

Bayes Classifiers

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CS 273P Machine Learning and Data Mining

Machine Learning

Bayes Classifiers

Naive Bayes Classifiers

Bayes Error

Gaussian Bayes Classifiers

A basic classifier

- Training data $D = \{x^{(i)}, y^{(i)}\}$, Classifier $f(x ; D)$
 - Discrete feature vector x
 - $f(x ; D)$ is a contingency table
- Ex: credit rating prediction (bad/good)
 - $X_1 = \text{income (low/med/high)}$
 - How can we make the most # of correct predictions?

Features	# bad	# good
X=0	42	15
X=1	338	287
X=2	3	5

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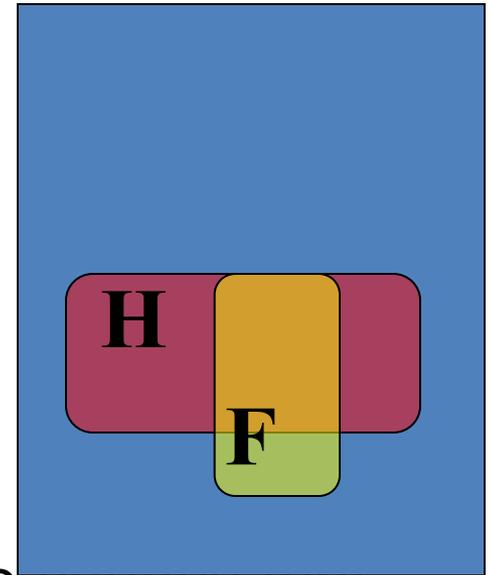
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- Ex: credit rating prediction (bad/good)
 - $X_1 = \text{income (low/med/high)}$
 - How can we make the most # of correct predictions?
 - Predict more likely outcome for each possible observation
 - Can normalize into probability:
 $p(y = \text{good} \mid X = c)$
 - How to generalize?

Features	# bad	# good
X=0	.7368	.2632
X=1	.5408	.4592
X=2	.3750	.6250

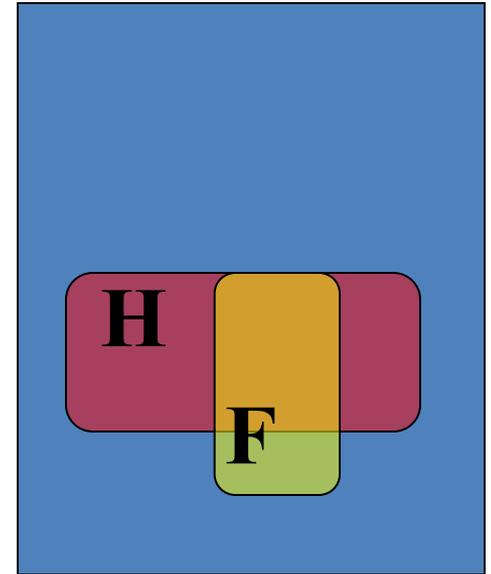
Bayes rule

- Two events: headache, flu
 - $p(H) = 1/10$
 - $p(F) = 1/40$
 - $p(H|F) = 1/2$
-
- You wake up with a headache – what is the chance that you have the flu?



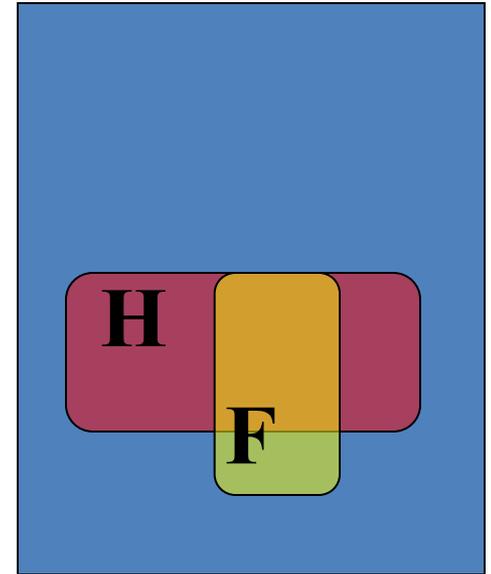
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- $P(F|H) = ?$



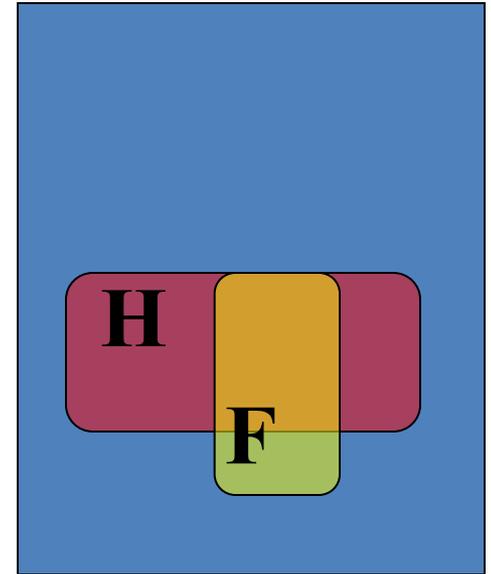
Bayes rule

- Two events: headache, flu
- $p(H) = 1/10$
- $p(F) = 1/40$
- $p(H|F) = 1/2$
- $P(H \& F) = p(F) p(H|F)$
 $= (1/2) * (1/40) = 1/80$
- $P(F|H) = ?$



Bayes rule

- Two events: headache, flu
- $p(H) = 1/10$
- $p(F) = 1/40$
- $p(H|F) = 1/2$
- $P(H \& F) = p(F) p(H|F)$
 $= (1/2) * (1/40) = 1/80$
- $P(F|H) = p(H \& F) / p(H)$
 $= (1/80) / (1/10) = 1/8$



Classification and probability

- Suppose we want to model the data
- Prior probability of each class, $p(y)$
 - E.g., fraction of applicants that have good credit
- Distribution of features given the class, $p(x | y=c)$
 - How likely are we to see “x” in users with good credit?
- Joint distribution

$$p(y|x)p(x) = p(x, y) = p(x|y)p(y)$$

- Bayes Rule:

$$\Rightarrow p(y|x) = p(x|y)p(y)/p(x)$$

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

(Use the rule of total probability to calculate the denominator!) 

Bayes classifiers

- Learn “class conditional” models
 - Estimate a probability model for each class
- Training data, D
 - Split by class, $D_c = \{ x^{(j)} : y^{(j)} = c \}$
- Estimate $p(x | y=c)$ using D_c
- For a discrete x , this recalculates the same table...

Features	# bad	# good
X=0	42	15
X=1	338	287
X=2	3	5



$p(x y=0)$	$p(x y=1)$
42 / 383	15 / 307
338 / 383	287 / 307
3 / 383	5 / 307



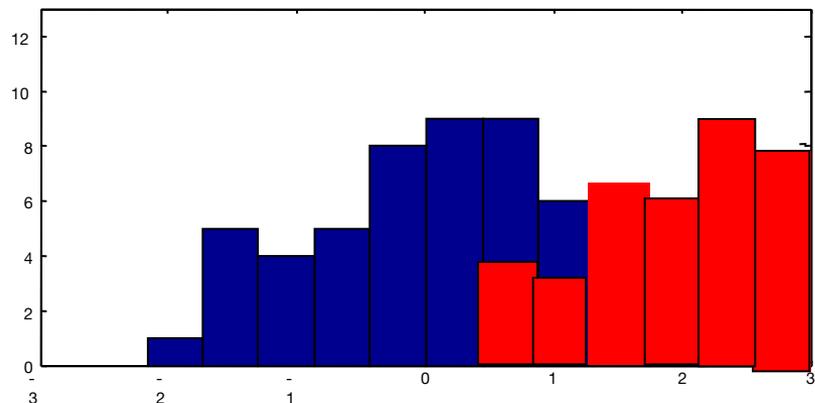
$p(y=0 x)$	$p(y=1 x)$
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$p(y)$	383/690	307/690
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Bayes classifiers

- Learn “class conditional” models
 - Estimate a probability model for each class
- Training data
 - Split by class
 - $D_c = \{ x^{(j)} : y^{(j)} = c \}$
- Estimate $p(x | y=c)$ using D_c

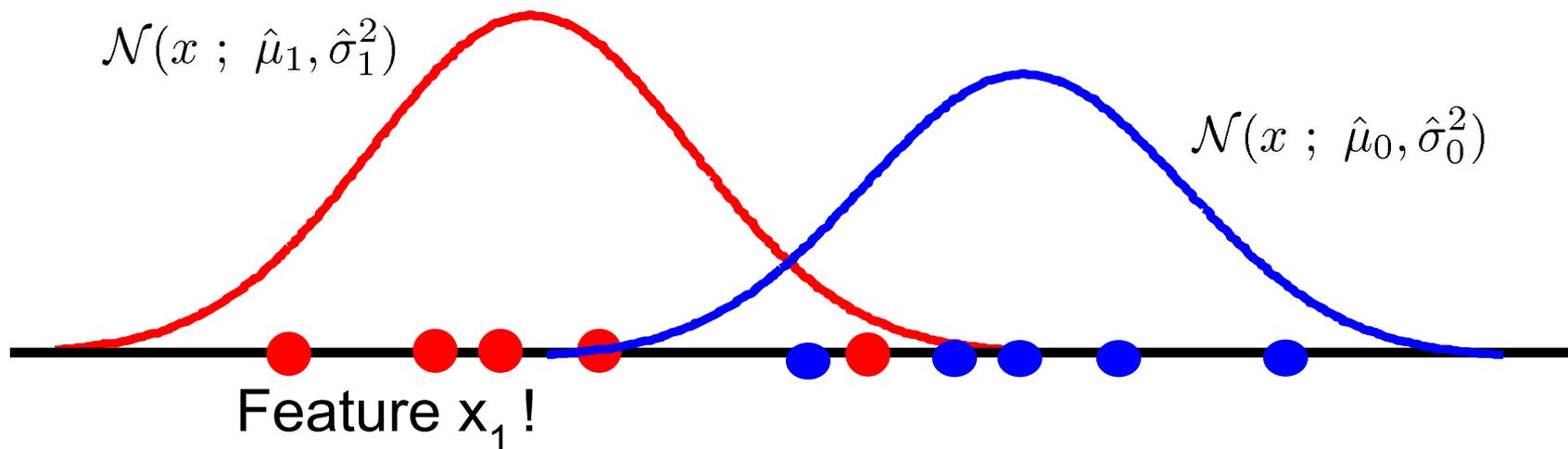
- For continuous x , can use any density estimate we like
 - Histogram
 - Gaussian
 - ...



Gaussian models

- Estimate parameters of the Gaussians from the data

$$\hat{\mu} = \frac{1}{m} \sum_j x^{(j)} \quad \hat{\sigma}^2 = \frac{1}{m} \sum_j (x^{(j)} - \mu)^2$$



Multivariate Gaussian models

- Similar to univariate case

$$\mathcal{N}(\underline{x}; \underline{\mu}, \Sigma) = \frac{1}{(2\pi)^{d/2}} |\Sigma|^{-1/2} \exp \left\{ -\frac{1}{2} (\underline{x} - \underline{\mu})^T \Sigma^{-1} (\underline{x} - \underline{\mu}) \right\}$$

$\underline{\mu}$ = length-d column vector

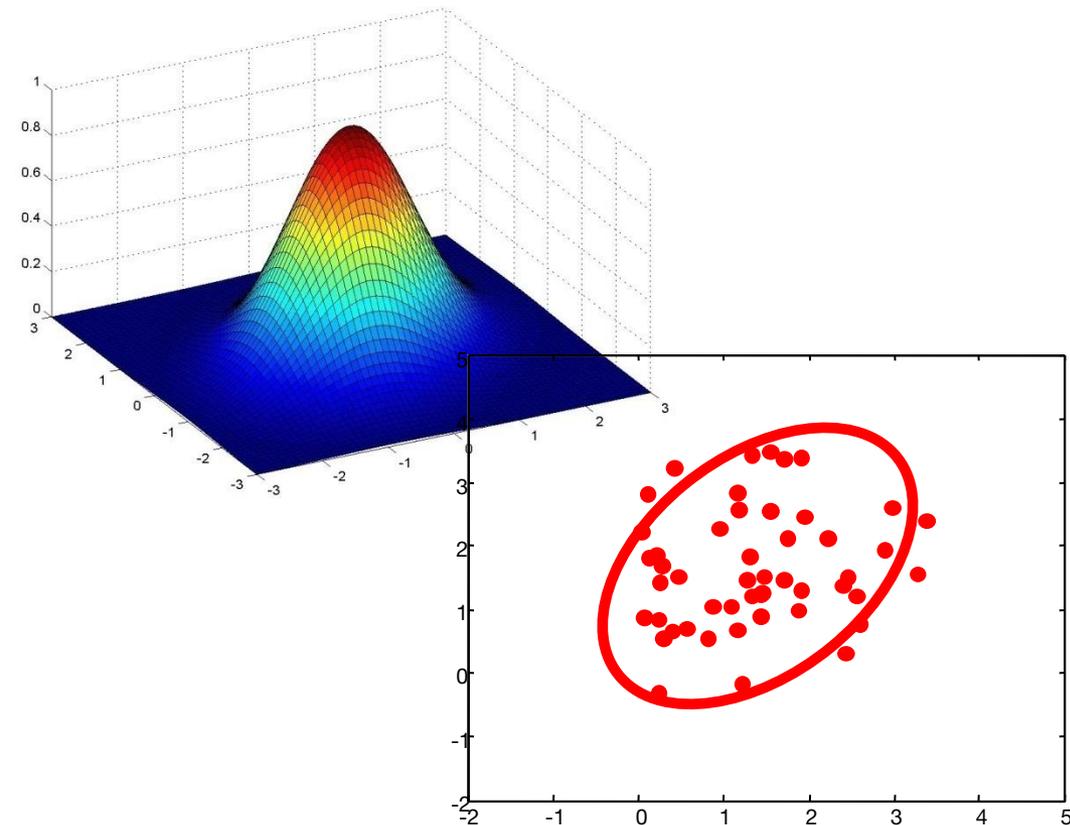
Σ = d x d matrix

$|\Sigma|$ = matrix determinant

Maximum likelihood estimate:

$$\hat{\underline{\mu}} = \frac{1}{m} \sum_j \underline{x}^{(j)}$$

$$\hat{\Sigma} = \frac{1}{m} \sum_j (\underline{x}^{(j)} - \hat{\underline{\mu}})^T (\underline{x}^{(j)} - \hat{\underline{\mu}})$$



Example: Gaussian Bayes for Iris Data

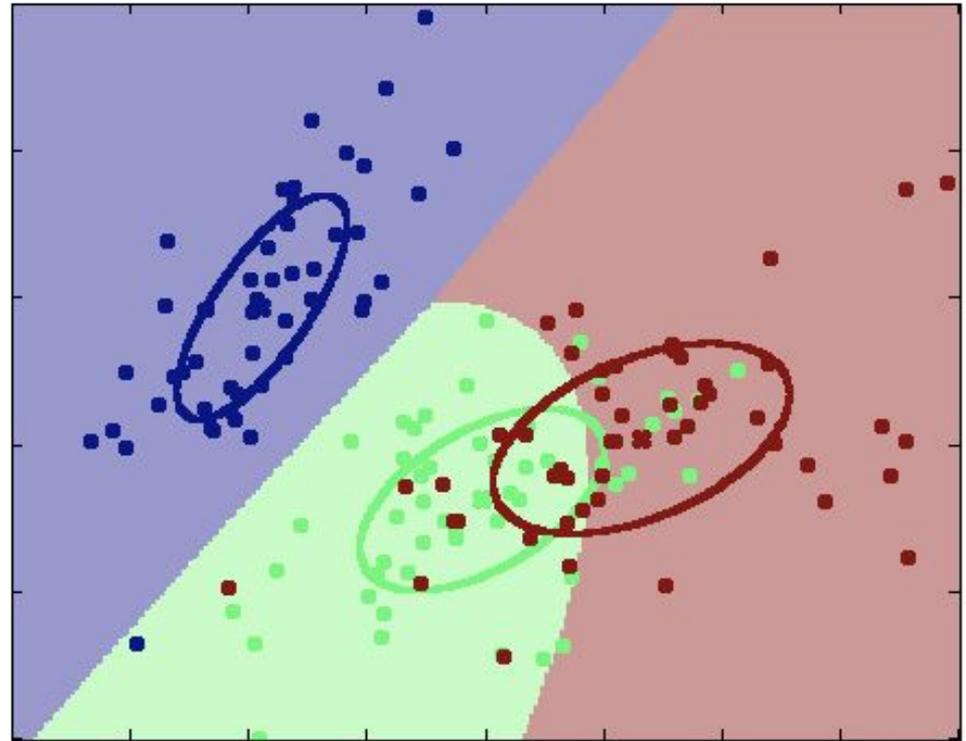
- Fit Gaussian distribution to each class {0,1,2}

$$p(y) = \text{Discrete}\left(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}\right)$$

$$p(x_1, x_2 | y = 0) = \mathcal{N}(x; \mu_0, \Sigma_0)$$

$$p(x_1, x_2 | y = 1) = \mathcal{N}(x; \mu_1, \Sigma_1)$$

$$p(x_1, x_2 | y = 2) = \mathcal{N}(x; \mu_2, \Sigma_2)$$



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Bayes classifiers

- Estimate $p(y) = [p(y=0) , p(y=1) \dots]$
- Estimate $p(x | y=c)$ for each class c
- Calculate $p(y=c | x)$ using Bayes rule
- Choose the most likely class c

- For a discrete x , can represent as a contingency table...
 - What about if we have more discrete features?

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X=0	42	15
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$p(x y=0)$	$p(x y=1)$
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$p(y)$	383/690	307/690
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Joint distributions

- Make a truth table of all combinations of values

A	B	C
0	0	0
0	0	1
0	1	0
0	1	1
1	0	0
1	0	1
1	1	0
1	1	1

Joint distributions

- Make a truth table of all combinations of values
- For each combination of values, determine how probable it is
- Total probability must sum to one
- How many values did we specify?

A	B	C	$p(A,B,C y=1)$
0	0	0	0.50
0	0	1	0.05
0	1	0	0.01
0	1	1	0.10
1	0	0	0.04
1	0	1	0.15
1	1	0	0.05
1	1	1	0.10

Overfitting and density estimation

- Estimate probabilities from the data
 - E.g., how many times (what fraction) did each outcome occur?
- $M \text{ data} \ll 2^N \text{ parameters?}$
- What about the zeros?
 - We learn that certain combinations are impossible?
 - What if we see these later in test data?
- Overfitting!

A	B	C	$p(A,B,C y=1)$
0	0	0	4/10
0	0	1	1/10
0	1	0	0/10
0	1	1	0/10
1	0	0	1/10
1	0	1	2/10
1	1	0	1/10
1	1	1	1/10

Overfitting and density estimation

- Estimate probabilities from the data
 - E.g., how many times (what fraction) did each outcome occur?

A	B	C	p(A,B,C y=1)
0	0	0	4/10
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0	1	0	0/10
0	1	1	0/10
1	0	0	1/10
1	0	1	2/10
1	1	0	1/10
1	1	1	1/10

- M data $\ll 2^n$ parameters?

- What about the zeros?

- We learn that certain combinations are impossible?
- What if we see these later in test data?

- One option: regularize

- Normalize to make sure $\hat{p}(a, b, c) \propto (M_{abc} + \alpha)$

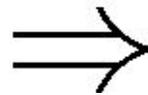
Overfitting and density estimation

- Another option: reduce the model complexity
 - E.g., **assume that features are independent of one another**
- Independence:
- $p(a,b) = p(a) p(b)$
- $p(x_1, x_2, \dots, x_N | y=1) = p(x_1 | y=1) p(x_2 | y=1) \dots p(x_N | y=1)$
- Only need to estimate each individually

A	$p(A y=1)$
0	.4
1	.6

B	$p(B y=1)$
0	.7
1	.3

C	$p(C y=1)$
0	.1
1	.9



A	B	C	$p(A,B,C y=1)$
0	0	0	.4 * .7 * .1
0	0	1	.4 * .7 * .9
0	1	0	.4 * .3 * .1
0	1	1	...
1	0	0	
1	0	1	
1	1	0	
1	1	1	

Example: Naïve Bayes

Observed Data:

x_1	x_2	y
1	1	0
1	0	0
1	0	1
0	0	0
0	1	1
1	1	0
0	0	1
1	0	1

$$\hat{p}(y = 1) = \frac{4}{8} = (1 - \hat{p}(y = 0))$$

$$\hat{p}(x_1, x_2 | y = 0) = \hat{p}(x_1 | y = 0) \hat{p}(x_2 | y = 0)$$

$$\hat{p}(x_1 = 1 | y = 0) = \frac{3}{4}$$

$$\hat{p}(x_1 = 1 | y = 1) = \frac{2}{4}$$

$$\hat{p}(x_2 = 1 | y = 0) = \frac{2}{4}$$

$$\hat{p}(x_2 = 1 | y = 1) = \frac{1}{4}$$

Prediction given some observation $x = (1,1)$?

$$\hat{p}(y = 1) \hat{p}(x = 11 | y = 1) <$$

$$\frac{4}{8} \times \frac{2}{4} \times \frac{1}{4} >$$

$$\hat{p}(y = 0) \hat{p}(x = 11 | y = 0)$$

$$\frac{4}{8} \times \frac{3}{4} \times \frac{2}{4}$$

Decide class 0

Example: Naïve Bayes

Observed Data:

x_1	x_2	y
1	1	0
1	0	0
1	0	1
0	0	0
0	1	1
1	1	0
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$$\hat{p}(x_1, x_2 | y = 0) = \hat{p}(x_1 | y = 0) \hat{p}(x_2 | y = 0)$$

$$\hat{p}(x_1 = 1 | y = 0) = \frac{3}{4} \qquad \hat{p}(x_1 = 1 | y = 1) = \frac{2}{4}$$

$$\hat{p}(x_2 = 1 | y = 0) = \frac{2}{4} \qquad \hat{p}(x_2 = 1 | y = 1) = \frac{1}{4}$$

$$\begin{aligned} \hat{p}(y = 1 | x_1 = 1, x_2 = 1) &= \frac{\frac{4}{8} \times \frac{2}{4} \times \frac{1}{4}}{\frac{3}{4} \times \frac{2}{4} \times \frac{4}{8} + \frac{2}{4} \times \frac{1}{4} \times \frac{4}{8}} \\ &= \frac{1}{4} \end{aligned}$$

Example: Joint Bayes

Observed Data:

x_1	x_2	y
1	1	0
1	0	0
1	0	1
0	0	0
0	1	1
1	1	0
0	0	1
1	0	1

$$\hat{p}(y = 1) = \frac{4}{8} = (1 - \hat{p}(y = 0))$$

$$\hat{p}(x_1, x_2 | y = 0) =$$

x_1	x_2	$p(x y=0)$
0	0	1/4
0	1	0/4
1	0	1/4
1	1	2/4

$$\hat{p}(x_1, x_2 | y = 1) =$$

x_1	x_2	$p(x y=1)$
0	0	1/4
0	1	1/4
1	0	2/4
1	1	0/4

$$\hat{p}(y = 1 | x_1 = 1, x_2 = 1) = \frac{\frac{4}{8} \times 0}{\frac{2}{4} \times \frac{4}{8} + 0 \times \frac{4}{8}} = 0$$

Naïve Bayes models

- Variable y to predict, e.g. “auto accident in next year?”
- We have **many** co-observed vars $\mathbf{x}=[x_1 \dots x_n]$
 - Age, income, education, zip code, ...
- Want to learn $p(y | x_1 \dots x_n)$, to predict y
 - Arbitrary distribution: $O(d^n)$ values!
- Naïve Bayes:
 - $p(y|\mathbf{x})= p(\mathbf{x}|y) p(y) / p(\mathbf{x})$; $p(\mathbf{x}|y) = \prod_i p(x_i|y)$
 - Covariates are independent given “cause”
- Note: may not be a good model of the data
 - Doesn't capture correlations in x 's
 - Can't capture some dependencies
- But in practice it often does quite well!

Naïve Bayes models for spam

- $y \in \{\text{spam, not spam}\}$
- $X =$ observed words in email
 - Ex: [“the” ... “probabilistic” ... “lottery”...]
 - “1” if word appears; “0” if not
- 1000’s of possible words: 2^{1000s} parameters?
- # of atoms in the universe: » 2^{270} ...
- Model words **given** email type as independent
- Some words more likely for spam (“lottery”)
- Some more likely for real (“probabilistic”)
- Only 1000’s of parameters now...

Naïve Bayes Gaussian models

$$p(x_1) = \frac{1}{Z} \exp \left\{ -\frac{1}{2\sigma_1^2} (x_1 - \mu_1)^2 \right\}$$

$$p(x_2) = \frac{1}{Z_2} \exp \left\{ -\frac{1}{2\sigma_2^2} (x_2 - \mu_2)^2 \right\}$$

$$p(x_1)p(x_2) = \frac{1}{Z_1 Z_2} \exp \left\{ -\frac{1}{2} (\underline{x} - \underline{\mu})^T \Sigma^{-1} (\underline{x} - \underline{\mu}) \right\}$$

$$\underline{\mu} = [\mu_1 \ \mu_2]$$

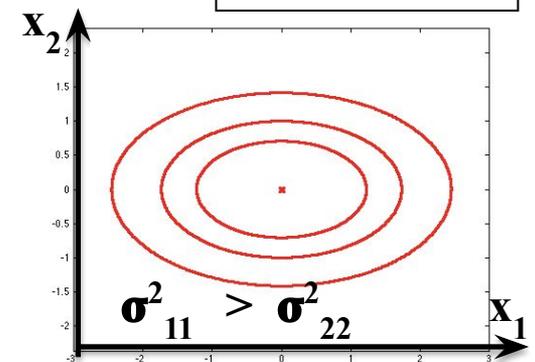
$$\Sigma = \text{diag}(\sigma_1^2, \sigma_2^2)$$

$$\Sigma = \begin{bmatrix} \sigma_{11}^2 & 0 \\ 0 & \sigma_{22}^2 \end{bmatrix}$$

Again, reduces the number of parameters of the model:

Bayes: $n^2/2$

Naïve Bayes: n



You should know...

- Bayes rule; $p(y | x)$
- Bayes classifiers
 - Learn $p(x | y=C)$, $p(y=C)$
- Naïve Bayes classifiers
 - Assume features are independent given class:
$$p(x | y=C) = p(x_1 | y=C) p(x_2 | y=C) \dots$$
- Maximum likelihood (empirical) estimators for
 - Discrete variables
 - Gaussian variables
 - Overfitting; simplifying assumptions or regularization

Machine Learning

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Gaussian Bayes Classifiers

A Bayes classifier

- Given training data, compute $p(y=c | x)$ and choose largest
- What's the (training) error rate of this method?

Features	# bad	# good
X=0	42	15
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A Bayes classifier

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- What's the (training) error rate of this method?

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Gets these examples wrong:

$$\text{Pr[error]} = (15 + 287 + 3) / (690)$$

(empirically on training data:
better to use test data)

Bayes Error Rate

- Suppose that we knew the true probabilities:

$$p(x, y) \Rightarrow p(y), p(x|y = 0), p(x|y = 1)$$

- Observe any x : $\Rightarrow p(y = 0|x)$ (at any x)

$$p(y = 1|x)$$

- Optimal decision at that particular x is:

$$\hat{y} = f(x) = \arg \max_c p(y = c|x)$$

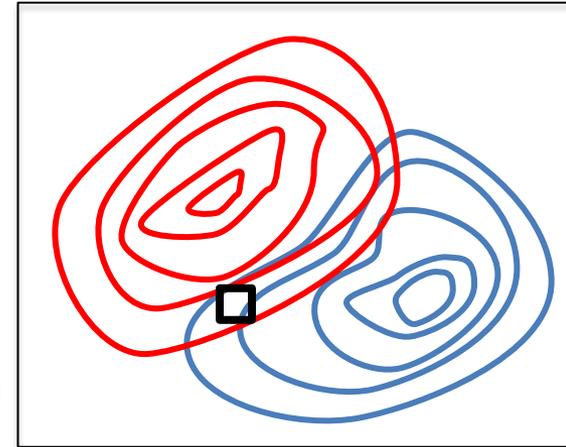
- Error rate is:

$$\mathbb{E}_{xy}[y \neq \hat{y}] = \mathbb{E}_x[1 - \max_c p(y = c|x)] = \text{“Bayes error rate”}$$

- This is **the best that any classifier can do!**
- Measures fundamental hardness of separating y -values given only features x

- Note: conceptual only!

- Probabilities $p(x,y)$ must be estimated from data
- Form of $p(x,y)$ is not known and may be very complex

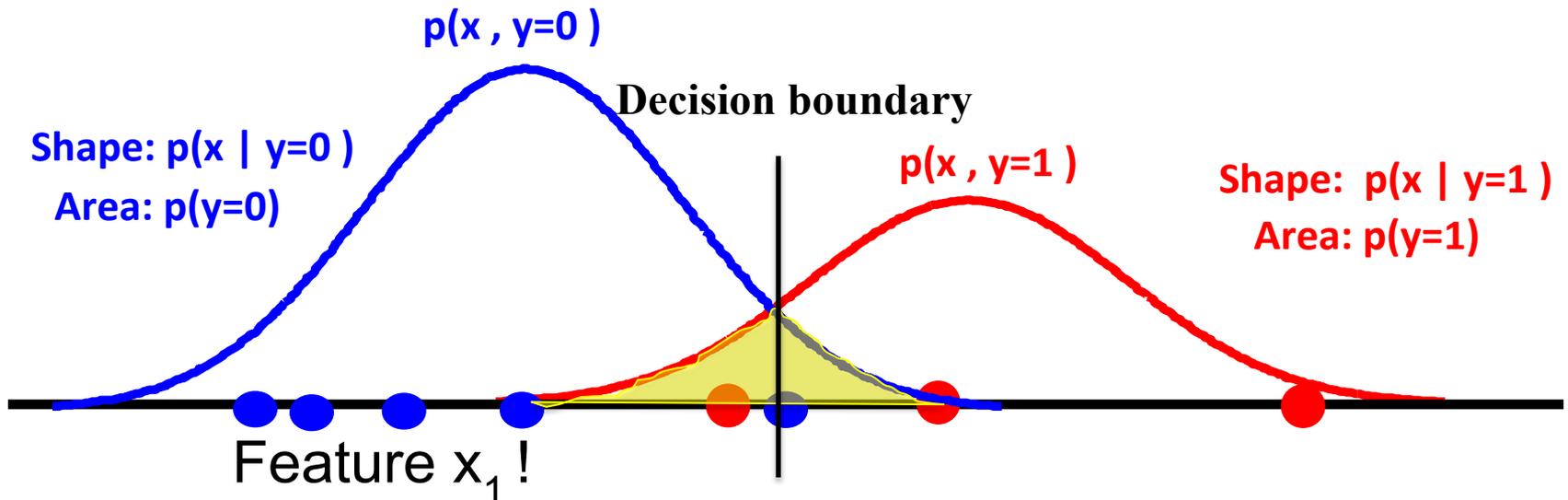


A Bayes classifier

- Bayes classification decision rule compares probabilities:

$$\begin{aligned} p(y = 0|x) &< p(y = 1|x) \\ &> \\ \Rightarrow p(y = 0, x) &< p(y = 1, x) \\ &> \end{aligned}$$

- Can visualize this nicely if x is a scalar:

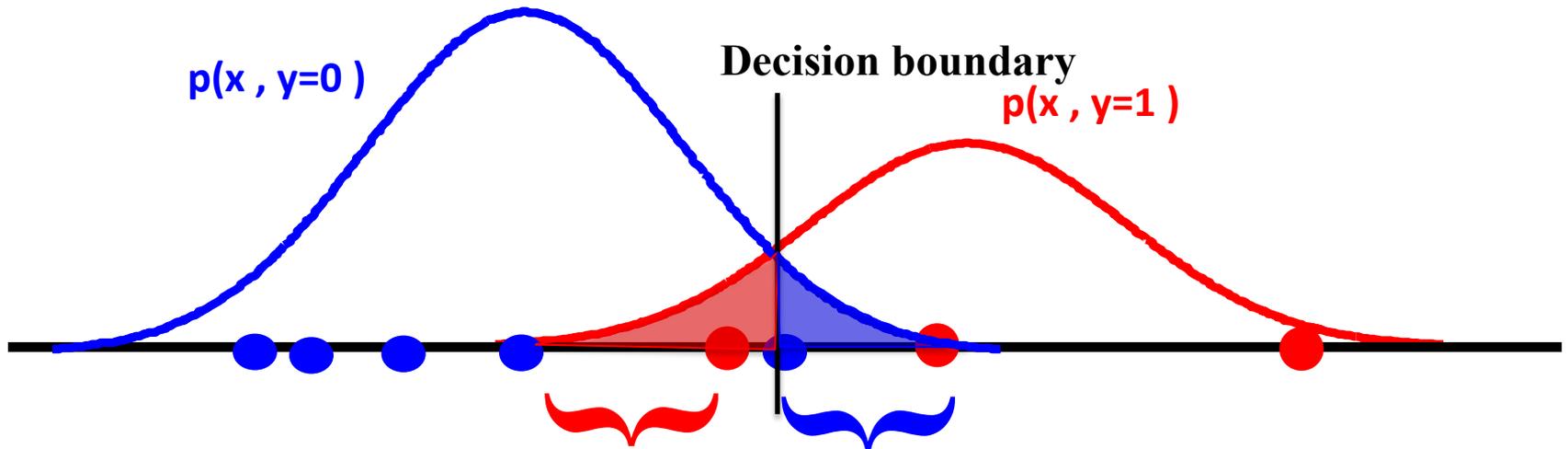


A Bayes classifier

- Not all errors are created equally...
- Risk associated with each outcome?

Add multiplier alpha:

$$\alpha p(y = 0, x) \begin{matrix} < \\ > \end{matrix} p(y = 1, x)$$



Type 2 errors: false negatives

Type 1 errors: false positives

False negative rate: $(\# y=1, \hat{y}=0) / (\#y=1)$

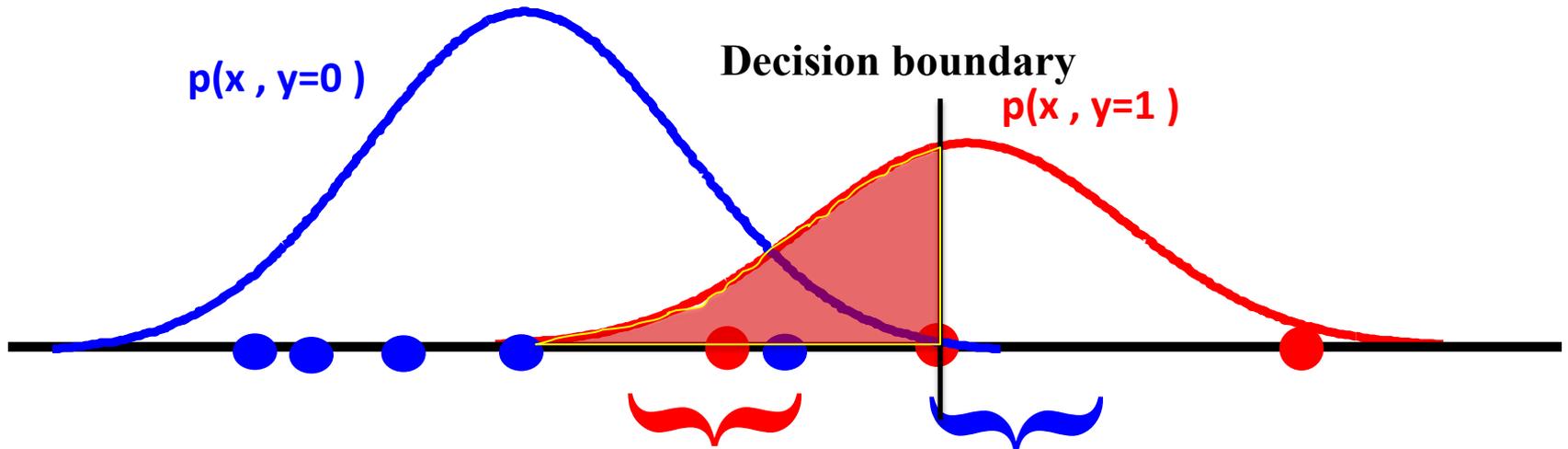
False positive rate: $(\# y=0, \hat{y}=1) / (\#y=0)$

A Bayes classifier

- Increase alpha: prefer class 0
- Spam detection

Add multiplier alpha:

$$\alpha p(y = 0, x) \begin{matrix} < \\ > \end{matrix} p(y = 1, x)$$



Type 2 errors: false negatives

Type 1 errors: false positives

False negative rate: $(\# y=1, \hat{y}=0) / (\#y=1)$

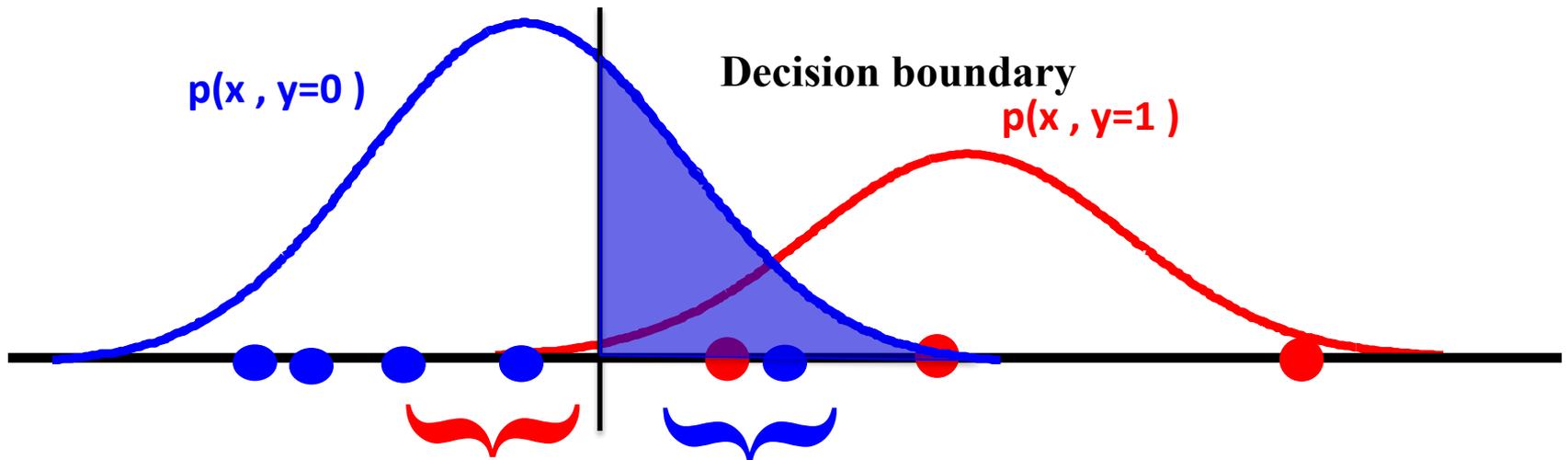
False positive rate: $(\# y=0, \hat{y}=1) / (\#y=0)$

A Bayes classifier

- Decrease alpha: prefer class 1
- Cancer detection

Add multiplier alpha:

$$\alpha p(y = 0, x) \begin{matrix} < \\ > \end{matrix} p(y = 1, x)$$



Type 2 errors: false negatives

Type 1 errors: false positives

False negative rate: $(\# y=1, \hat{y}=0) / (\#y=1)$ False positive rate: $(\# y=0, \hat{y}=1) / (\#y=0)$

Measuring errors

- Confusion matrix
- Can extend to more classes

	Predict 0	Predict 1
Y=0	380	5
Y=1	338	3

- True positive rate: $\#(y=1, \hat{y}=1) / \#(y=1)$ -- “sensitivity”
- False negative rate: $\#(y=1, \hat{y}=0) / \#(y=1)$
- False positive rate: $\#(y=0, \hat{y}=1) / \#(y=0)$
- True negative rate: $\#(y=0, \hat{y}=0) / \#(y=0)$ -- “specificity”

Likelihood ratio tests

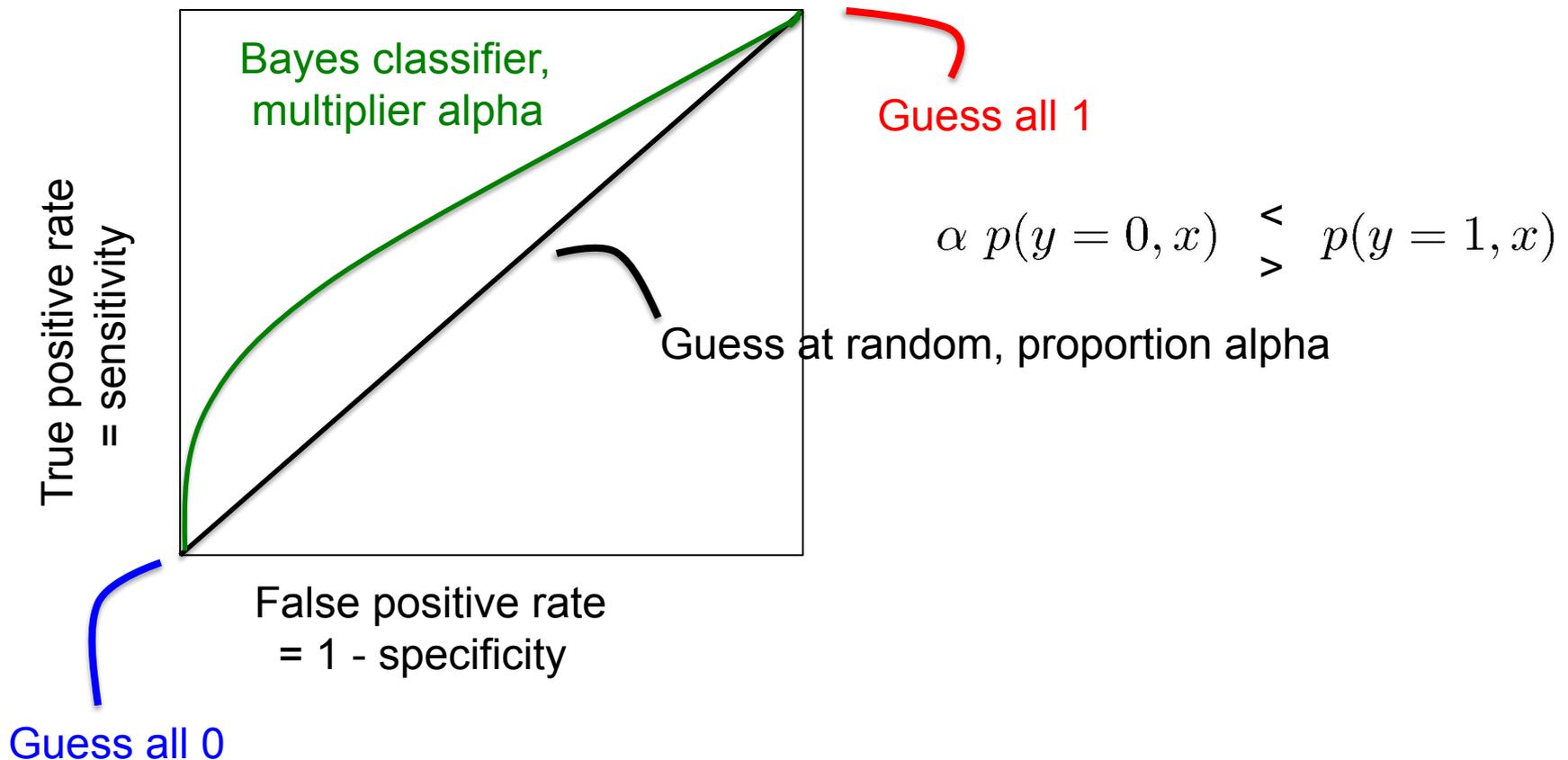
- Connection to classical, statistical decision theory:

$$p(y = 0, x) \underset{>}{<} p(y = 1, x) = \log \frac{p(y = 0)}{p(y = 1)} \underset{>}{<} \log \frac{p(x|y = 1)}{p(x|y = 0)}$$

- Likelihood ratio: relative support for observation “x” under “alternative hypothesis” $y=1$, compared to “null hypothesis” $y=0$
“log likelihood ratio”
- Can vary the decision threshold: $\gamma \underset{>}{<} \log \frac{p(x|y = 1)}{p(x|y = 0)}$
- Classical testing:
 - Choose gamma so that FPR is fixed (“p-value”)
 - Given that $y=0$ is true, what’s the probability we decide $y=1$?

ROC Curves

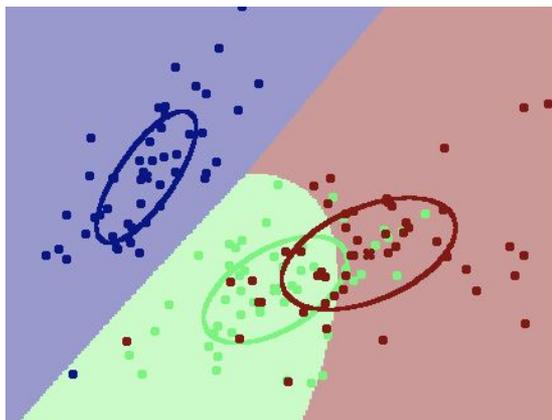
- Characterize performance as we vary the decision threshold?



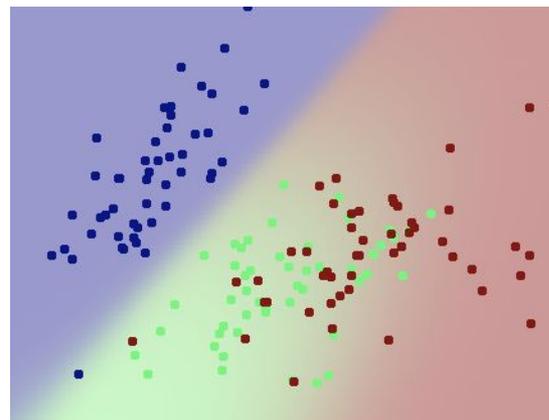
Demo of ROC

<http://www.navan.name/roc/>

Probabilistic vs. Discriminative learning



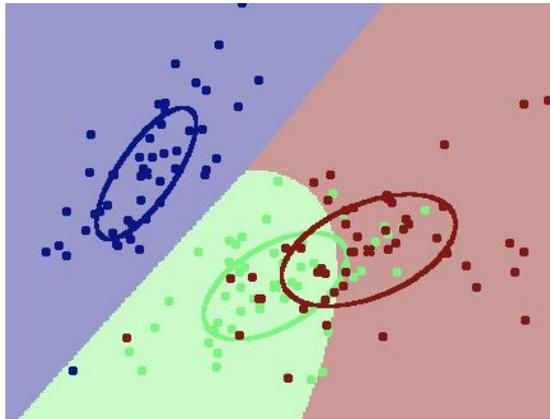
“Discriminative” learning:
Output prediction $\hat{y}(x)$



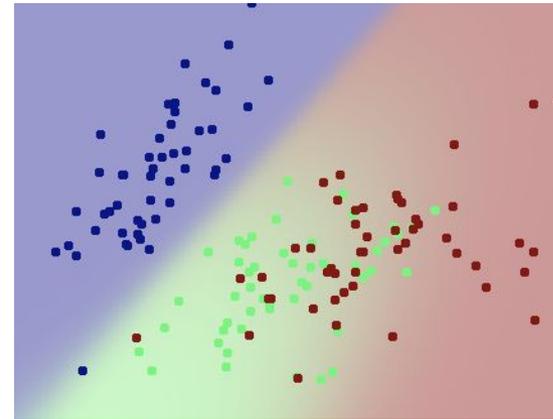
“Probabilistic” learning:
Output probability $p(y|x)$
(*expresses confidence in outcomes*)

- “Probabilistic” learning
 - Conditional models just explain y : $p(y|x)$
 - Generative models also explain x : $p(x,y)$
 - Often a component of unsupervised or semi-supervised learning
 - Bayes and Naïve Bayes classifiers are generative models

Probabilistic vs. Discriminative learning



“Discriminative” learning:
Output prediction $\hat{y}(x)$



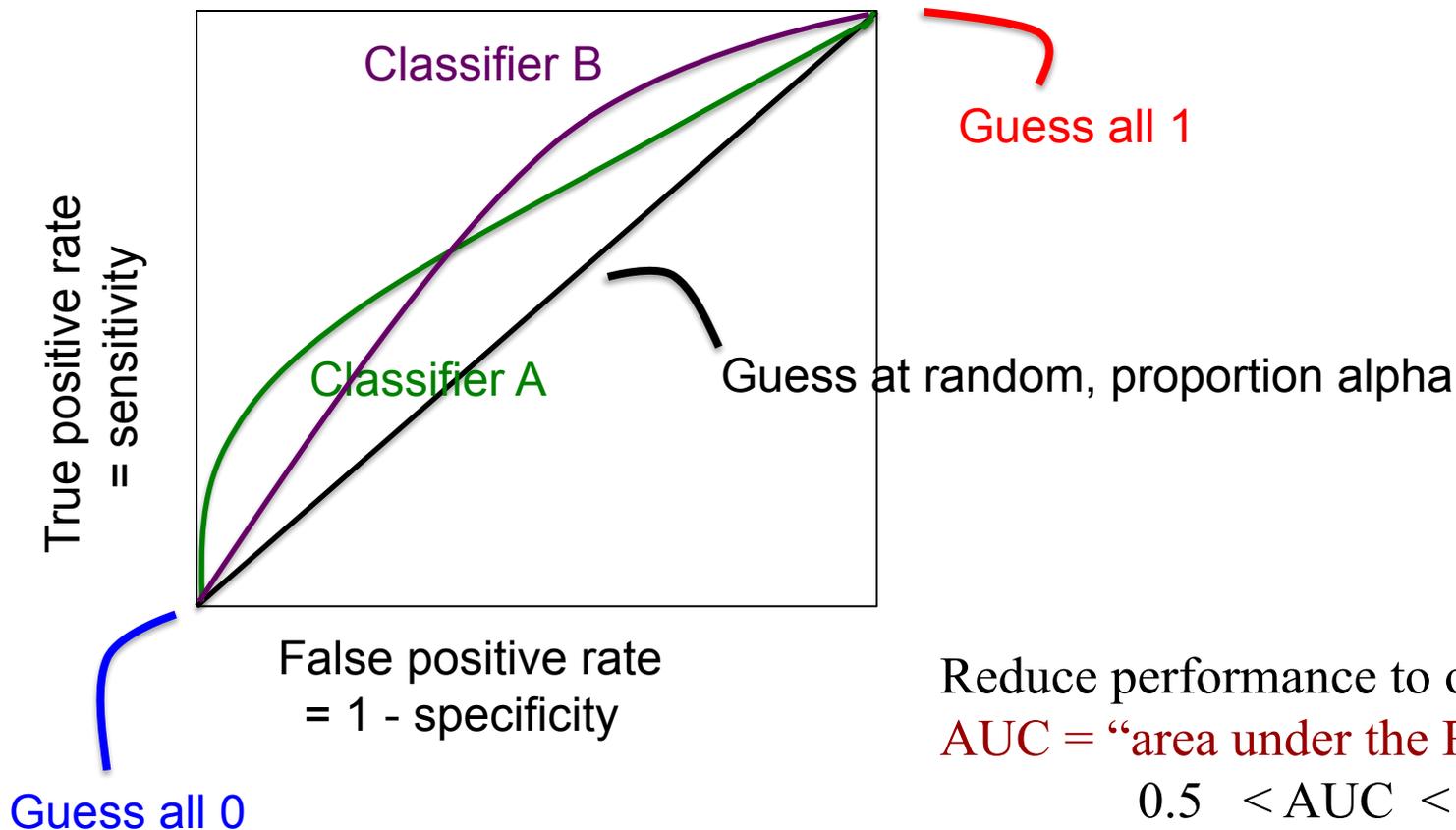
“Probabilistic” learning:
Output probability $p(y|x)$
(expresses confidence in outcomes)

- Can use ROC curves for discriminative models also:
 - Some notion of confidence, but doesn't correspond to a probability
 - In our code: “predictSoft” (vs. hard prediction, “predict”)

```
>> learner = gaussianBayesClassify(X,Y); % build a classifier
>> Ysoft = predictSoft(learner, X); % N x C matrix of confidences
>> plotSoftClassify2D(learner,X,Y); % shaded confidence plot
```

ROC Curves

- Characterize performance as we vary our confidence threshold?



Reduce performance to one number?

AUC = "area under the ROC curve"

$$0.5 < \text{AUC} < 1$$

Machine Learning

Bayes Classifiers

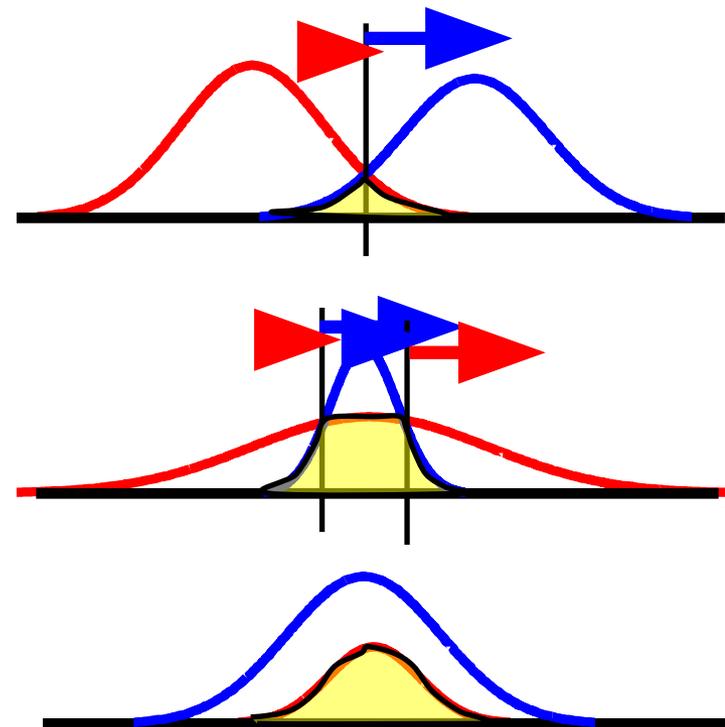
Naive Bayes Classifiers

Bayes Error

Gaussian Bayes Classifiers

Gaussian models

- “Bayes optimal” decision
 - Choose most likely class
- Decision boundary
 - Places where probabilities equal
- What shape is the boundary?



Gaussian models

- Bayes optimal decision boundary
 - $p(y=0 | x) = p(y=1 | x)$
 - Transition point between $p(y=0|x) >/< p(y=1|x)$
- Assume Gaussian models with equal covariances

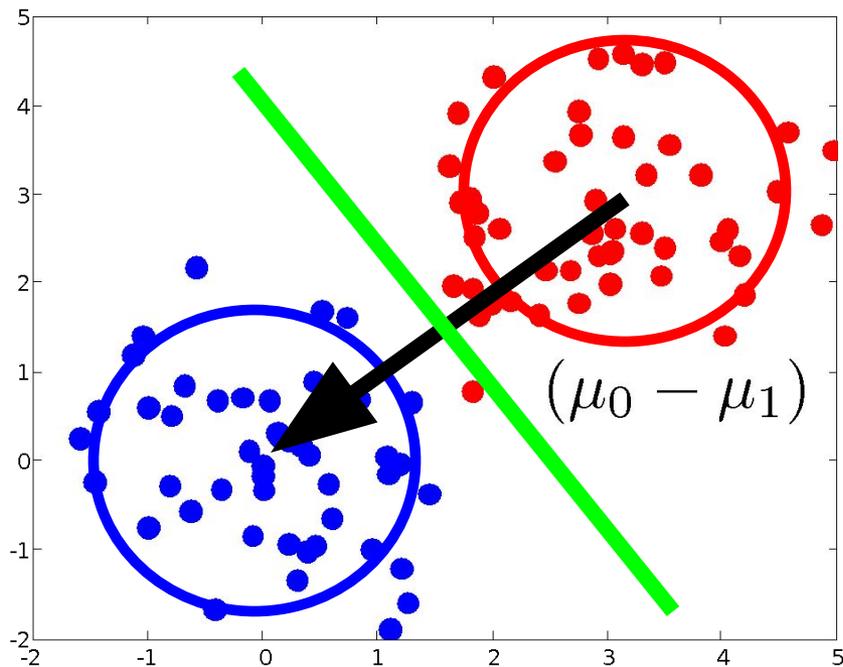
$$\mathcal{N}(\underline{x} ; \underline{\mu}, \Sigma) = \frac{1}{(2\pi)^{d/2}} |\Sigma|^{-1/2} \exp \left\{ -\frac{1}{2} (\underline{x} - \underline{\mu})^T \Sigma^{-1} (\underline{x} - \underline{\mu}) \right\}$$

$$\begin{aligned} 0 &< \log \frac{p(x|y=0) p(y=0)}{p(x|y=1) p(y=1)} = \log \frac{p(y=0)}{p(y=1)} + \\ &> & - .5(x \Sigma^{-1} x - 2\mu_0^T \Sigma^{-1} x + \mu_0^T \Sigma^{-1} \mu_0) \\ & & + .5(x \Sigma^{-1} x - 2\mu_1^T \Sigma^{-1} x + \mu_1^T \Sigma^{-1} \mu_1) \\ & = (\mu_0 - \mu_1)^T \Sigma^{-1} x + \text{constants} \end{aligned}$$

Gaussian example

- Spherical covariance: $\Sigma = \sigma^2 \mathbf{I}$
- Decision rule $= (\mu_0 - \mu_1)^T \Sigma^{-1} x + \text{constants}$

$$(\mu_0 - \mu_1)^T x \begin{matrix} < \\ > \end{matrix} C$$

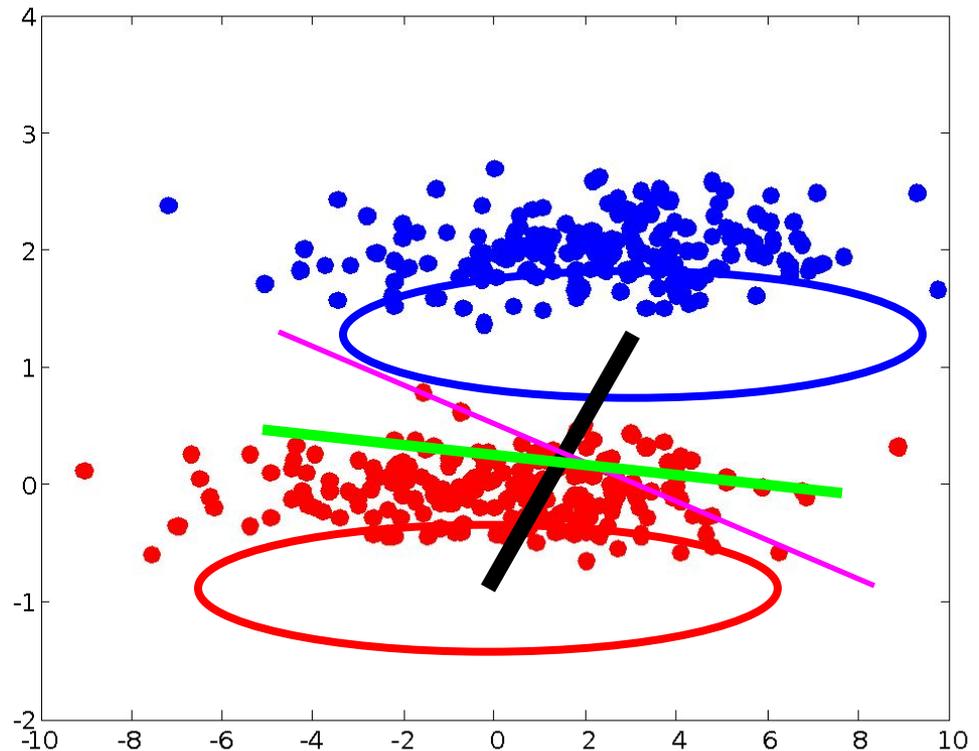


$$C = .5(\mu_0^T \Sigma^{-1} \mu_0 - \mu_1^T \Sigma^{-1} \mu_1) - \log \frac{p(y = 0)}{p(y = 1)}$$

Non-spherical Gaussian distributions

- Equal covariances => still linear decision rule
 - May be “modulated” by variance direction
 - Scales; rotates (if correlated)

Ex:
Variance
 $\begin{bmatrix} 3 & 0 \\ 0 & .25 \end{bmatrix}$



Class posterior probabilities

- Useful to also know class *probabilities*
- Some notation
 - $p(y=0)$, $p(y=1)$ – class *prior* probabilities
 - How likely is each class in general?
 - $p(x | y=c)$ – class conditional probabilities
 - How likely are observations “x” in that class?
 - $p(y=c | x)$ – class posterior probability
 - How likely is class c *given* an observation x?

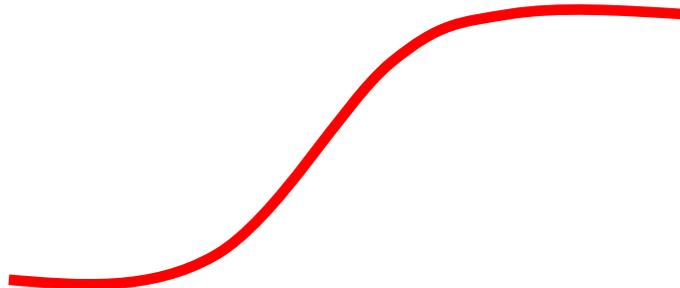
Class posterior probabilities

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 - How likely are observations “x” in that class?
 - $p(y=c | x)$ – class posterior probability
 - How likely is class *c* *given* an observation *x*?
- We can compute posterior using Bayes’ rule
 - $p(y=c | x) = p(x|y=c) p(y=c) / p(x)$
- Compute $p(x)$ using sum rule / law of total prob.
 - $p(x) = p(x|y=0) p(y=0) + p(x|y=1)p(y=1)$

Class posterior probabilities

- Consider comparing two classes
 - $p(x | y=0) * p(y=0)$ vs $p(x | y=1) * p(y=1)$
 - Write probability of each class as
 - $p(y=0 | x) = p(y=0, x) / p(x)$
 - $= p(y=0, x) / (p(y=0,x) + p(y=1,x))$
 - $= 1 / (1 + \exp(-a))$ (**)

 - $a = \log [p(x|y=0) p(y=0) / p(x|y=1) p(y=1)]$
 - (**) called the logistic function, or logistic sigmoid.



Gaussian models

- Return to Gaussian models with equal covariances

$$\mathcal{N}(\underline{x} ; \underline{\mu}, \Sigma) = \frac{1}{(2\pi)^{d/2}} |\Sigma|^{-1/2} \exp \left\{ -\frac{1}{2} (\underline{x} - \underline{\mu})^T \Sigma^{-1} (\underline{x} - \underline{\mu}) \right\}$$

$$0 < \log \frac{p(x|y=0) p(y=0)}{p(x|y=1) p(y=1)} > = (\mu_0 - \mu_1)^T \Sigma^{-1} x + \text{constants}$$

(**)

Now we also know that the probability of each class is given by:

$$p(y=0 | x) = \text{Logistic}(**) = \text{Logistic}(a^T x + b)$$

We'll see this form again soon...

Upcoming

- Sign up on Piazza
 - All course announcements will be done through Piazza! You may miss information announcements if you are not on Piazza.
- Homework 1 is up.
 - Meanwhile, get familiar with Python, Numpy, Matplotlib