7. Naïve Bayes classifier

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Naïve Bayes

Summary

- Bayes Rule
- Bayes Classifier
- Naïve Bayes classifier
- Comparing classifiers
- (Assignment 1)

Bayes' Rule

Bayes' Rule

Sum rule and marginal probability

- Given two random variables X and Y

$$p(X = x_i) = \sum_{j=1}^{N} p(X = x_i, Y = y_j)$$

- This is the sum rule, giving the marginal probability

Y \ X	1	2	3	4	P(Y)
2	0,06	0,026	0,051	0,012	0,189
3	0,045	0,001	0,046	0,016	0,152
4	0,035	0,015	0,065	0,045	0,218
5	0,006	0,033	0,057	0,039	0,157
6	0,029	0,004	0,054	0,035	0,127
P(X)	0,175	0,079	0,273	0,147	

Bayes' Rule

Product rule and joint probability

- The conditional probability of $Y = y_j$ given that $X = x_i$ is the fraction of $p(X = x_i, Y = y_j)$ in $p(X = x_i)$

$$p(Y = y_j|X = x_i) = \frac{p(X = x_i, Y = y_j)}{p(X = x_i)}$$

$$p(X = x_i, Y = y_j) = p(Y = y_j|X = x_i)p(X = x_i)$$

Summarizing:

$$\textit{sum rule} \qquad p(X) = \sum_{j=1}^{N} p(X, Y_j)$$

$$\textit{product rule} \qquad p(X, Y) = p(Y|X)p(X)$$

Bayes' rule

- Since $p(Y, X) = p(X, Y)$, applying the product rule

$$p(Y, X) = p(X, Y) \Leftrightarrow$$

$$p(Y|X)p(X) = p(X|Y)p(Y) \Leftrightarrow$$

$$p(Y|X) = \frac{p(Y)p(X|Y)}{p(X)}$$

Bayes' Rule

Frequentist interpretation

- Probability is frequency over infinite trials
- Bayes rule simply relates different frequency estimates:

$$p(Y|X) = \frac{p(Y)p(X|Y)}{p(X)}$$

Bayesian interpretation

- Probability measures (rational) certainty about truth of hypotheses
- Bayes' rule gives posterior probability from prior and evidence:

$$p(H|E) = \frac{p(H)p(E|H)}{p(E)}$$

Bayes' Rule

For classification

- We can consider the conditional probability of an example with features x belonging to class c to be:

$$p(C = c|X = x) = \frac{p(C = c)p(X = x|C = c)}{p(X = x)}$$

- Frequentist interpretation:
  - Frequencies over infinite trials
- Bayesian interpretation:
  - Confidence on hypothesis given the data
- Either way, we have to estimate these probabilities from the data

Bayes Classifier

Bayes Classifier

To classify, find most probable class:

$$p(C = c|X = x) = \frac{p(C = c)p(X = x|C = c)}{p(X = x)}$$

- (probable in the bayesian sense)

- Since $p(X = x)$ is independent of c, simplify to:

$$p(C = c|X = x) \propto p(C = c)p(X = x|C = c)$$

- And since

$$p(C = c)p(X = x|C = c) = p(C = c, X = x)$$

- all we need is the joint distribution of the classes and the feature value combinations.

Bayes Classifier

To classify, find most probable class:

$$C^{Bayes} = \underset{c \in \{0,1,\ldots,N\}}{\operatorname{argmax}} \; p(C = c, X = x)$$

- The Bayes Classifier is the ideal classifier
- If we know the joint distribution of classes and feature combinations we minimize the error.

- (That's the problem)

Bayes Classifier

Example: predict diabetes

- Questionnaires with 20 yes/no questions (food, exercise, etc..)
- Total of $2^{20} \sim 1$ million combinations
- We need (many) millions of examples to estimate $P(C, X)$
- The full Bayes Classifier is not practical

- We never have enough data to estimate the joint probability for all combinations of features

Naïve Bayes Classifier

Naïve Bayes Classifier

Assume conditional independence given class

- Example: the time two people arrive home are not independent variables because a strike affects both.
- But if we know that there was a strike, these variables become independent.
- This makes it easier to estimate the probabilities

Applying the product rule to $p(C, X)$

$$p(C_k, x_1, \ldots, x_n) = p(C_k)p(x_1|C_k)p(x_2|C_k, x_1)\ldots$$
$$p(x_n|C_k, x_1, x_2, \ldots, x_{n-1})$$

- But conditional independence given the class means that

$$p(x_n|C_k, x_1, x_2, \ldots, x_{n-1}) = p(x_n|C_k)$$

Naïve Bayes Classifier

So it all simplifies to:

$$p(C_k, x_1, \ldots, x_n) = p(C_k) \prod_{j=1}^{N} p(x_j|C_k)$$

- Taking the logarithm:

$$\ln p(C_k, x_1, \ldots, x_n) = \ln p(C_k) + \sum_{j=1}^{N} \ln p(x_j|C_k)$$

The Naïve Bayes Classifier is:

$$C^{Naïve\ Bayes} = \underset{k \in \{0,1,\ldots,K\}}{\operatorname{argmax}} \ln p(C_k) + \sum_{j=1}^{N} \ln p(x_j|C_k)$$

Naïve Bayes Classifier

$$\underset{k \in \{0,1,\ldots,K\}}{\operatorname{argmax}} \ln p(C_k) + \sum_{j=1}^{N} \ln p(x_j | C_k)$$

To train the Naïve Bayes Classifier:

- For each class, find the log probability distribution of features
- For each class, find the log of the prior probability

To classify:

- Find class for which the sum of the feature logs, plus the log of the prior, is greatest

Naïve Bayes Classifier

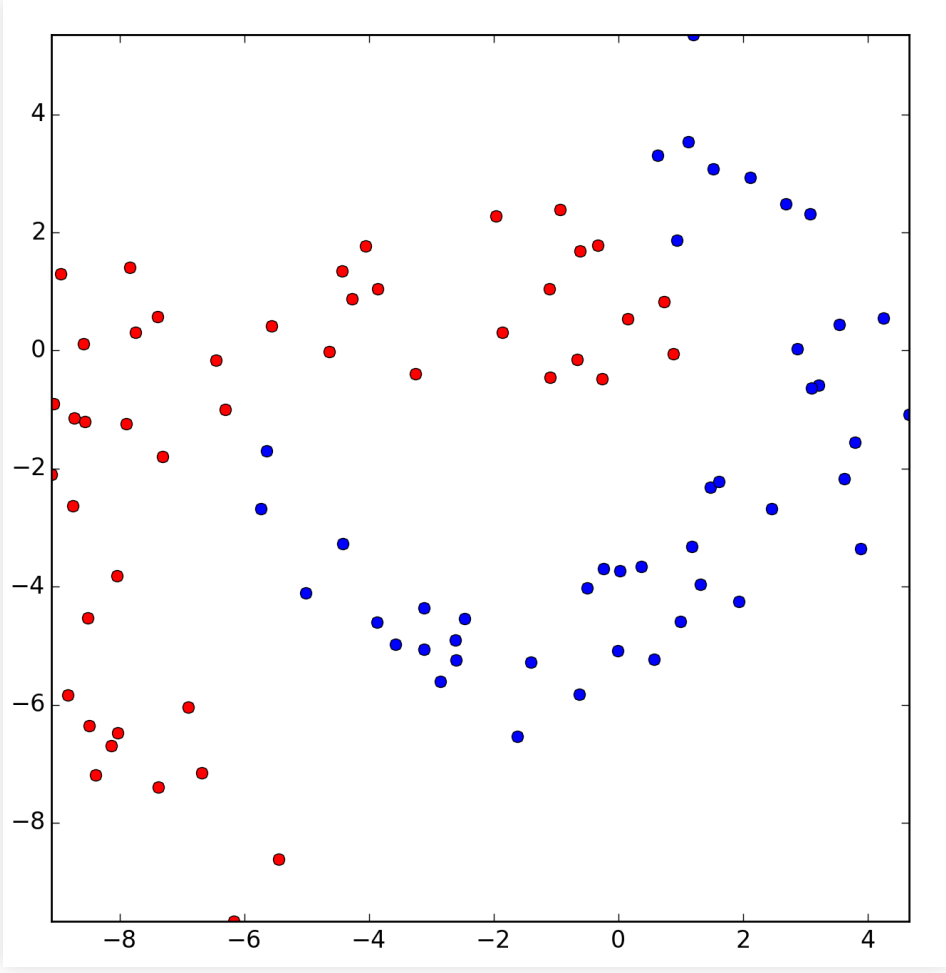
Example: predict diabetes

- Questionnaires with 20 yes/no questions (food, exercise, etc..)
- Split into healthy and diabetic
- Count yes/no fraction for each question in each class
- Predict: log fraction of healthy to diabetic (prior) plus sum of log feature fraction for each class

NB: example 1

NB, continuous

- Data set with two continous features and two classes



NB, continuous

Finding the distributions

- Parametric method: assume some distribution (e.g. Normal) and compute the parameters (e.g. mean and standard deviation):

$$p(x_j|C_k) = \frac{1}{\sigma_k\sqrt{2\pi}} e^{-\frac{(x-\mu_k)^2}{2\sigma_k^2}}$$

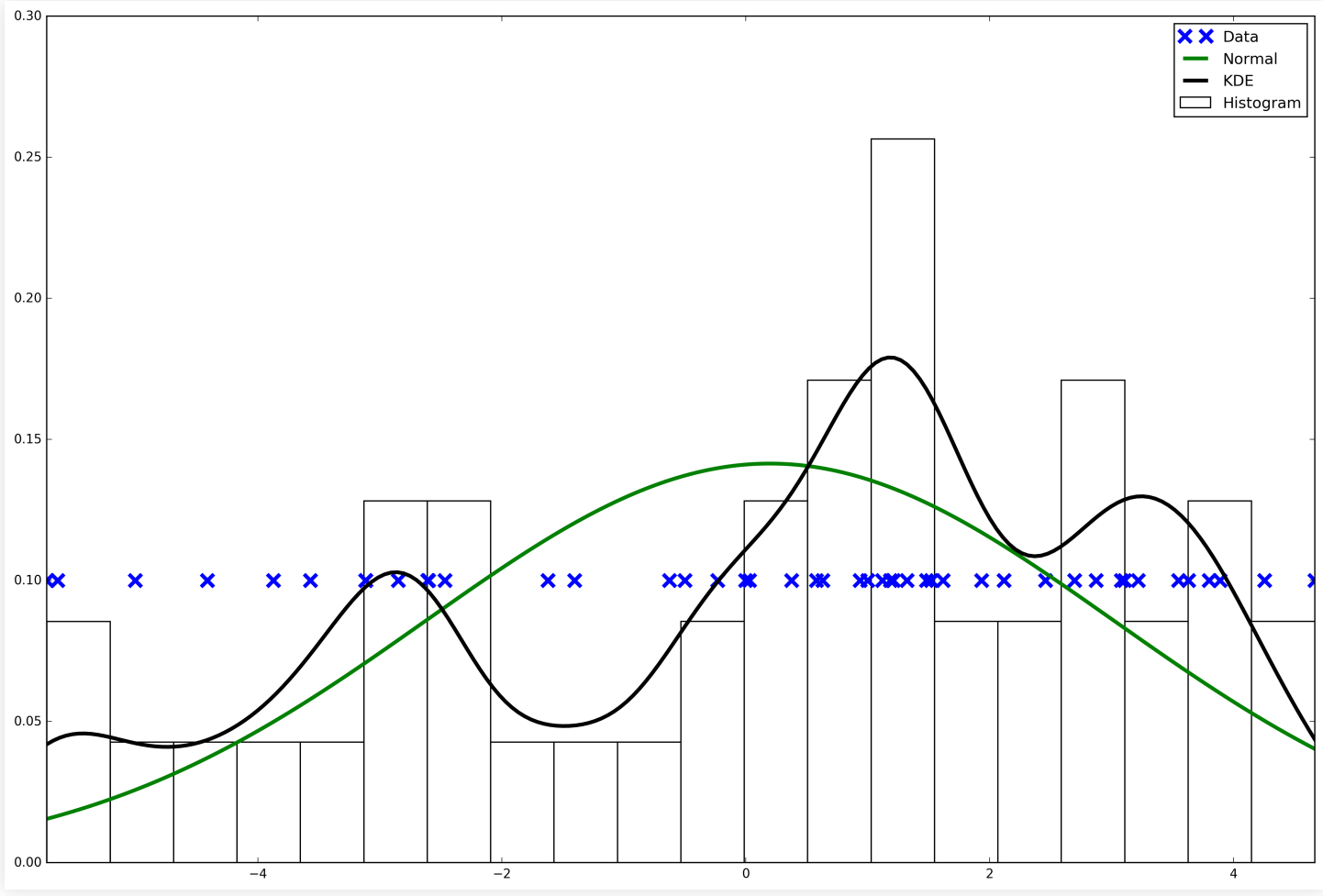
- Non-Parametric method: do not assume distribution. E.g. KDE.

Parametric vs Non-parametric

- Parametric models: completely defined by the chosen parameters
- Non-Parametric need additional data (e.g. k-NN, KDE).
- (Naïve Bayes can be either)

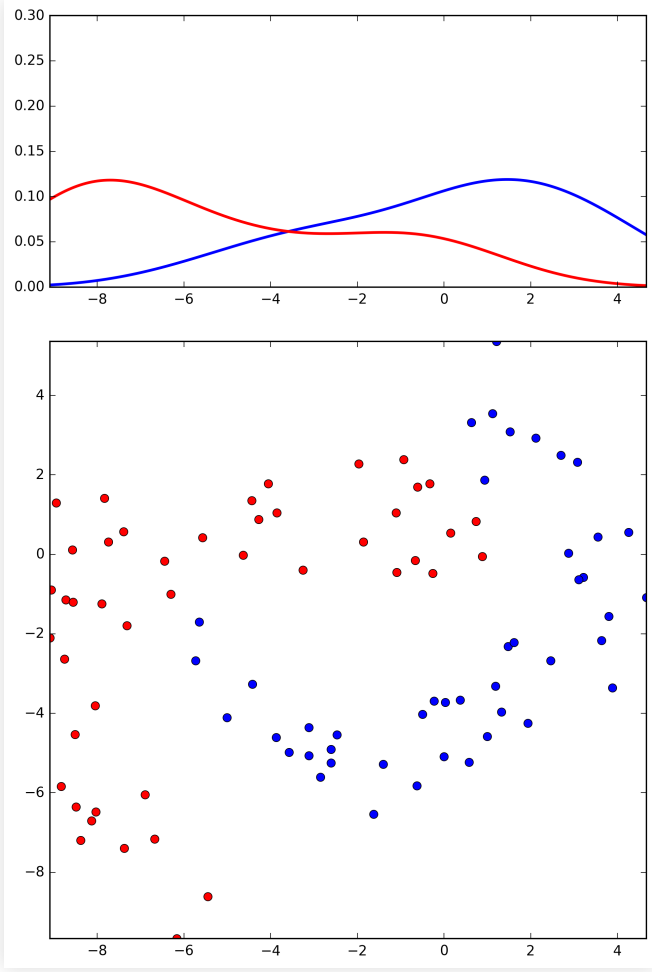
NB, continuous

- In our case, we'll choose a KDE



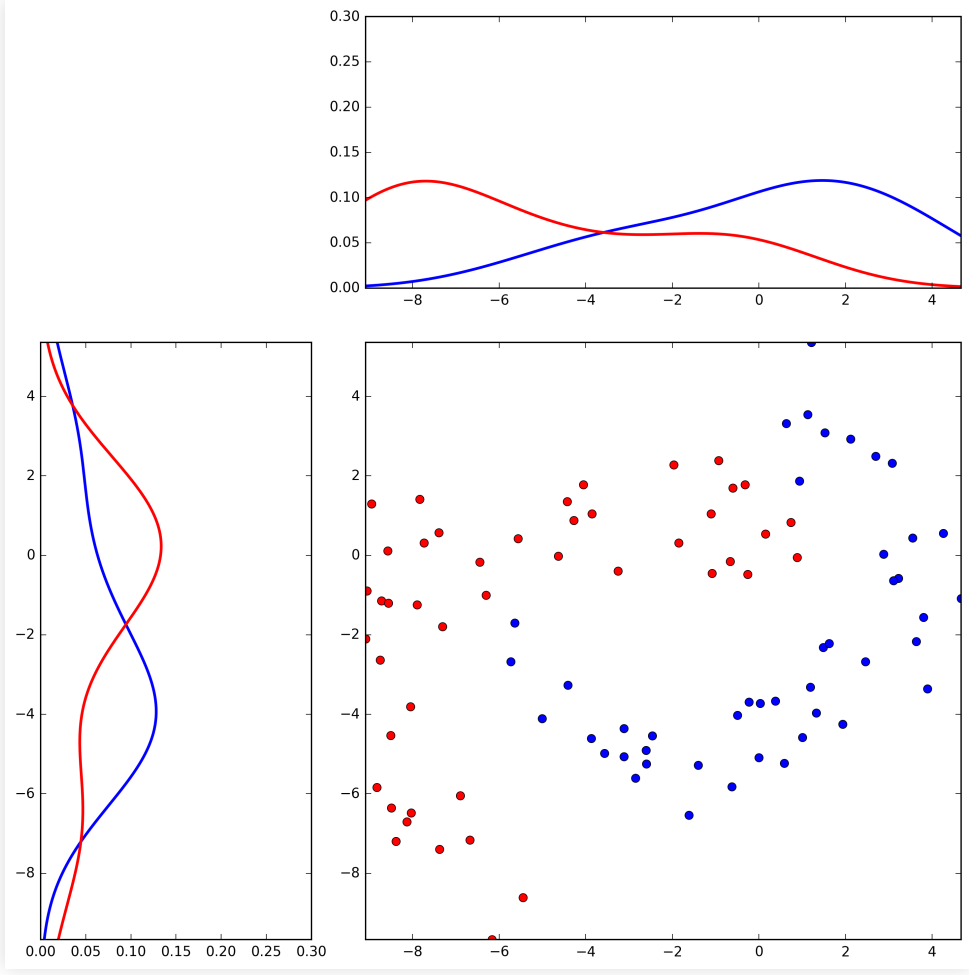
NB, continuous

- KDE for one feature, both classes:



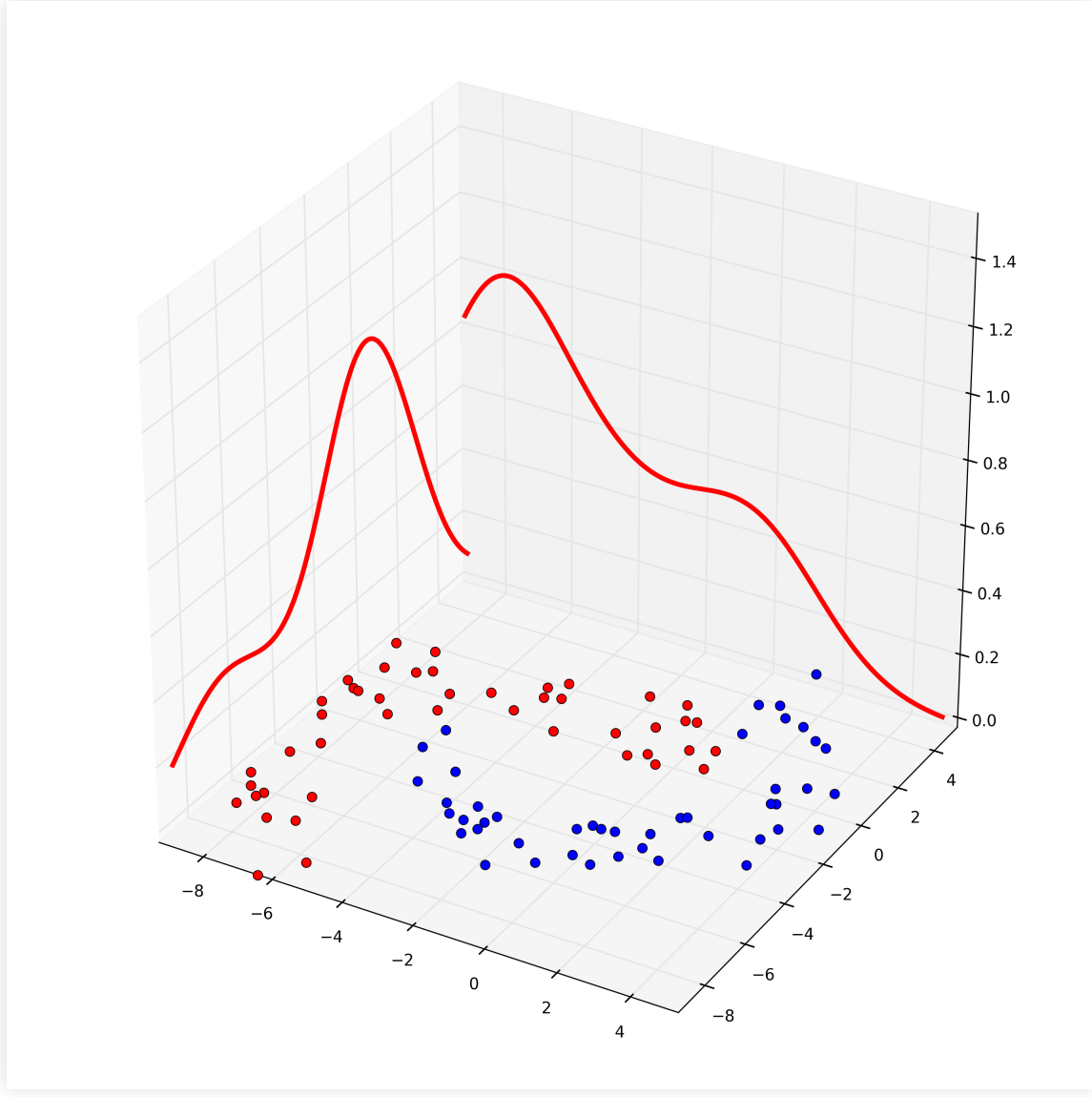
NB, continuous

- KDE for both features, both classes:



NB, continuous

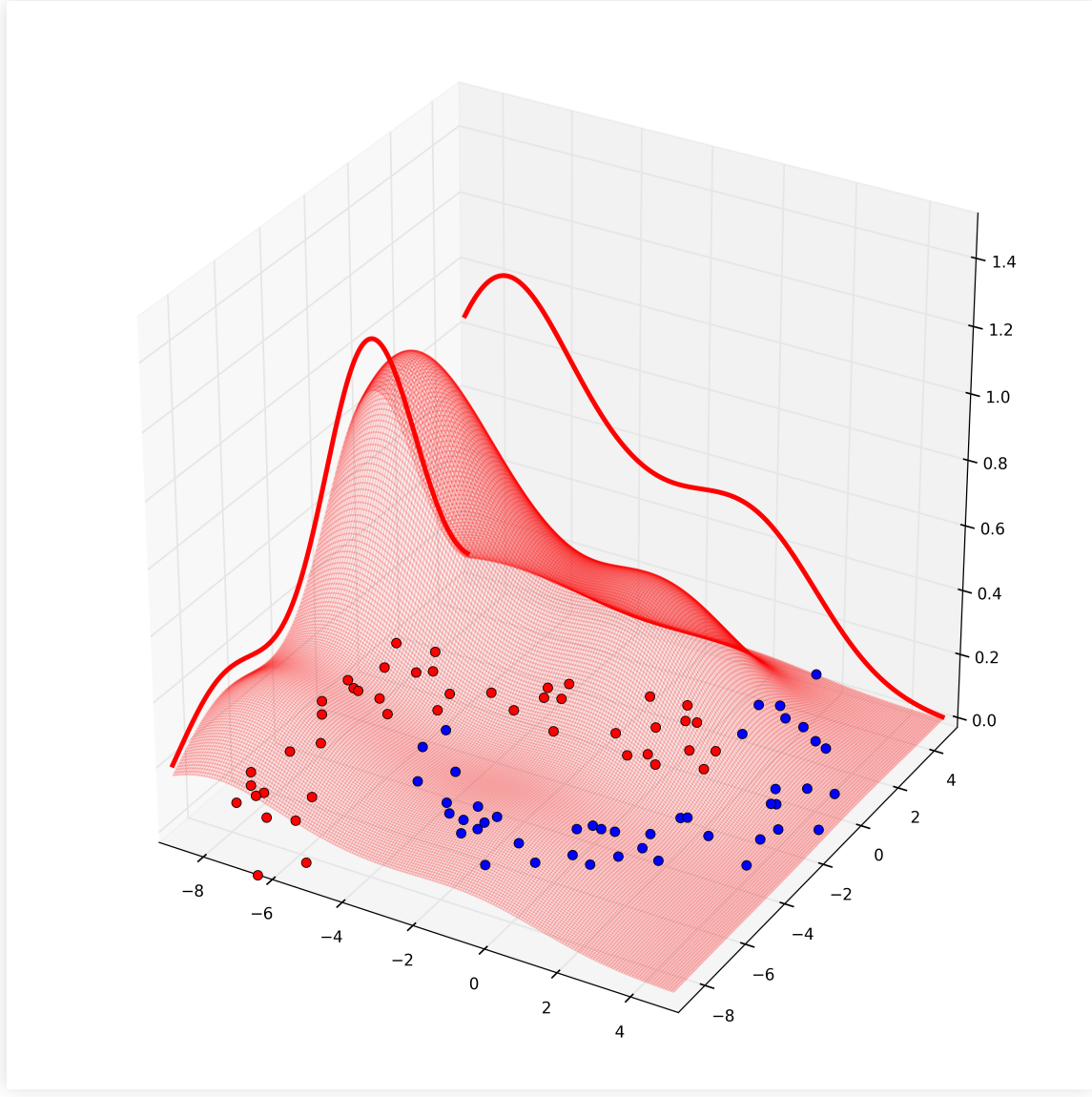
$$P(x_1, x_2|red)$$



NB, continuous

$$P(x_1, x_2|red) =$$

$$P(x_1|red)P(x_2|red)$$



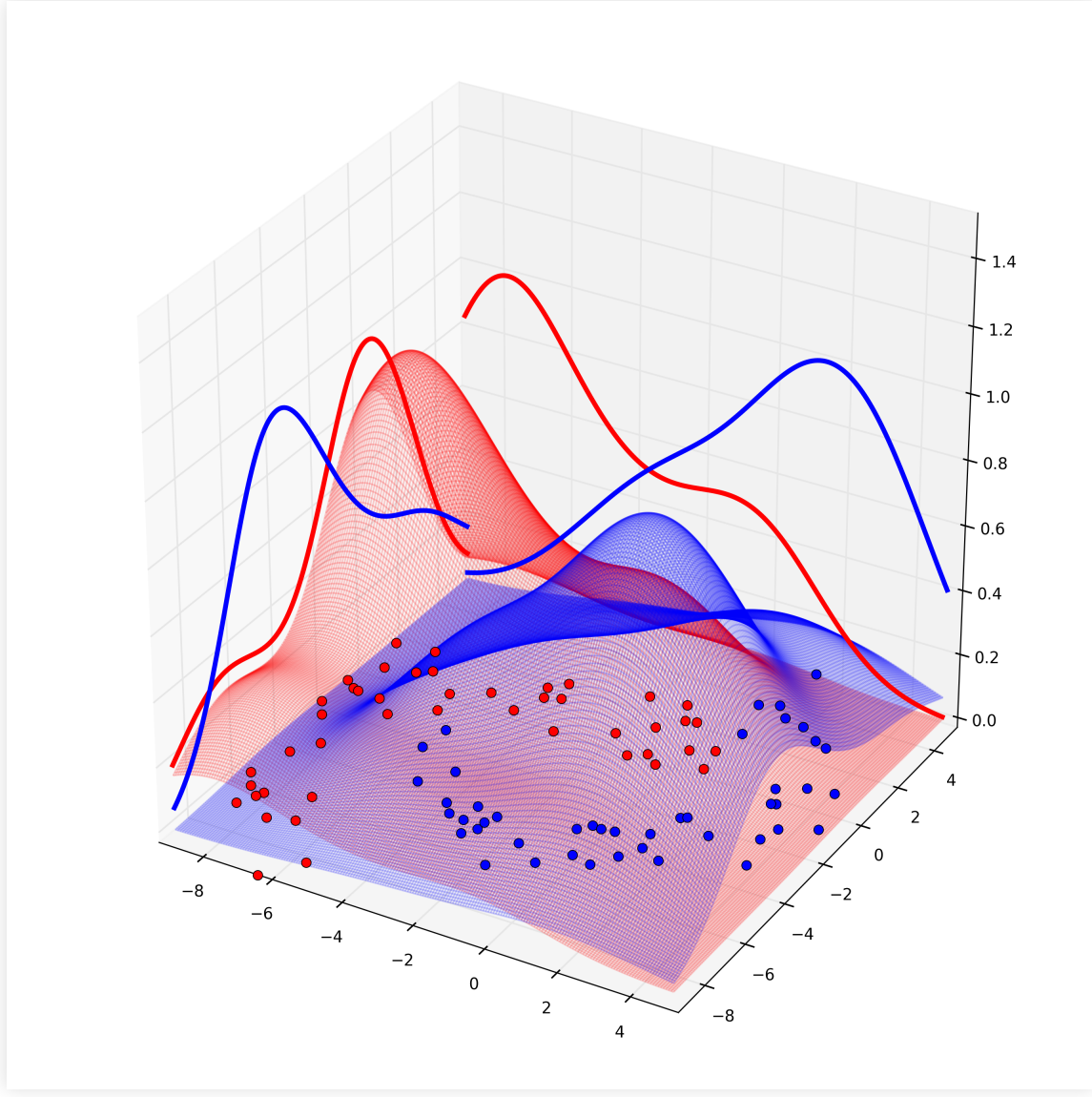
NB, continuous

$$P(x_1, x_2|red) =$$

$$P(x_1|red)P(x_2|red)$$

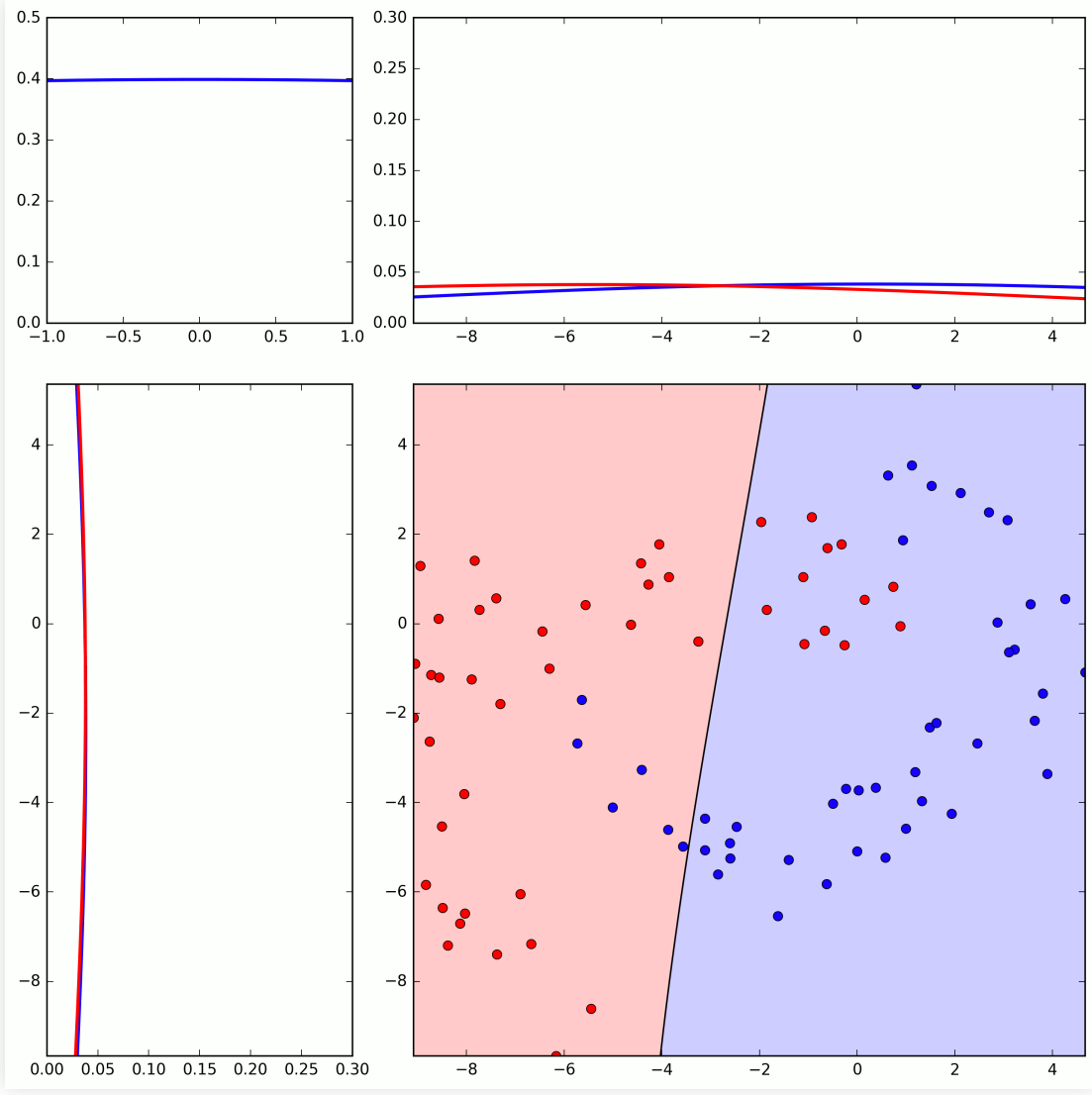
$$P(x_1, x_2|blue) =$$

$$P(x_1|blue)P(x_2|blue)$$



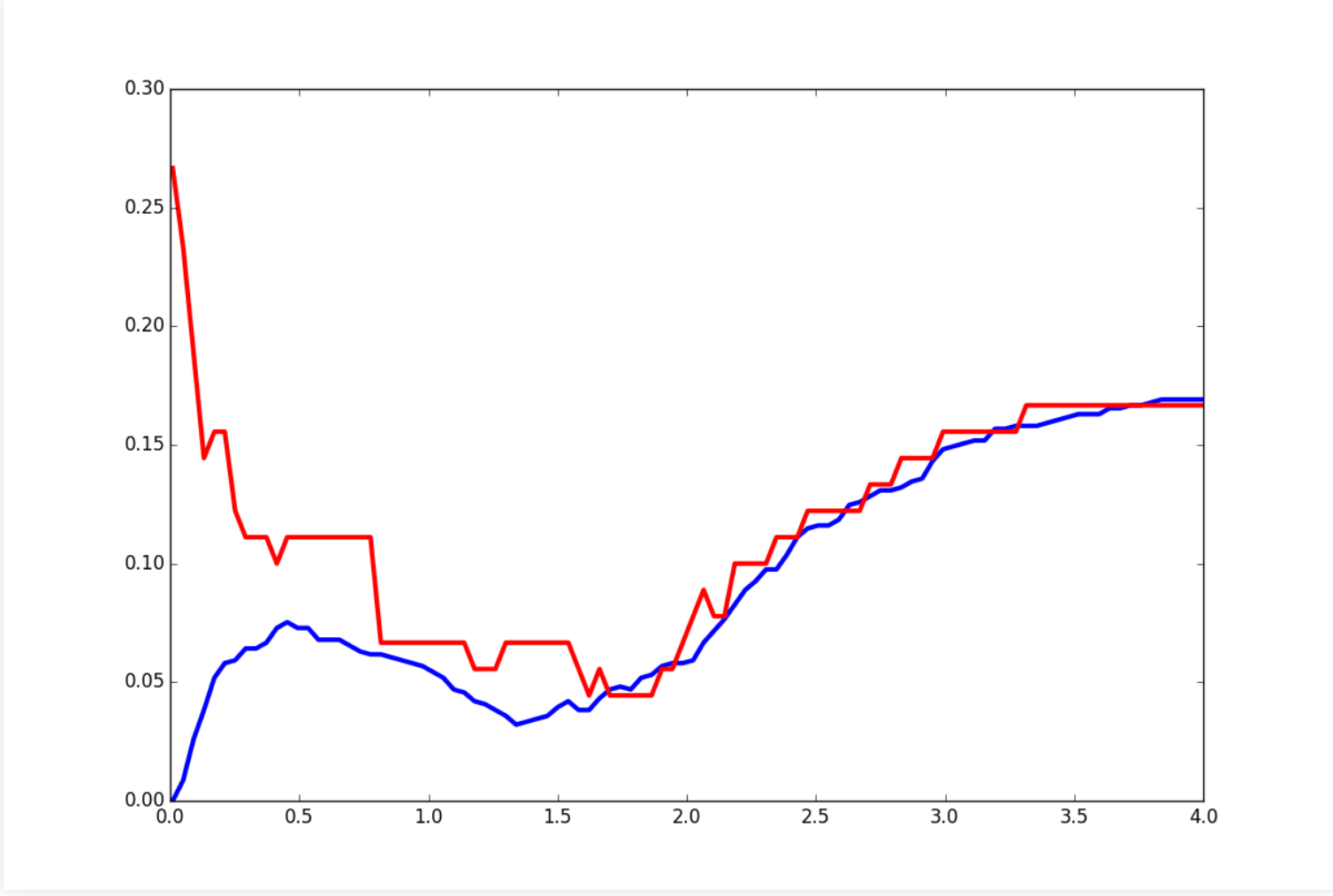
NB, continuous

- We need to adjust the kernel width



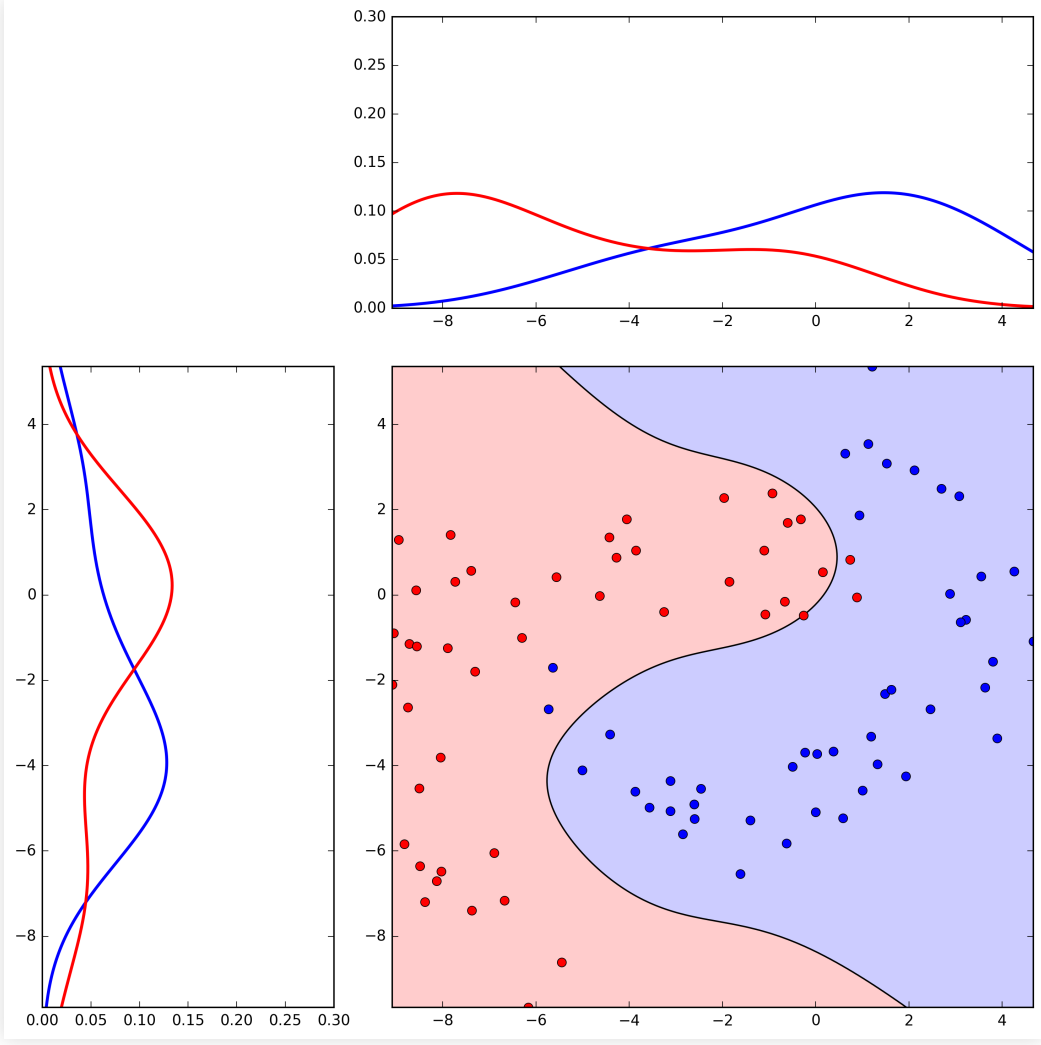
NB, continuous

- Cross-validation (10-fold)



NB, continuous

- Final result
  - $(h = 1.8)$



NB: example 2

NB, categorical

Mushroom edibility

- Data set with mushroom features and class (poisonous, edible)
- From http://archive.ics.uci.edu/ml/datasets/Mushroom

```
 1. cap-shape:                bell=b,conical=c,convex=x,flat=f,knobbed=k,sunken=s
 2. cap-surface:              fibrous=f,grooves=g,scaly=y,smooth=s
 3. cap-color:                brown=n,buff=b,cinnamon=c,gray=g,green=r,pink=p,purple=u,red=e,white=w,yellow=y
 4. bruises?:                 bruises=t,no=f
 5. odor:                     almond=a,anise=l,creosote=c,fishy=y,foul=f,musty=m,none=n,pungent=p,spicy=s
 6. gill-attachment:          attached=a,descending=d,free=f,notched=n
 7. gill-spacing:             close=c,crowded=w,distant=d
 8. gill-size:                broad=b,narrow=n
 9. gill-color:               black=k,brown=n,buff=b,chocolate=h,gray=g,green=r,orange=o,pink=p,purple=u,red=e,white=w,yellow=y
10. stalk-shape:              enlarging=e,tapering=t
11. stalk-root:               bulbous=b,club=c,cup=u,equal=e,rhizomorphs=z,rooted=r,missing=?
12. stalk-surface-above-ring: fibrous=f,scaly=y,silky=k,smooth=s
13. stalk-surface-below-ring: fibrous=f,scaly=y,silky=k,smooth=s
...
21. population:               abundant=a,clustered=c,numerous=n,scattered=s,several=v,solitary=y
22. habitat:                  grasses=g,leaves=l,meadows=m,paths=p,urban=u,waste=w,woods=d
```

NB, categorical

Data set on mushroom edibility (poisonous, edible)

```
p,x,s,n,t,p,f,c,n,k,e,e,s,s,w,w,p,w,o,p,k,s,u
e,x,s,y,t,a,f,c,b,k,e,c,s,s,w,w,p,w,o,p,n,n,g
e,b,s,w,t,l,f,c,b,n,e,c,s,s,w,w,p,w,o,p,n,n,m
p,x,y,w,t,p,f,c,n,n,e,e,s,s,w,w,p,w,o,p,k,s,u
e,x,s,g,f,n,f,w,b,k,t,e,s,s,w,w,p,w,o,e,n,a,g
[...]
```

- Note: for real applications, you can use the implementation of Naïve Bayes in the Scikit-learn library
- For the assignment you will implement your NB classifier.
- For the assignment, with continuous features, use KDE
- In this example we have categorical features, so we just compute the logarithms of the fractions

NB, categorical

List features values, adding "?"

```
def get_features():
    lines = open('agaricus-lepiota.features').readlines()
    features = []
    for lin in lines:
        ft_vals = '?'
        fragments = lin.split('=')
        for frag in fragments[1:]:
            ft_vals = ft_vals+frag[0]
        features.append(ft_vals)
    return features
```

```
1. cap-shape: bell=b,conical=c,convex=x,flat=f, knobbed=k,sunken=s
2. cap-surface: fibrous=f,grooves=g,scaly=y,smooth=s
[...]
21. population: abundant=a,clustered=c,numerous=n, scattered=s...
22. habitat: grasses=g,leaves=l,meadows=m,paths=p, urban=u,...
```

NB, categorical

List features values, adding "?"

```
def get_features():
    lines = open('agaricus-lepiota.features').readlines()
    features = []
    for lin in lines:
        ft_vals = '?'
        fragments = lin.split('=')
        for frag in fragments[1:]:
            ft_vals = ft_vals+frag[0]
        features.append(ft_vals)
    return features
```

```
In : get_features()
Out:
 ['?bcxfks', '?fgys', '?nbcgrpuewy', '?tf', '?alcyfmnps', '?adfn',
  '?cwd', '?bn', '?knbhgropuewy', '?et', '?bcuezr?', '?fyks', '?fyks',
  '?nbcgopewy', '?nbcgopewy', '?pu', '?nowy', '?not', '?ceflnpsz',
  '?knbhrouwy', '?acnsvy', '?glmpuwd']
```

NB, categorical

- Load data and shuffle rows

```
def load_data(features,class_codes):
    lines = open('agaricus-lepiota.data').readlines()
    feat_vals = np.zeros((len(lines),22)).astype(int)  # to store indexes
    classes = np.zeros(len(lines))
    for row,lin in enumerate(lines):
        s = lin.replace(',','').strip()
        classes[row] = class_codes.index(s[0])
        for column,fv in enumerate(s[1:]):
            feat_vals[row,column] = features[column].index(fv)
    ixs = list(range(feat_vals.shape[0]))
    np.random.shuffle(ixs)
    return feat_vals[ixs,:],classes[ixs]
```

- Note: take care not to scramble features and class labels

NB, categorical

- Build "histogram" with $\ln p(x_i|C_c)$
- (count frequencies)
- What to do if some feature does not appear? $p(x_i|C_c) = 0$.
- Solution:additive smoothing

$$\hat{p}(x_j = k) = \frac{count(k) + \alpha}{N + \alpha d}$$

- (we'll use $\alpha = 1$)

```
def make_hists(data,features):
    hists = []
    for feat in features:
        hists.append(np.ones(len(feat)))
    for row in range(data.shape[0]):
        for column in range(data.shape[1]):
            hists[column][data[row,column]] +=1
    for ix in range(len(hists)):
        hists[ix] = np.log(hists[ix]/float(data.shape[0]+len(features[ix])))
    return hists
```

NB, categorical

Split train and test sets

- We'll do stratified sampling to keep same proportion of classes in training and test sets (poisonous and edible)
- No need for cross-validation; we are not adjusting parameters

- We could use cross-validation instead of a test set if we had fewer data
- You can use train_test_split from sklearn.model_selection

```
def split_data(features,test_fraction):
    feat_vals,classes = load_data(features,'ep')
    edible = feat_vals[classes==0,:]
    poison = feat_vals[classes==1,:]
    e_test_points = int(test_fraction*edible.shape[0])
    e_train = edible[e_test_points:,:]
    e_test = edible[:e_test_points,:]
    p_test_points = int(test_fraction*poison.shape[0])
    p_train = poison[p_test_points:,:]
    p_test = poison[:p_test_points,:]
    return e_train,p_train,e_test,p_test
```

NB, categorical

Classify examples

```
def classify(e_class,e_log,p_class,p_log,feat_mat):
    classes = np.zeros(feat_mat.shape[0])
    for row in range(feat_mat.shape[0]):
        e_sum = e_log
        p_sum = p_log
        for column in range(feat_mat.shape[1]):
            e_sum = e_sum + e_class[column][int(feat_mat[row,column])]
            p_sum = p_sum + p_class[column][int(feat_mat[row,column])]
        if e_sum<p_sum:
            classes[row]=1
    return classes
```

NB, categorical

- The complete function

```
def do_bayes():
    features = get_features()
    e_train,p_train,e_test,p_test = split_data(features,0.5)
    e_hists = make_hists(e_train,features)
    p_hists = make_hists(p_train,features)
    tot_len = e_train.shape[0]+p_train.shape[0]
    e_log = np.log(float(e_train.shape[0])/tot_len)
    p_log = np.log(float(p_train.shape[0])/tot_len)
    c_e = classify(e_hists,e_log,p_hists,p_log,e_test)
    c_p = classify(e_hists,e_log,p_hists,p_log,p_test)
    errors = sum(c_e)+sum(1-c_p)
    error_perc = float(errors)/(len(c_e)+len(c_p))*100
    print(f'{errors:.0f} errors; {error_perc:.2f}% error rate')
    print('\tE\tP')
    print(f'E\t{sum(1-c_e):.0f}\t{sum(1-c_p):.0f}')
    print(f'P\t{sum(c_e):.0f}\t{sum(c_p):.0f}')
```

```
191 errors; 4.70% error rate
        E       P
E       2091    178
P       13      1780
```

NB, categorical

Confusion matrix

- Eating poisonous mushrooms is more costly...

Mushroom class		
Prediction	Edible	Poisonous
Edible	2091	178
Poisonous	13	1780

Naïve Bayes

Discriminative classifiers

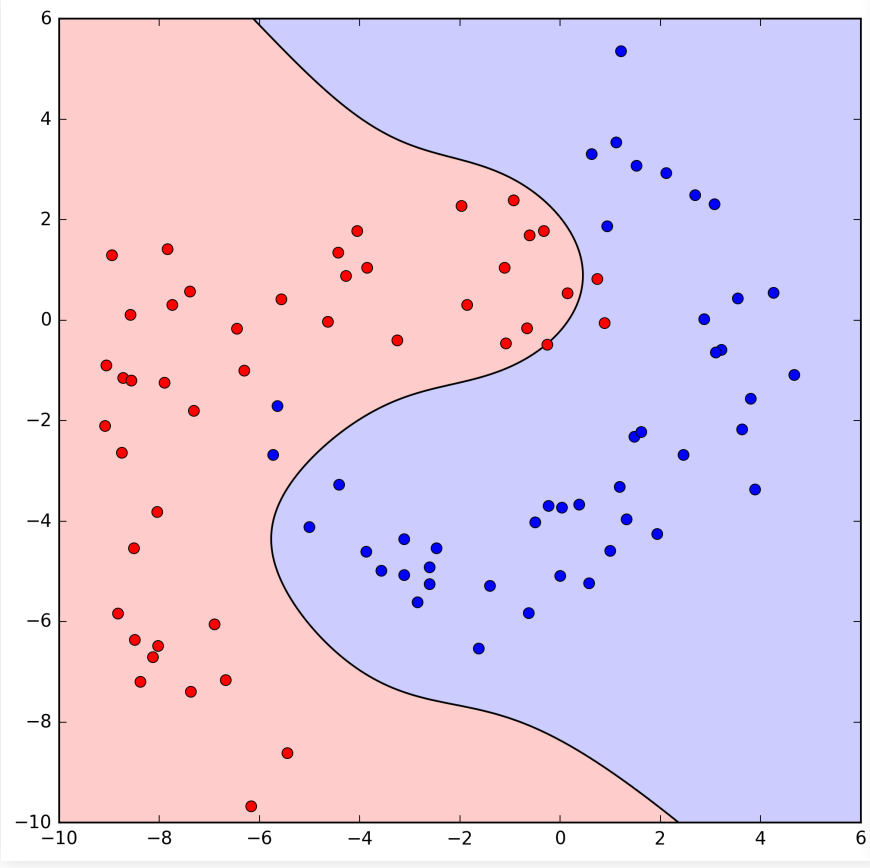
- Classifiers such as logistic regression compute a conditional probability for the class given the features.
- This is directly what we need to discriminate examples.

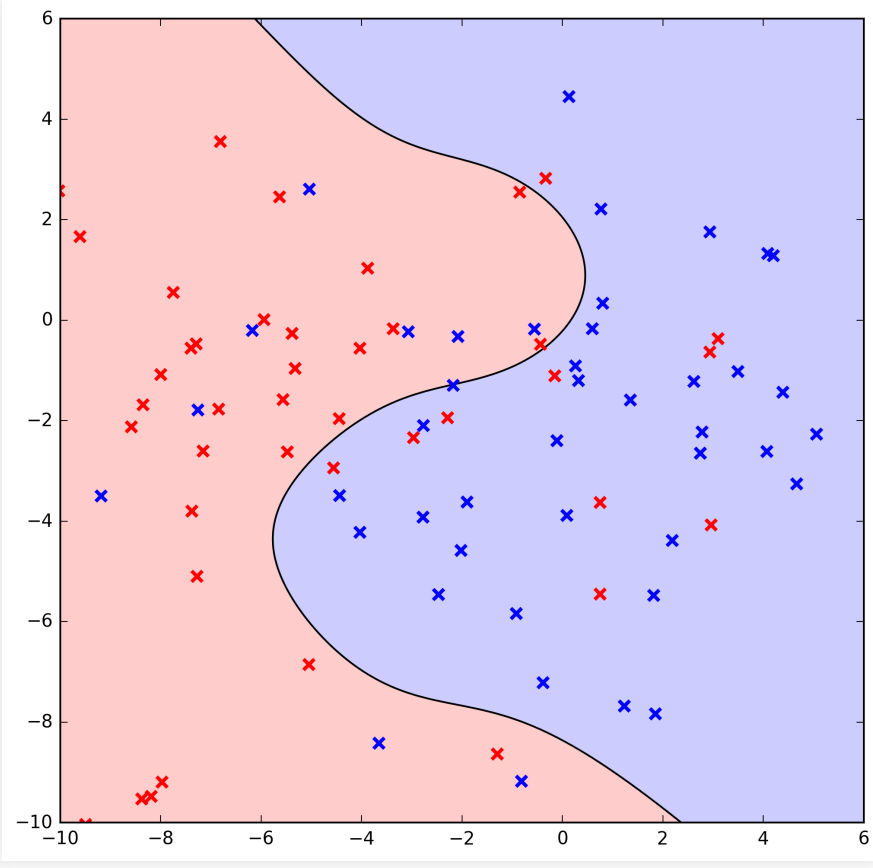
Generative classifiers

- Naïve Bayes classifier is a generative classifier
- These compute the joint probability distribution, allowing us to generate synthetic examples from the trained hypothesis

Naïve Bayes

- Learning from points on the left, generate points on the right

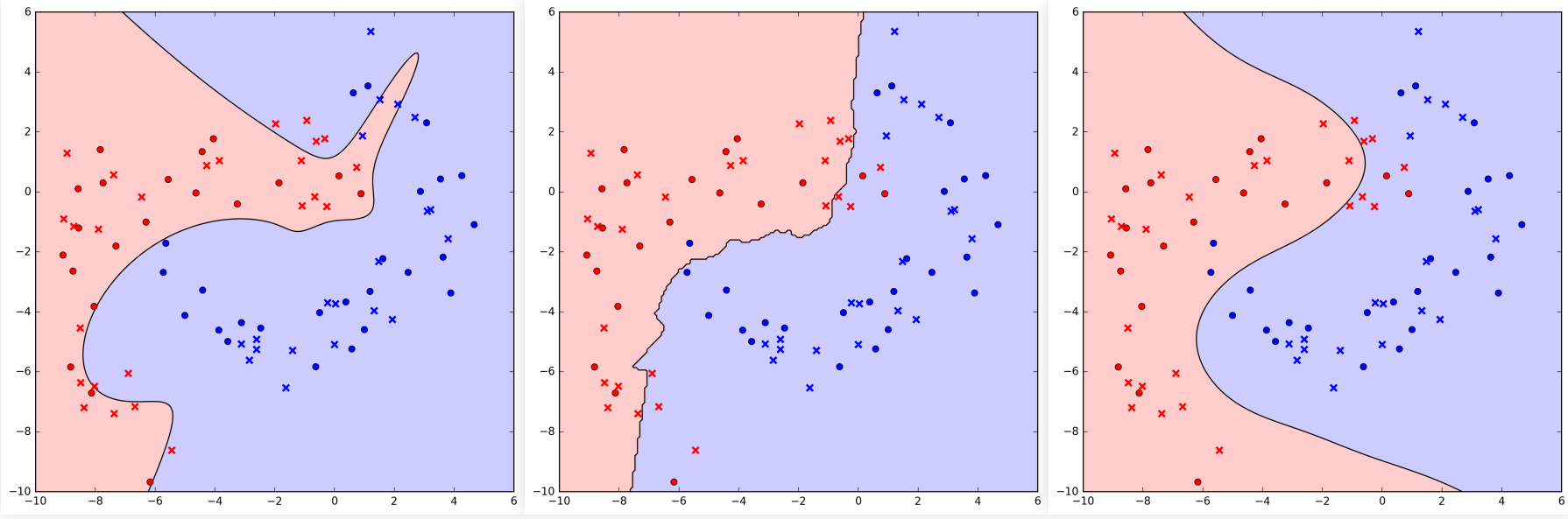




Comparing classifiers

Comparing classifiers

- Log.Reg., k-NN, Naïve Bayes



- Test set, 45 points
- Logistic Regression, 10 errors; k-NN, 6 errors; Naïve Bayes, 1 error

Which one is better?

Comparing classifiers

Aproximate normal test

- Assume errors normally distributed around true error rate:

$$\frac{X - Np_0}{\sqrt{Np_0(1-p_0)}} \approx Z$$

- Test if intervals are disjoint with some confidence level (e.g. 95%)

$$X - 1.96\sigma \leq Np_0 \leq X + 1.96\sigma \quad \sigma \approx \sqrt{N\frac{X}{N}(1-\frac{X}{N})}$$

- Logistic Regression: 10 ± 5.4
- k-NN: 6 ± 3.5
- Naïve Bayes: 1 ± 1.9

Comparing classifiers

Better alternative: McNemar's test

- e_{01} and e_{10}: count examples wrong in one and correct in the other

$$\frac{(|e_{01} - e_{10}| - 1)^2}{e_{01} + e_{10}} \approx \chi_1^2$$

- McNemar's test, 95% confidence, significant difference if:

$$\frac{(|e_{01} - e_{10}| - 1)^2}{e_{01} + e_{10}} \geq 3.84$$

- Logistic Regression vs kNN = 0.8
- kNN vs Naïve Bayes = 2.3
- Naïve Bayes vs Logistic Regression = 7.11
- Conclusion: Naïve Bayes likely better than Logistic Regression

Processing Data

Processing Data

Data can come in many forms

- Target values: Classification vs Regression
- Continuous or discrete features
- Different distributions

Main goal: predict for new examples

- Train on some data, validate and test on other data

How about rescaling?

- Should we compute scale parameters (normalization, standardization) for training set or training folds?

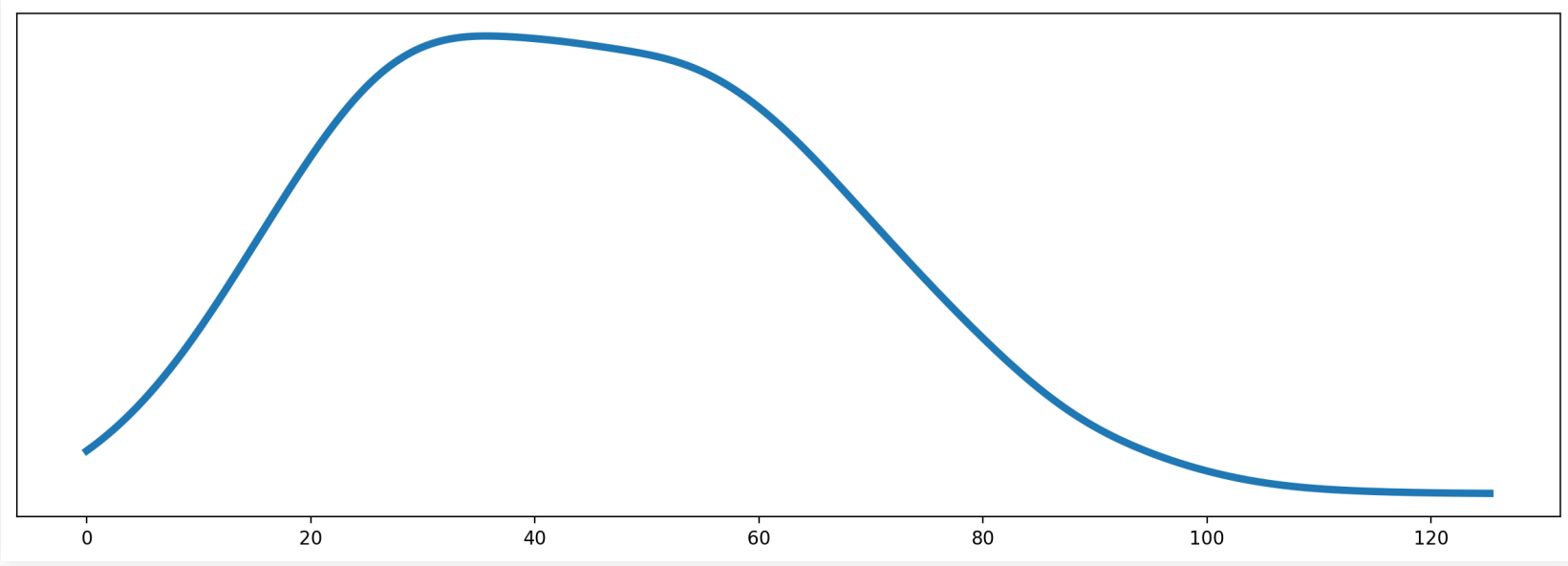
Processing Data

Rescaling parameters

- In theory: these are parameters computed from data
- We should compute on training data and apply to validation or test
- However, statistics like the mean converge rapidly
- In practice it makes little difference, so we do it only once
- (In general...)

Rescaling parameters

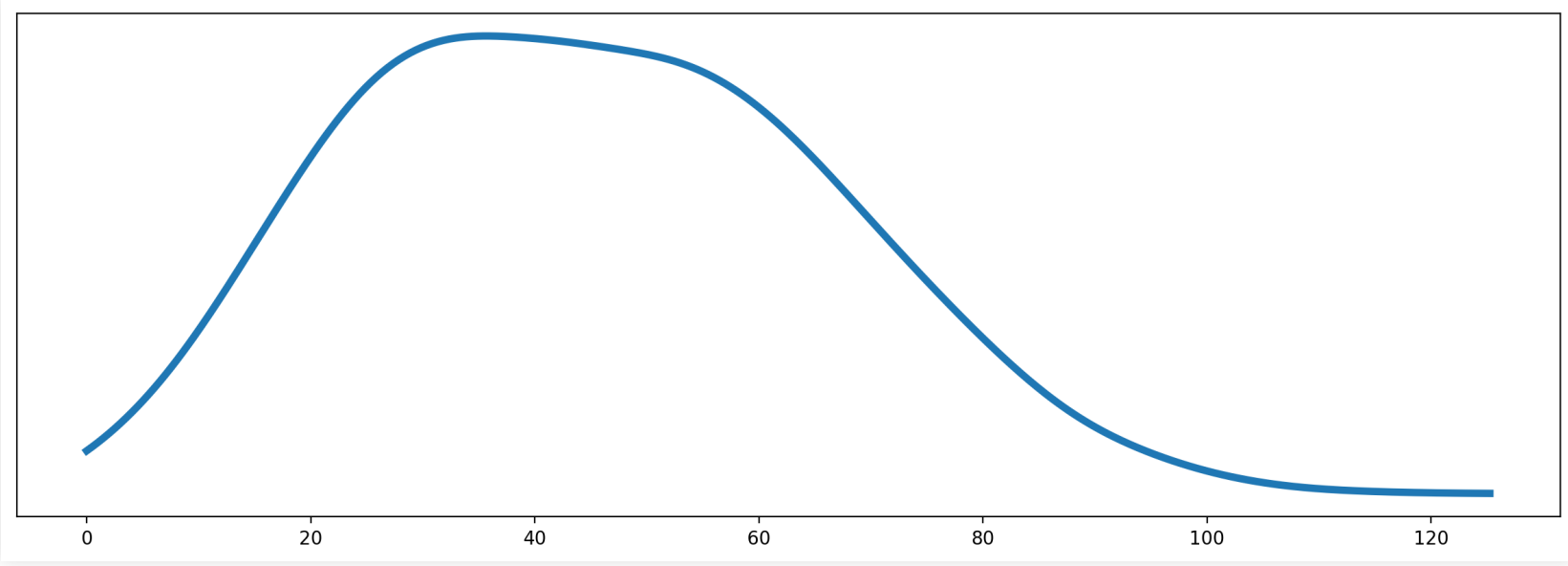
- Example: 2000 points, split 1000/1000, compute mean



- Means diverge by 0.014 of standard deviation
- Computing for each training fold or whole set nearly the same

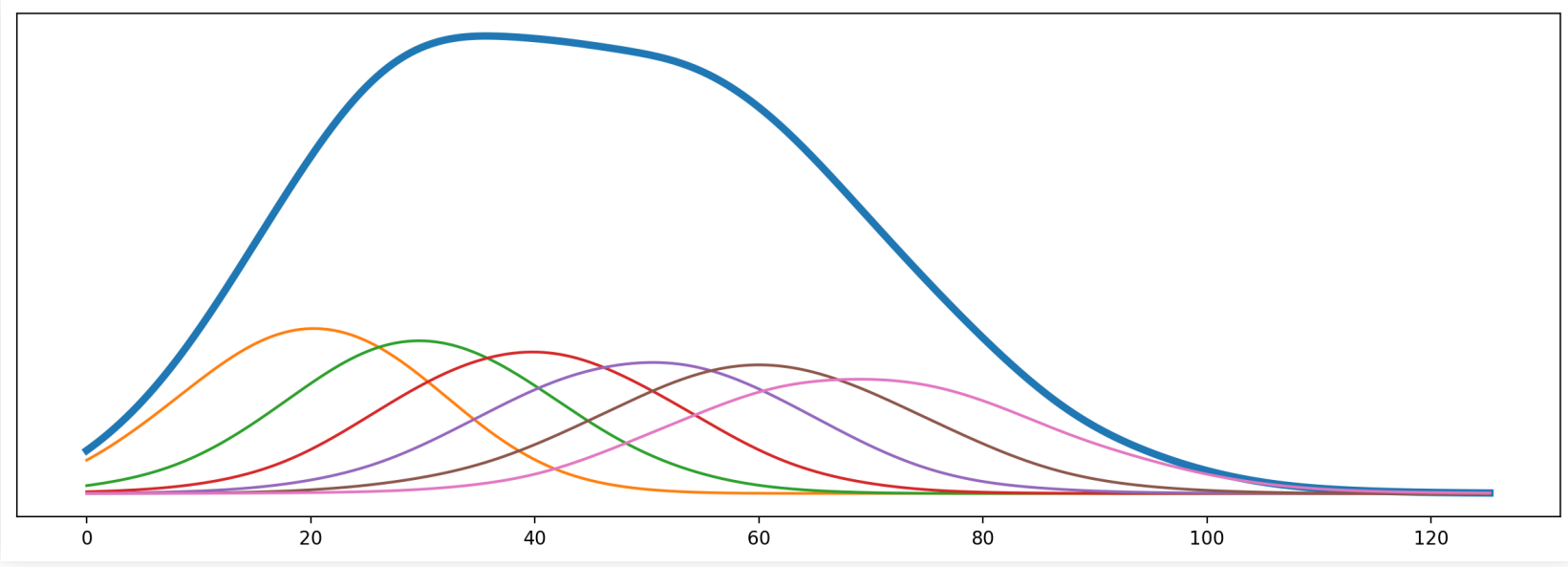
Splitting the data

- But things may be more complicated.
- Example: 2000 values, money spent on transportation



Splitting the data

- Data comes from 6 different cities
- Example: 2000 values, money spent on transportation



- How should we split the data and compute scaling parameters?

Processing Data

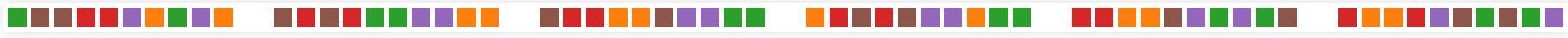
- Case 1:

- Examples can come from any city
- We want to predict for new examples in these cities

- We can shuffle the data and if the data set is large enough we can rescale everything once

- For cross validation or testing, better to stratify

- Keep the same proportion of data from each city

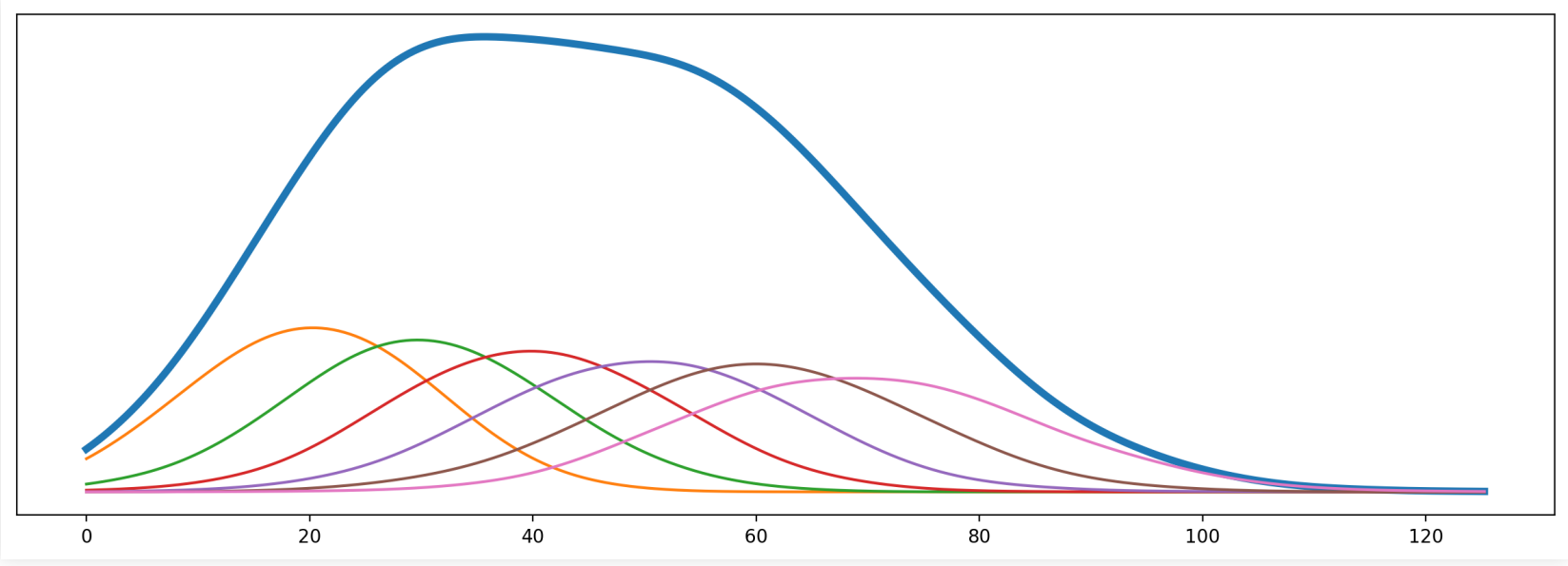


Processing Data

- Case 2:

- We know the city each example comes from
- We want to predict for new examples in other cities

- Different cities have different distributions

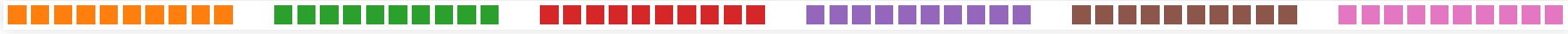


Processing Data

- Case 2:

- We know the city each example comes from
- We want to predict for new examples in other cities

- Different cities have different distributions
- We need to consider the generalization from some cities to others
- We should split by city (and eventually shuffle before training)



- Rescaling should be done for training data only because statistics will differ

Processing Data

What to take from this

- Do not memorize recipes
- This may lead you to incorrect results
- Understand what you are doing
- Main focus of this course

Assignment 1

Assignment 1

Classify bank notes

- Four features (from scans of bank notes), continuous
- Do not expand (that was for illustrating the concept)
- Three classifiers:

- Naïve Bayes with KDE (yours), Gaussian NB and Logistic Regression (sklearn)

- Implement Naïve Bayes using KDE from Scikit-Learn
- Optimize parameters (KDE bandwidth and C for Logistic Regression)
- Compare using approximate normal and McNemar's test
- Submit code, plots and answered question form

- English or Português

- Check page for instructions (and updates)

Summary

Summary

- Bayes Classifier and Naïve Bayes Classifier
- Parametric and non-parametric models
- Generative and Discriminative classifiers
- Comparing classifiers
- Processing data: understand what you are dealing with

Further reading

- Bishop, Section 1.2
- Alpaydin, Section 14.6
- Mitchell, Section 6.9
- Marsland, Section 8.1.2