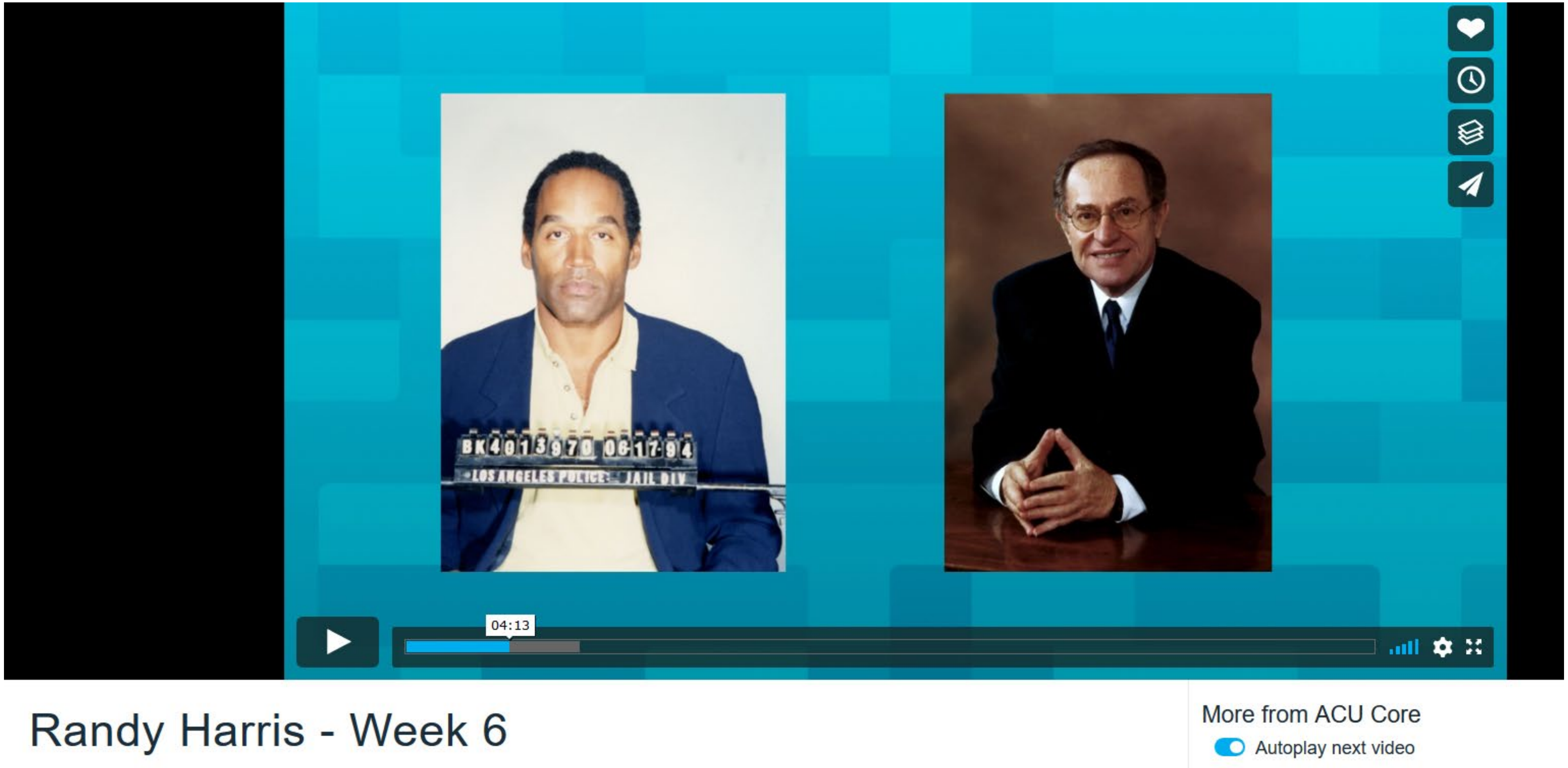


Bayesian Statistics

Bayesian Statistics

So what can I do if I have an equation for the probability distributions?

A great option is to apply Bayes’ Theorem to get the probabilities of each class https://vimeo.com/71446628



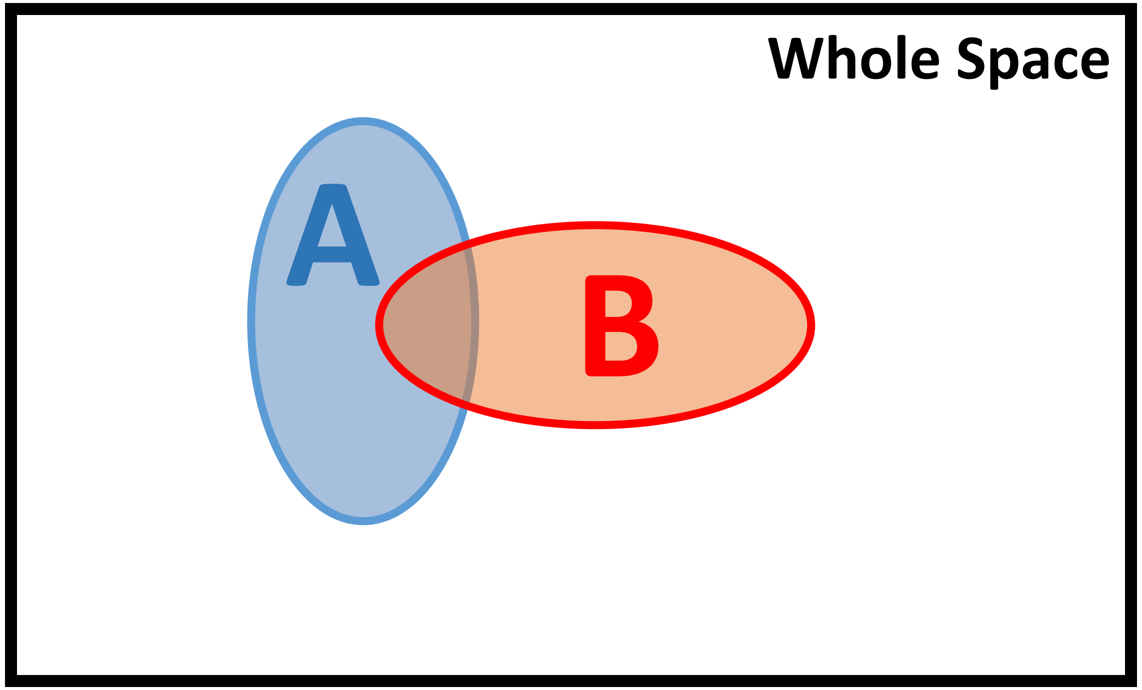
Randy Harris - Week 6

Randy Harris
September 30, 2013
(Start at 4:00 mark)

Graphical Derivation of Bayes’ Theorem

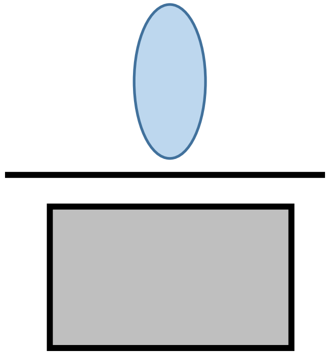
Source: http://www.science20.com/quantum_diaries_survivor/you_bayesian

Define subsets A and B

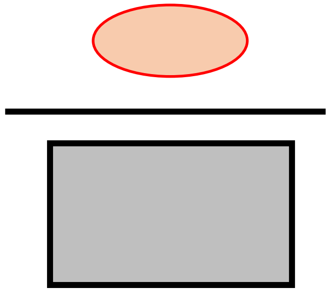


Basic Probabilities:

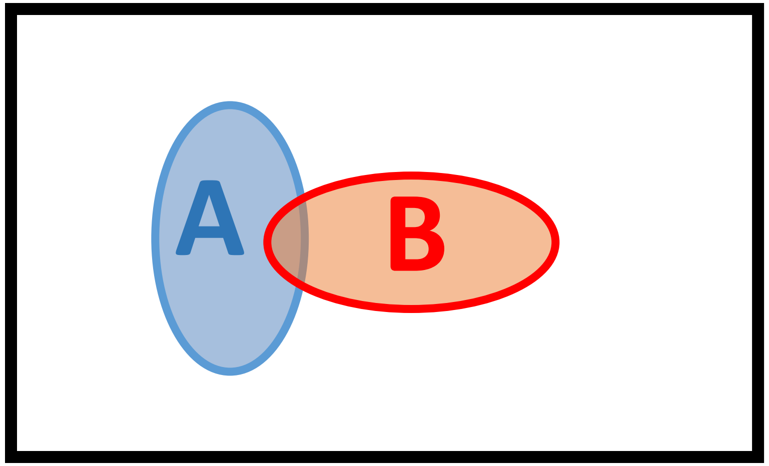
P(A) =



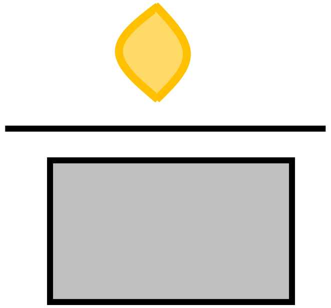
P(B) =



Combined Probabilities

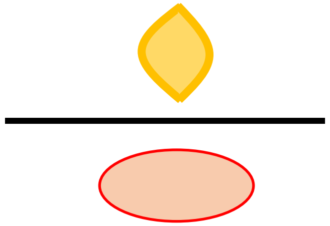


Intersection:

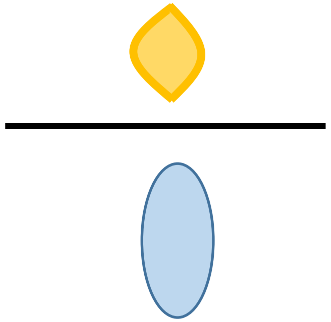
P(A∩B) = 

A **and** B

Conditional Probabilities:

P(A|B) = 

A **given** B

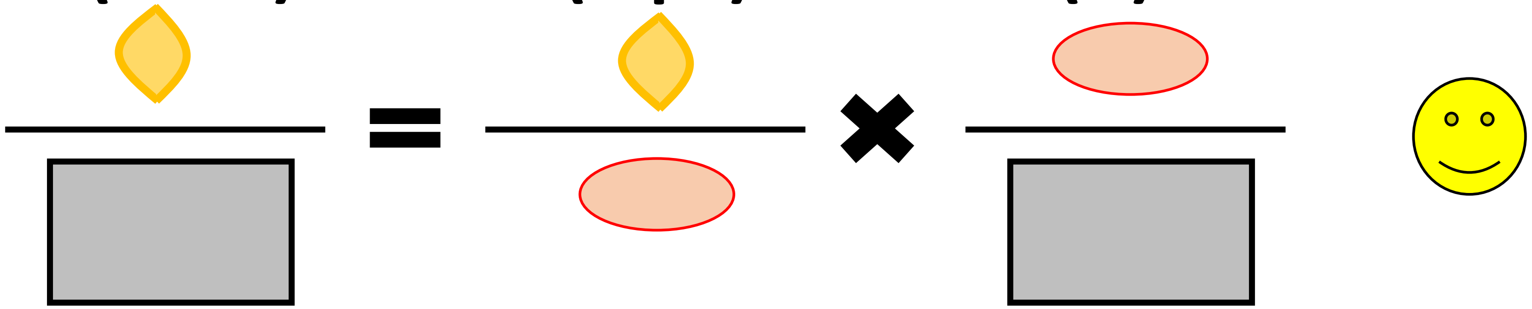
P(B|A) = 

B **given** A

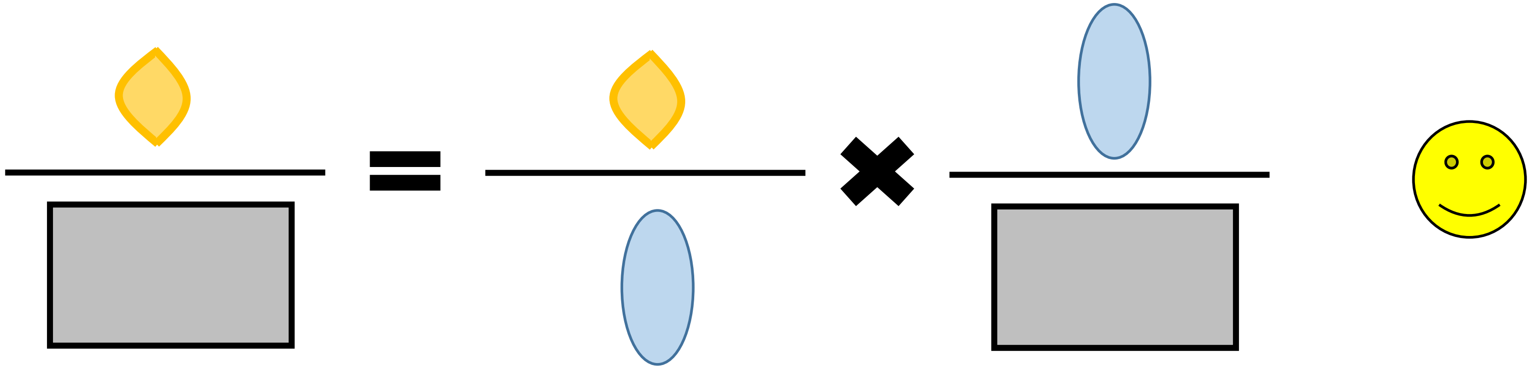
Derivation:

$$P(A \cap B) = P(A|B) * P(B) = P(B|A) * P(A)$$

Check 1: **P(A∩B) = P(A|B) * P(B)**

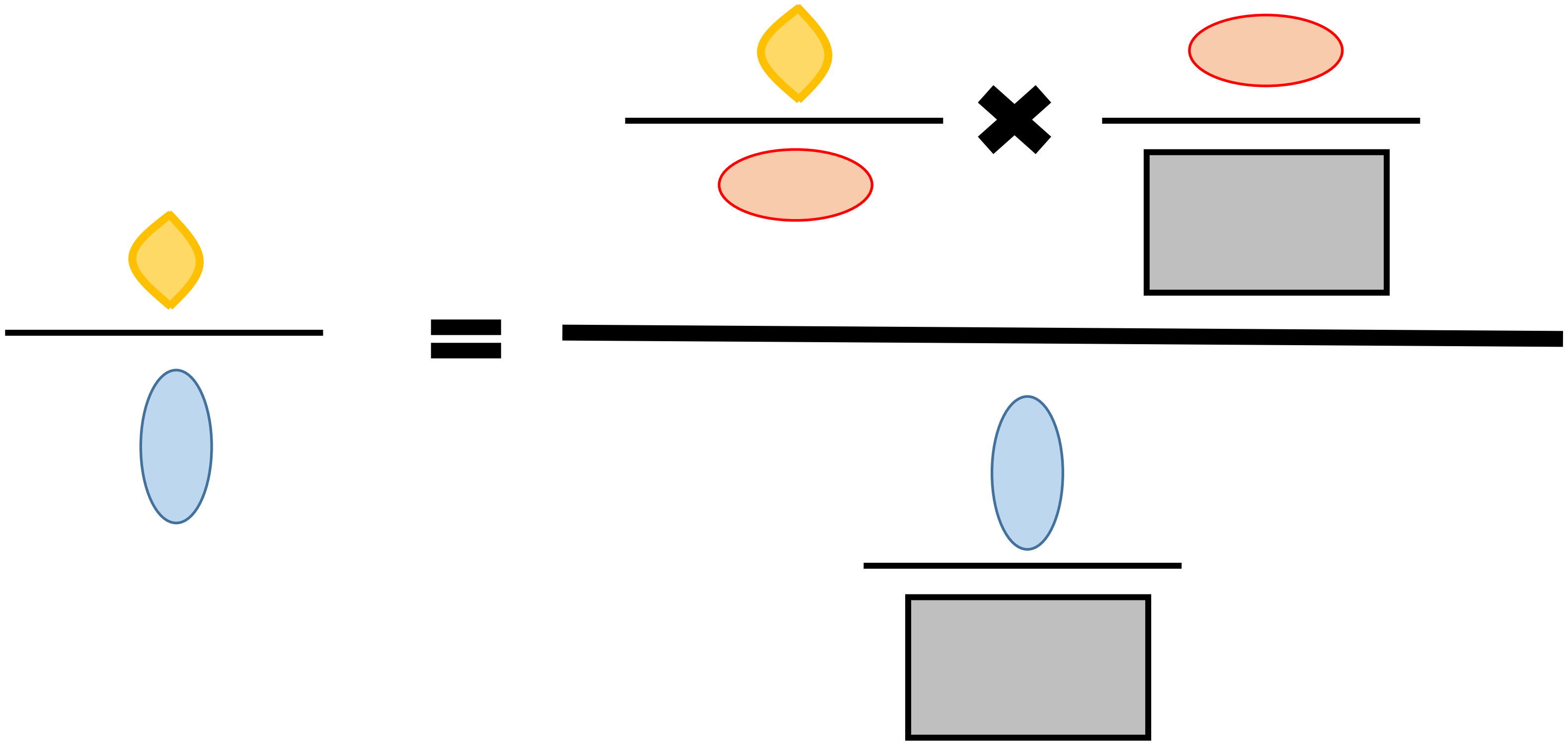


Check 2: **P(A∩B) = P(B|A) * P(A)**

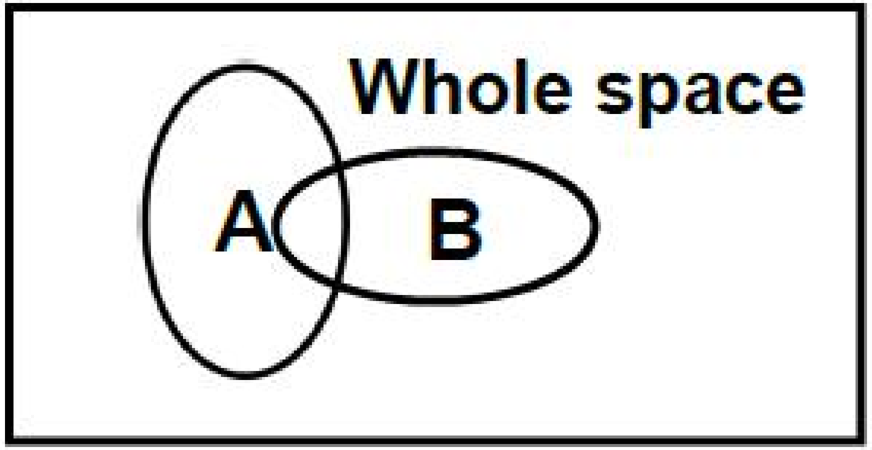


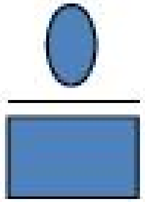
Final “Proof”:

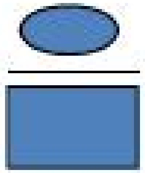
$$P(B|A) = \frac{P(A \cap B)}{P(A)} = \frac{P(A|B)\ P(B)}{P(A)}$$

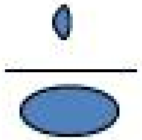


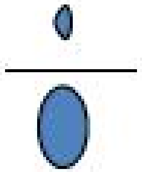
P, Conditional P, and Derivation of Bayes' Theorem in Pictures

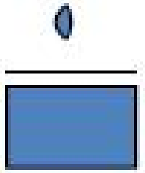


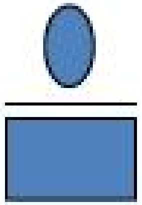
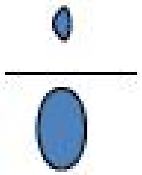
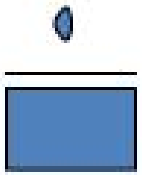
$P(A)$ = 

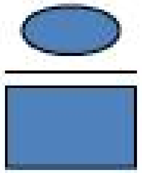
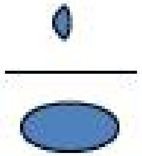
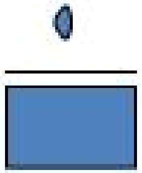
$P(B)$ = 

$P(A|B)$ = 

$P(B|A)$ = 

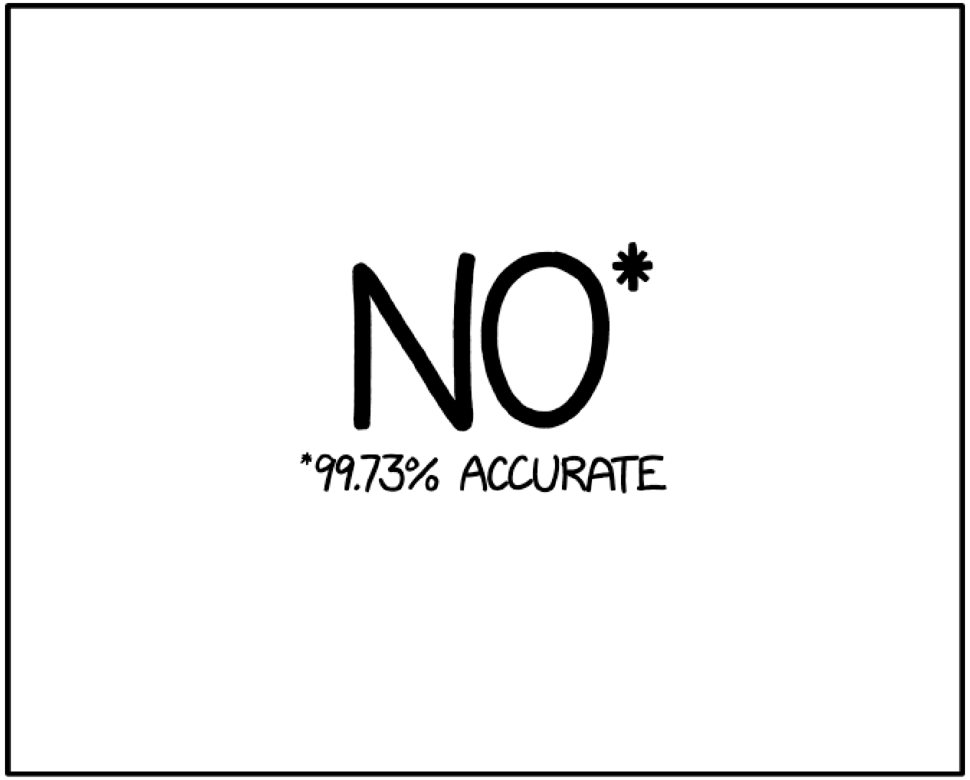
$P(A \cap B)$ = 

$P(A) \times P(B|A)$ =  ×  =  = $P(A \cap B)$

$P(B) \times P(A|B)$ =  ×  =  = $P(A \cap B)$

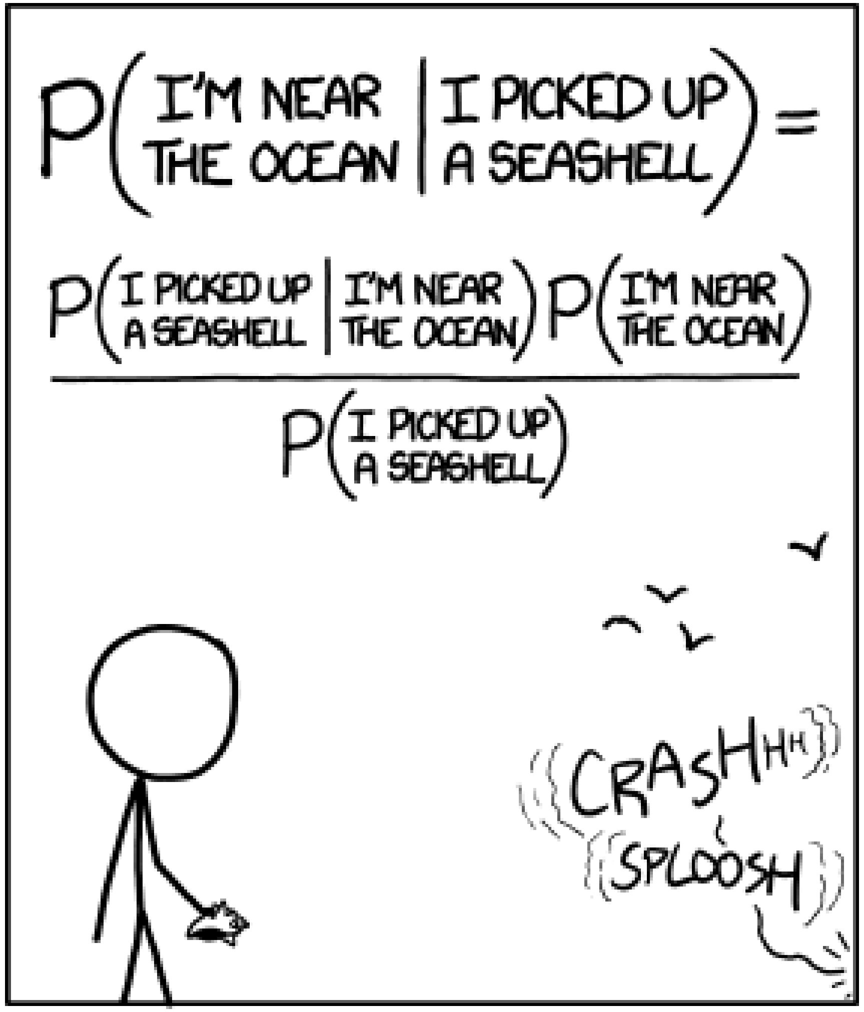
$\Rightarrow P(B|A) = P(A|B) \times P(B) / P(A)$

Is it Christmas?



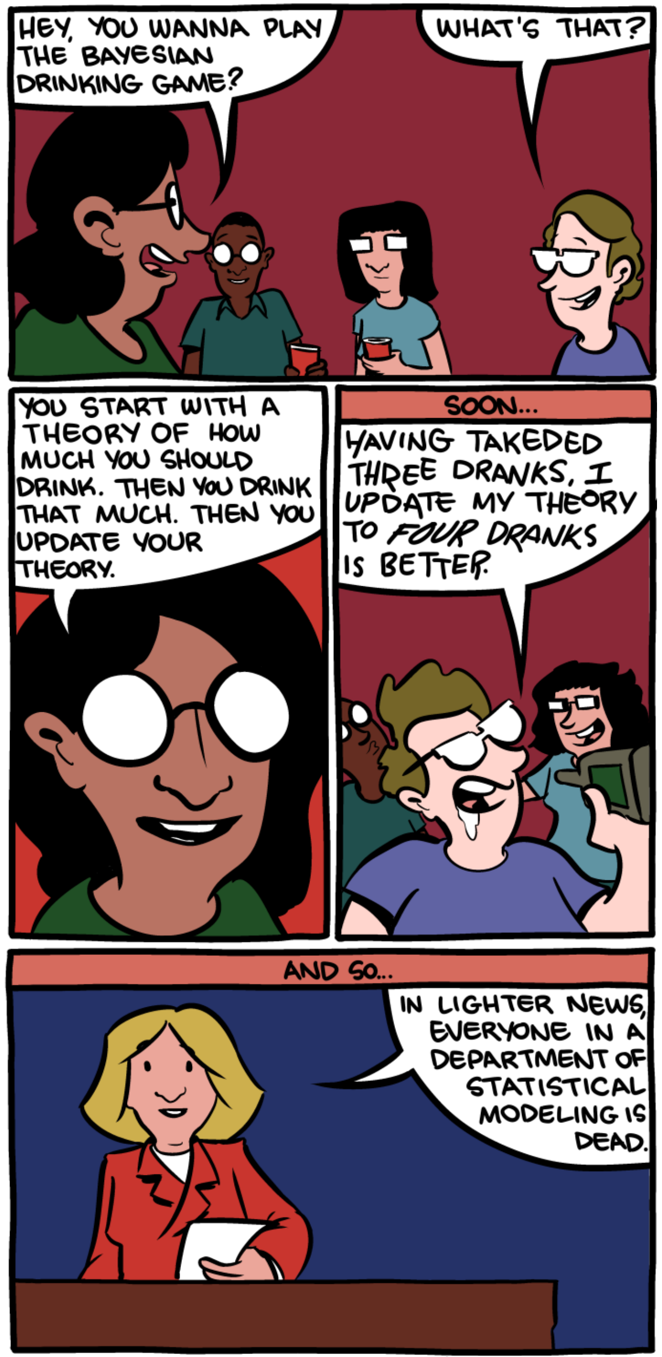
XKCD.COM PRESENTS A NEW "IS IT CHRISTMAS" SERVICE TO COMPETE WITH ISITCHRISTMAS.COM

https://xkcd.com/2236/


P(I'M NEAR THE OCEAN | I PICKED UP A SEASHELL) =
P(I PICKED UP A SEASHELL | I'M NEAR THE OCEAN) P(I'M NEAR THE OCEAN)
P(I PICKED UP A SEASHELL)
CRASHHH
SPLOOSH

STATISTICALLY SPEAKING, IF YOU PICK UP A SEASHELL AND *DON'T* HOLD IT TO YOUR EAR, YOU CAN PROBABLY HEAR THE OCEAN.

https://xkcd.com/1236/


HEY, YOU WANNA PLAY THE BAYESIAN DRINKING GAME?
WHAT'S THAT?
YOU START WITH A THEORY OF HOW MUCH YOU SHOULD DRINK. THEN YOU DRINK THAT MUCH. THEN YOU UPDATE YOUR THEORY.
SOON...
HAVING TAKEDED THREE DRANKS, I UPDATE MY THEORY TO *FOUR* DRANKS IS BETTER.
AND SO...
IN LIGHTER NEWS, EVERYONE IN A DEPARTMENT OF STATISTICAL MODELING IS DEAD.

smbc-comics.com

Bayesian Statistics for Classifiers

Bayes Theorem in Classification

Prior
Prob of target y

Likelihood
Prob of features X given target y, measured in training data

$$P(y \mid x_1, \dots, x_n) = \frac{P(y) P(x_1, \dots, x_n \mid y)}{P(x_1, \dots, x_n)}$$

Posterior
Prob of target y given features X

Evidence
Prob of features X, only purpose is normalization so we can just ignore this!

Example: $$P(salmon|10\ cm) = \frac{P(10\ cm|salmon)\, P(salmon)}{P(10\ cm)}$$

A plague of Zombieitis has swept the land.

Priors: 5% of population is sick: $P(well) = 0.95,\ P(sick) = 0.05$

Test has 3% false + and 2% false – rates:

$$P(+|well) = 0.03, \qquad P(-|well) = 0.97$$
$$P(-|sick) = 0.02, \qquad P(+|sick) = 0.98$$

We need $P(sick|+) = \frac{P(+|sick)P(sick)}{P(+)}$, so first find $P(+)$ by tediously adding all possibilities

$$P(+\cap\, well) = P(+|well)P(well) = (0.03)(0.95) = 0.0285$$

$$P(+\cap\, sick) = P(+|sick)P(sick) = (0.98)(0.05) = 0.0490$$

$P(+) = P(+\cap\, well) + P(+\cap\, sick) = 0.0775$

$$P(sick|+) = \frac{P(+|sick)P(sick)}{P(+)} = \frac{(0.98)(0.05)}{(0.0775)} = \mathbf{0.632}$$

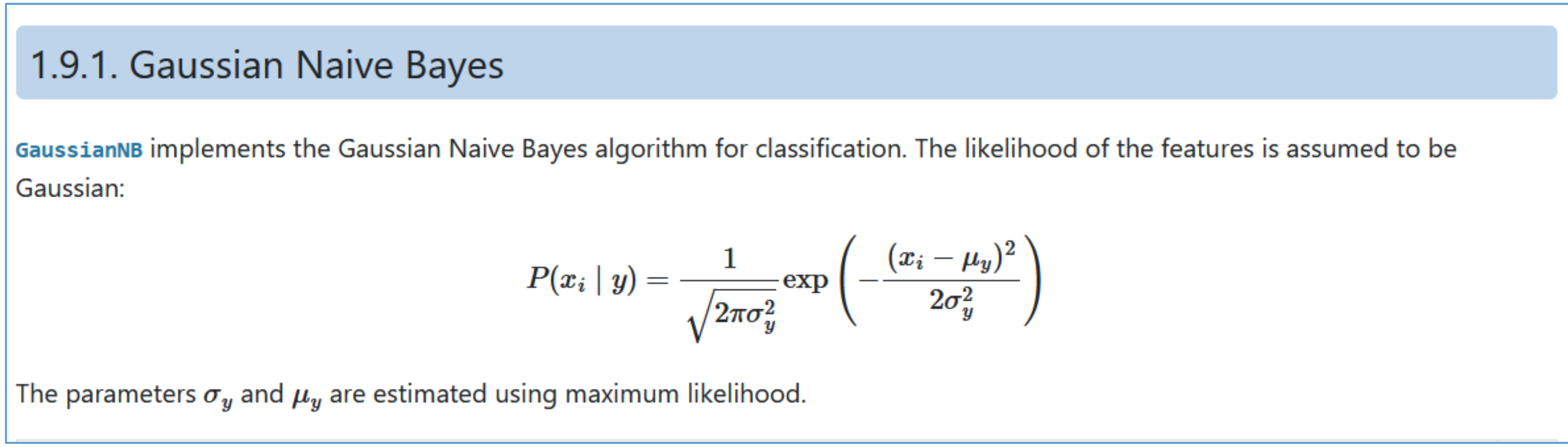
A positive test only gives 63% odds of being sick!

https://scikit-learn.org/stable/modules/naive_bayes.html#gaussian-naive-bayes

$$P(y \mid x_1, \dots, x_n) = \frac{P(y) P(x_1, \dots, x_n \mid y)}{P(x_1, \dots, x_n)}$$

Each feature is fit separately (as a 1D fit), so total prob of getting this sample is the product of all of these 1D gaussians.

$$P(y \mid x_1, \dots, x_n) = \frac{P(y) \prod_{i=1}^{n} P(x_i \mid y)}{P(x_1, \dots, x_n)}$$



1.9.1. Gaussian Naive Bayes

`GaussianNB` implements the Gaussian Naive Bayes algorithm for classification. The likelihood of the features is assumed to be Gaussian:

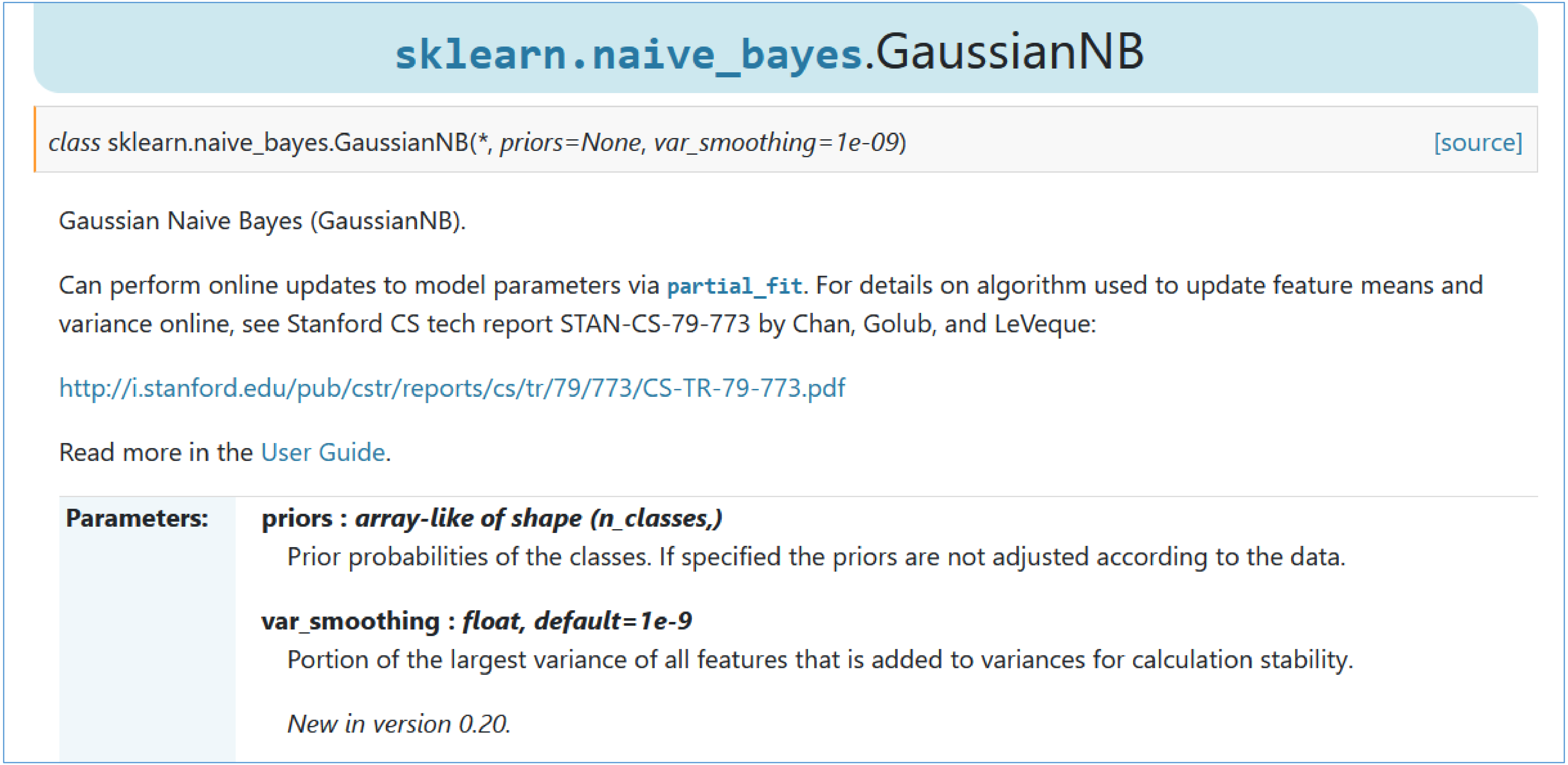
$$P(x_i \mid y) = \frac{1}{\sqrt{2\pi\sigma^2_y}} \exp\left(-\frac{(x_i - \mu_y)^2}{2\sigma^2_y}\right)$$

The parameters σ_y and μ_y are estimated using maximum likelihood.

Since the denominator P(x1,..xn) is a constant, we ignore it and just choose the largest numerator

$$\hat{y} = \arg\max_y P(y) \prod_{i=1}^{n} P(x_i \mid y),$$

https://scikit-learn.org/stable/modules/generated/sklearn.naive_bayes.GaussianNB.html



sklearn.naive_bayes.GaussianNB

class sklearn.naive_bayes.GaussianNB(*, *priors=None*, *var_smoothing=1e-09*) [source]

Gaussian Naive Bayes (GaussianNB).

Can perform online updates to model parameters via `partial_fit`. For details on algorithm used to update feature means and variance online, see Stanford CS tech report STAN-CS-79-773 by Chan, Golub, and LeVeque:

http://i.stanford.edu/pub/cstr/reports/cs/tr/79/773/CS-TR-79-773.pdf

Read more in the User Guide.

Parameters:

priors : *array-like of shape (n_classes,)*

Prior probabilities of the classes. If specified the priors are not adjusted according to the data.

var_smoothing : *float, default=1e-9*

Portion of the largest variance of all features that is added to variances for calculation stability.

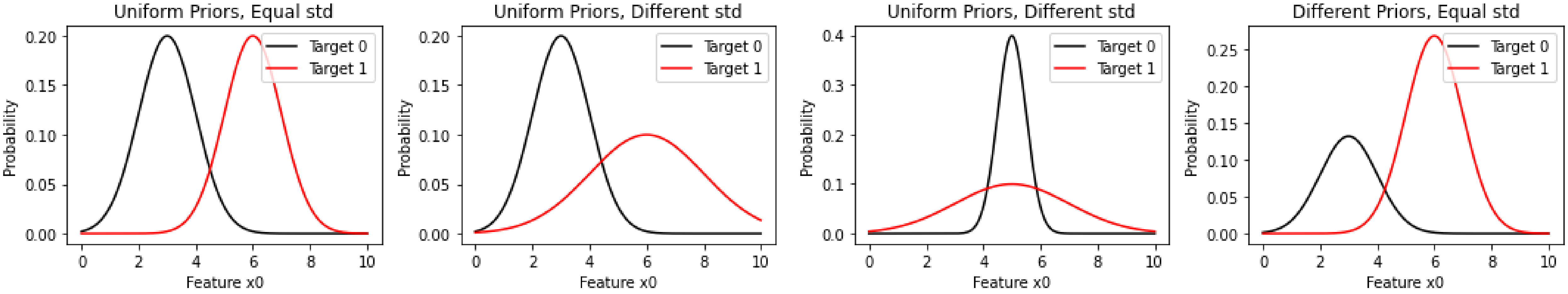
New in version 0.20.

1-D Examples

$$\hat{y} = \arg\max_{y} P(y) \prod_{i=1}^{n} P(x_i \mid y),$$

$$P(x_i \mid y) = \frac{1}{\sqrt{2\pi\sigma_y^2}} \exp\left(-\frac{(x_i - \mu_y)^2}{2\sigma_y^2}\right)$$

1) Use the μ and σ for each feature to construct a Gaussian
2) Draw the Gaussian times the prior $P(y)P(x_i|y)$
3) To classify, just pick which probability is biggest!



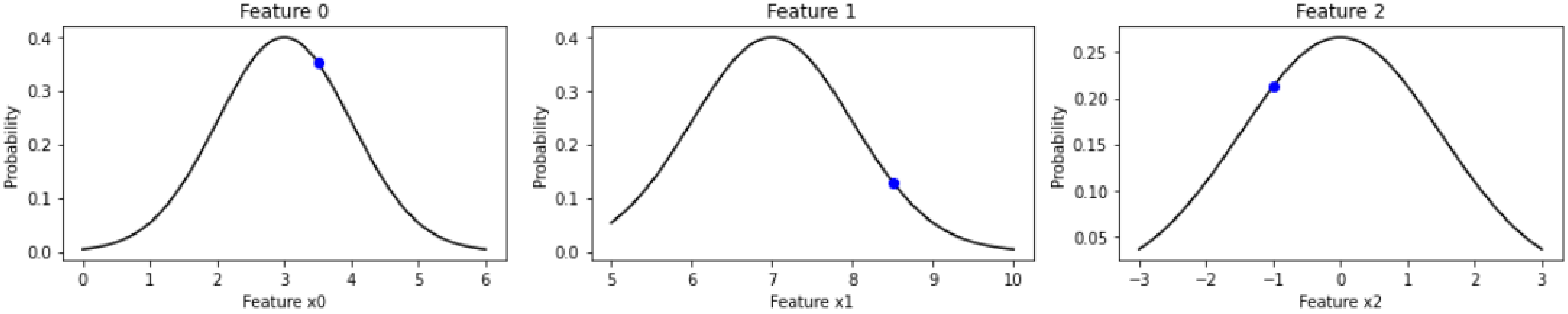
Black = y_0 salmon

Red = y_1 bass

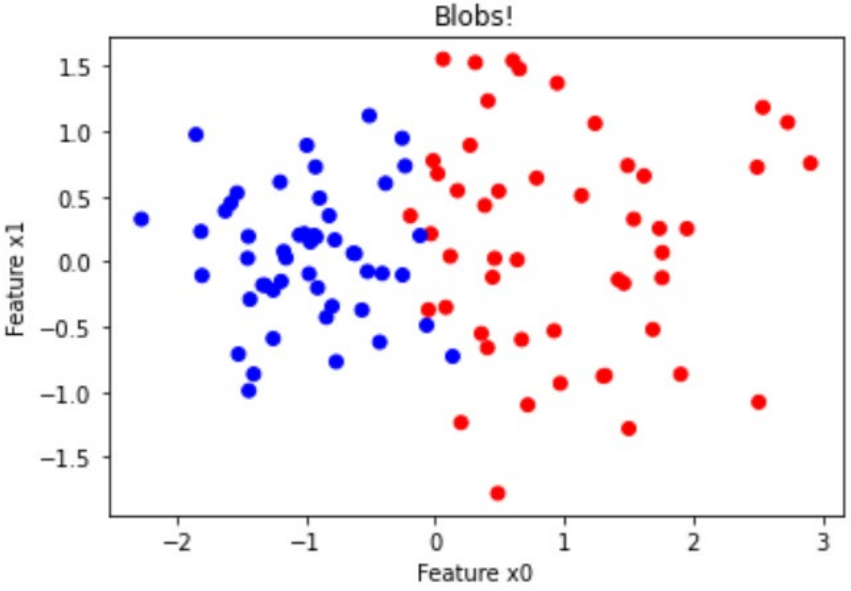
Higher D

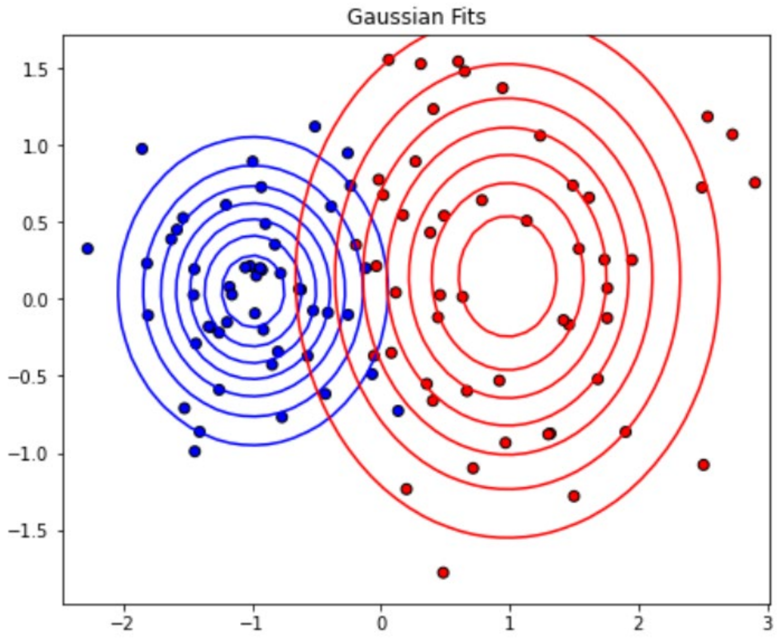
In finding the probability of a sample belonging to a certain class, first look at the Gaussian for each feature which is most likely to be near the mean. We expect that the further it gets away from the mean, the less likely it is to belong to this target.

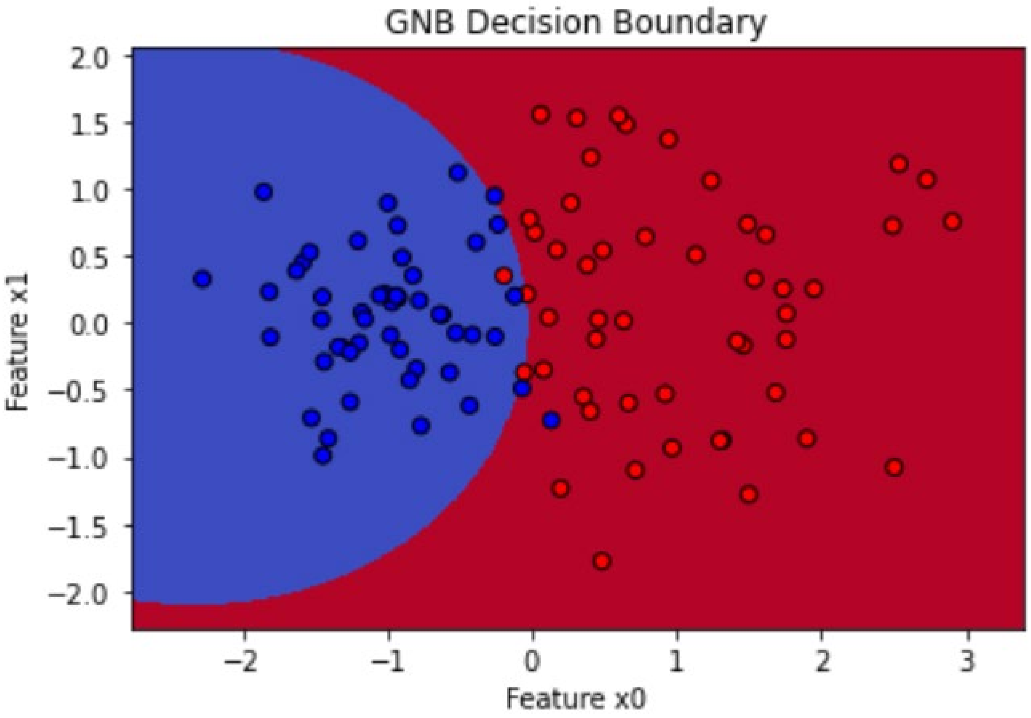
For multiple features, since we **assume** the features are independent we just multiply the probabilities for each feature together!



https://github.com/mdaugherity/MachineLearning2022/blob/main/Tutorial_10_Bayesian_Classifier.ipynb





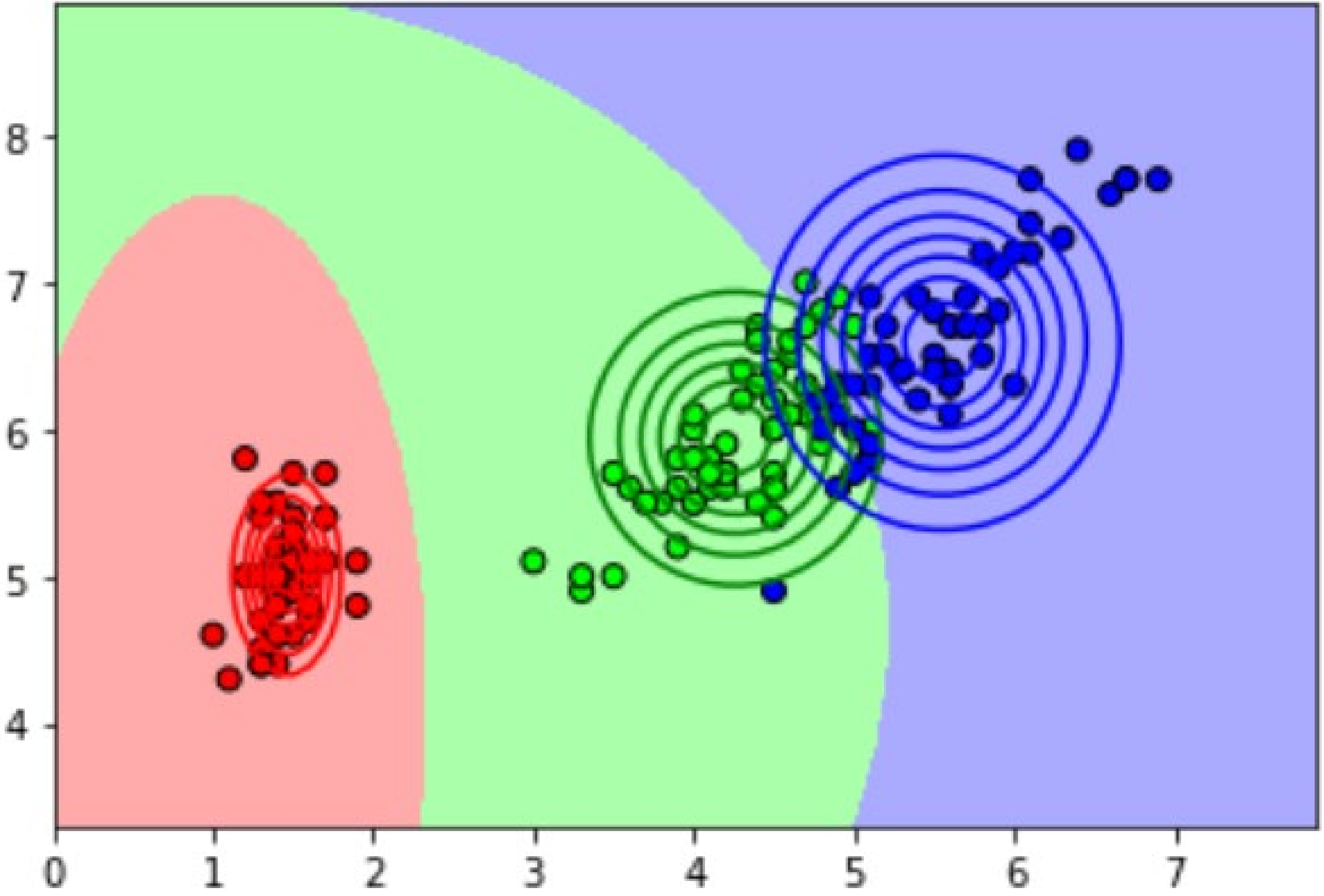


Classifier just picks which Gaussian is tallest at any given point!

- Equivalent choosing smallest number of σ's away from mean
- Priors weight the relative heights for each target

https://github.com/mdaugherity/MachineLearning2022/blob/main/Tutorial_10_Bayesian_Classifier.ipynb

Two feature Iris data



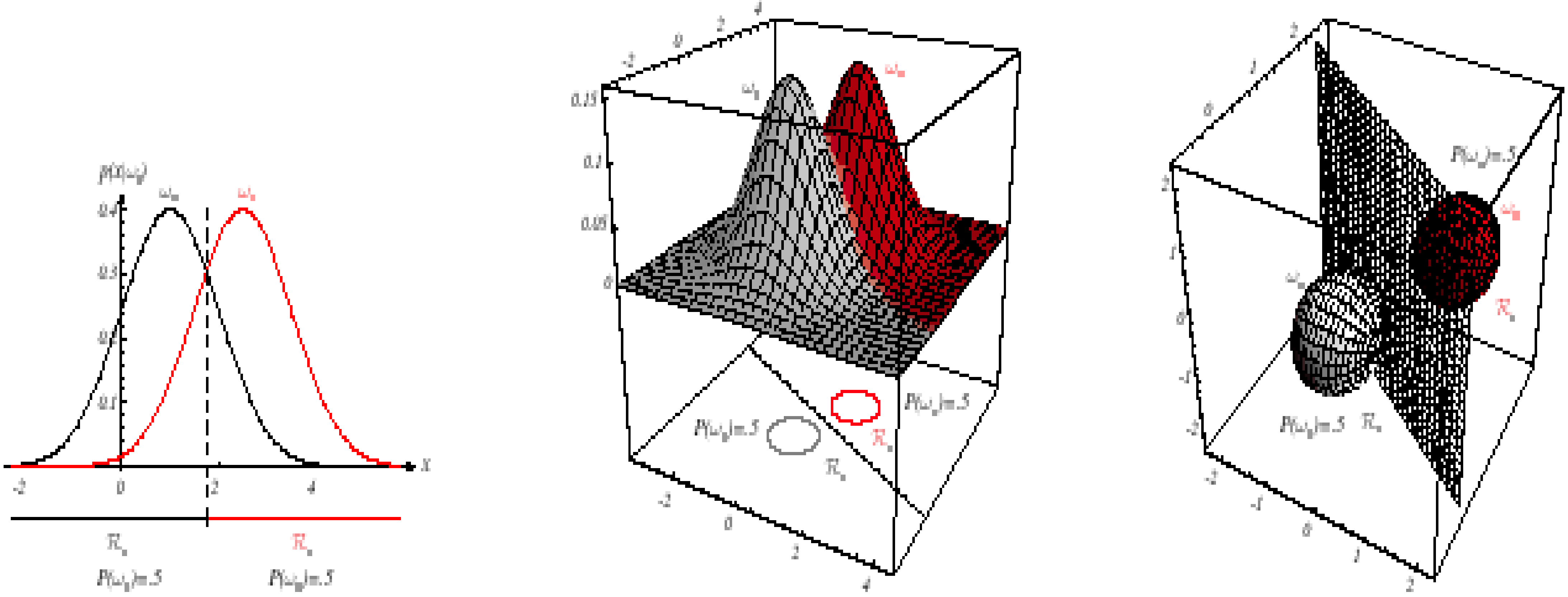


FIGURE 2.10. If the covariance matrices for two distributions are equal and proportional to the identity matrix, then the distributions are spherical in d dimensions, and the boundary is a generalized hyperplane of $d-1$ dimensions, perpendicular to the line separating the means. In these one-, two-, and three-dimensional examples, we indicate $p(\mathbf{x}|\omega_i)$ and the boundaries for the case $P(\omega_1) = P(\omega_2)$. In the three-dimensional case, the grid plane separates $\mathcal{R}_1$ from $\mathcal{R}_2$. From: Richard O. Duda, Peter E. Hart, and David G. Stork, *Pattern Classification*. Copyright © 2001 by John Wiley & Sons, Inc.

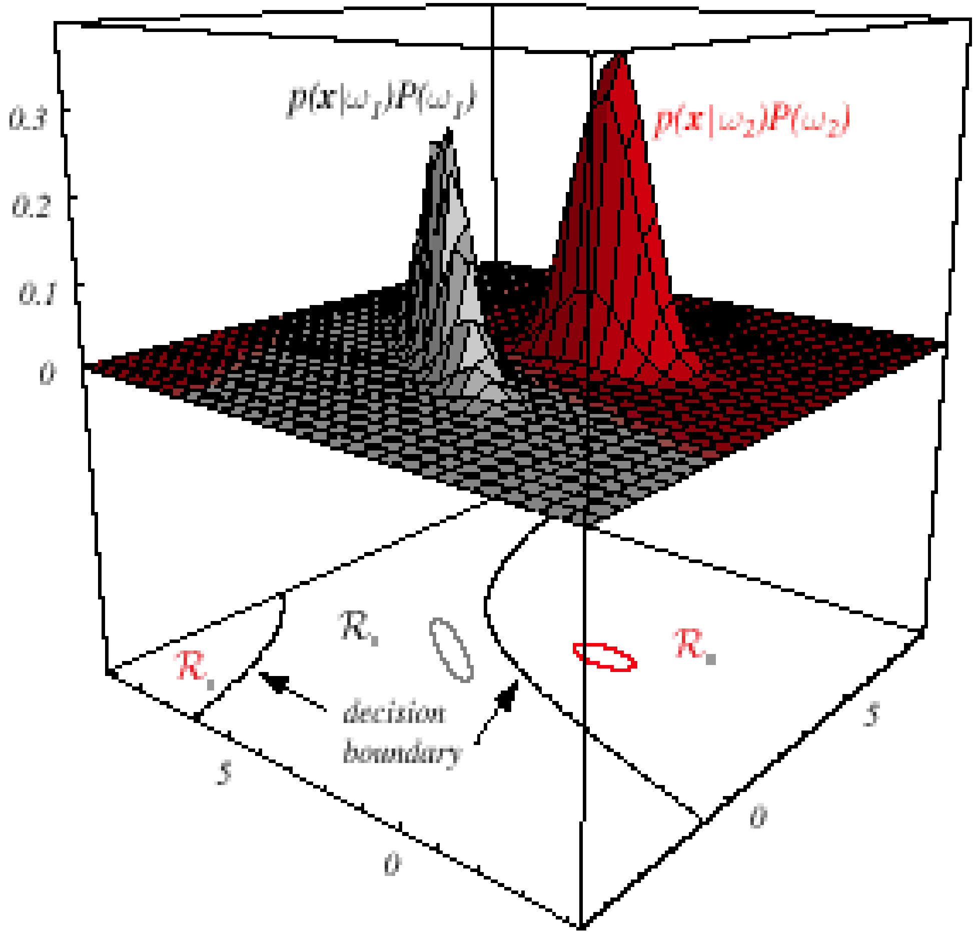


FIGURE 2.6. In this two-dimensional two-category classifier, the probability densities are Gaussian, the decision boundary consists of two hyperbolas, and thus the decision region $\mathcal{R}_2$ is not simply connected. The ellipses mark where the density is $1/e$ times that at the peak of the distribution. From: Richard O. Duda, Peter E. Hart, and David G. Stork, *Pattern Classification*. Copyright © 2001 by John Wiley & Sons, Inc.

Summary

Pros:

- Bayesian Classifiers actually use real statistics!
- Few parameters
- Fast and memory efficient
- Gaussian works surprisingly well on many problems

Cons:

- Some problems just aren’t Gaussian

Classifier Comparison

Name	sklearn	Algorithm	Params	Training	Pros	Cons	Notes
Nearest Neighbors (kNN)	neighbors.KNeighborsClassifier	Finds "closest" point in training data	n_neighbors=5 voting weights = (uniform / distance)	Easy! Just copies training data	• Simple to use • Understandable	• SLOW for big datasets	• Always scores 100% on training when k=1 • Increasing k averages over outliers
Decision Tree	tree.DecisionTreeClassifier	Like 20 questions, learns rules (yes/no questions on one feature at a time) that minimizes impurity	max_depth = None	Easy! Default max_depth=None will overfit	• Understandable • Super fast classification	• Overfits by default • "Stair-step" decision boudaries	• Limit max_depth!
Gaussian Naïve Bayes	naive_bayes.GaussianNB	Fits 1D gauss to each feature	None (but see note about priors)	Easy! Just finds mean and var of each feature	• Simple to use • Understandable • Great if your data is gaussian	• Terrible if your problem isn't gaussian	• Priors learned from y by default, can specify other values