CSE 375 Machine Learning and Pattern Recognition

07. Bayesian Classifiers & Naïve Bayes

Slides Credit: Erik Sudderth, Alex Ihler & Sameer Singh

Contents

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 = 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

A basic classifier

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- Example: credit rating prediction (bad/good)
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  - Predict more likely outcome for each possible observation

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

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

- Training data $D=\{x^{(i)},y^{(i)}\}$, Classifier $f(x\,;D)$
  - Discrete feature vector x
  - $f(x\,;D)$ is a contingency table
- Example: credit rating prediction (bad/good)
  - X_1 = 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: $p(y=good|X=c)$
  - How to generalize?

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

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

(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
  - Split by class
  - $D_c = \{ x^{(j)} : y^{(j)} = c \}$
- Estimate $p(x \mid y=c)$ 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(y)	383/690	307/690

$\Rightarrow$

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

$\Rightarrow$

p(y=0|x)	p(y=1|x)
.7368	.2632
.5408	.4592
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Bayes classifiers

- Learn "class conditional" models
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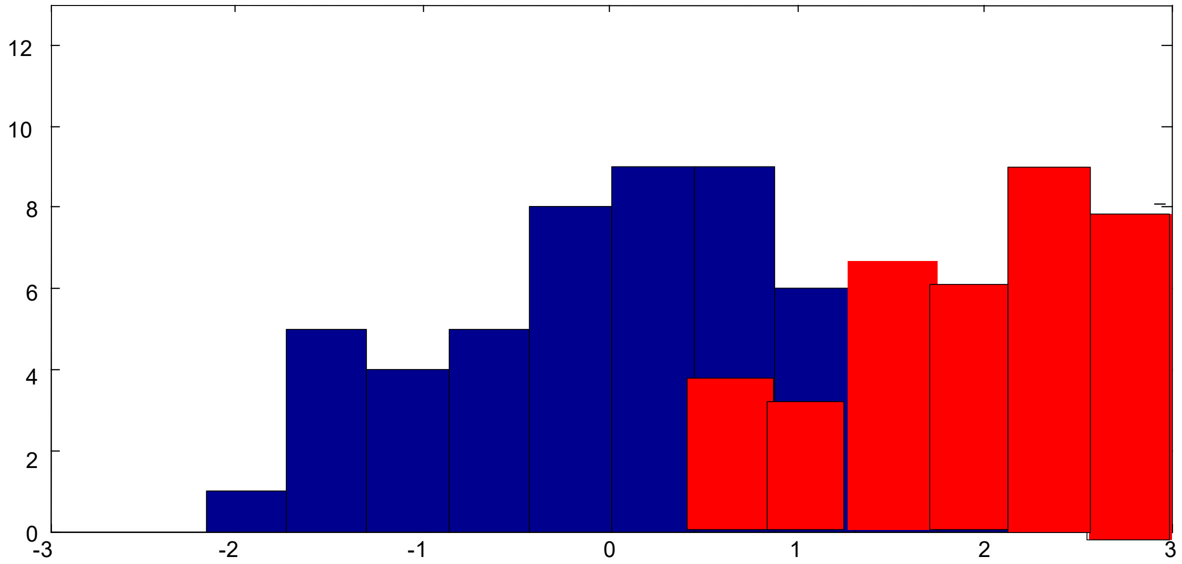
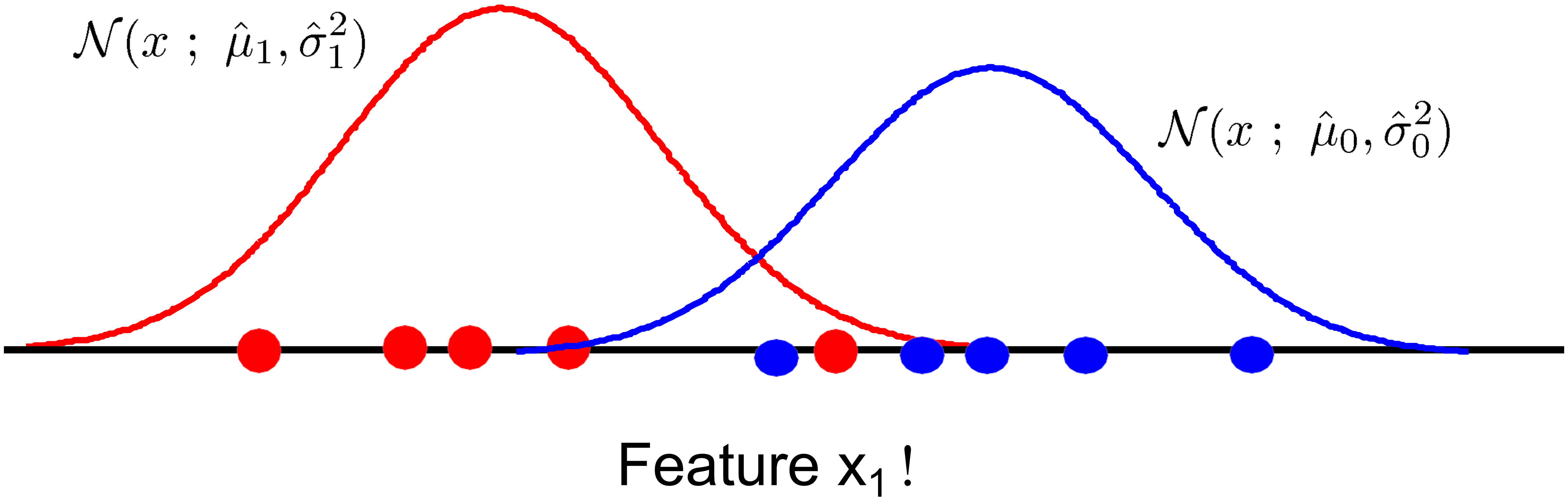


- For continuous x, can use any density estimate we like
  - Histogram
  - Gaussian
  - …

Gaussian models

- Estimate parameters of the Gaussians from the data

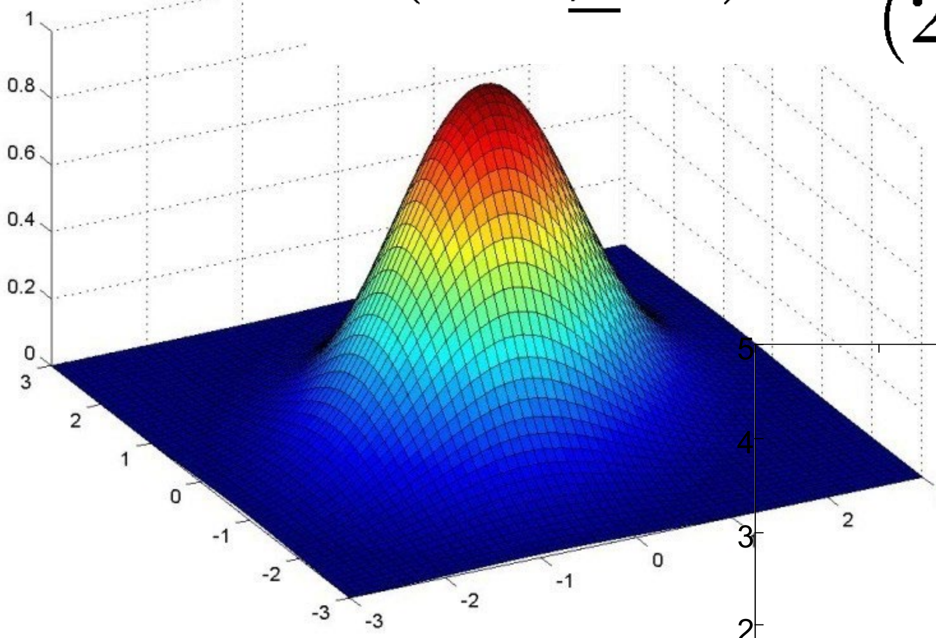
$$\alpha = \frac{m_1}{m} = \hat{p}(y = c_1) \qquad \hat{\mu} = \frac{1}{m} \sum_j x^{(j)} \qquad \hat{\sigma}^2 = \frac{1}{m} \sum_j (x^{(j)} - \mu)^2$$

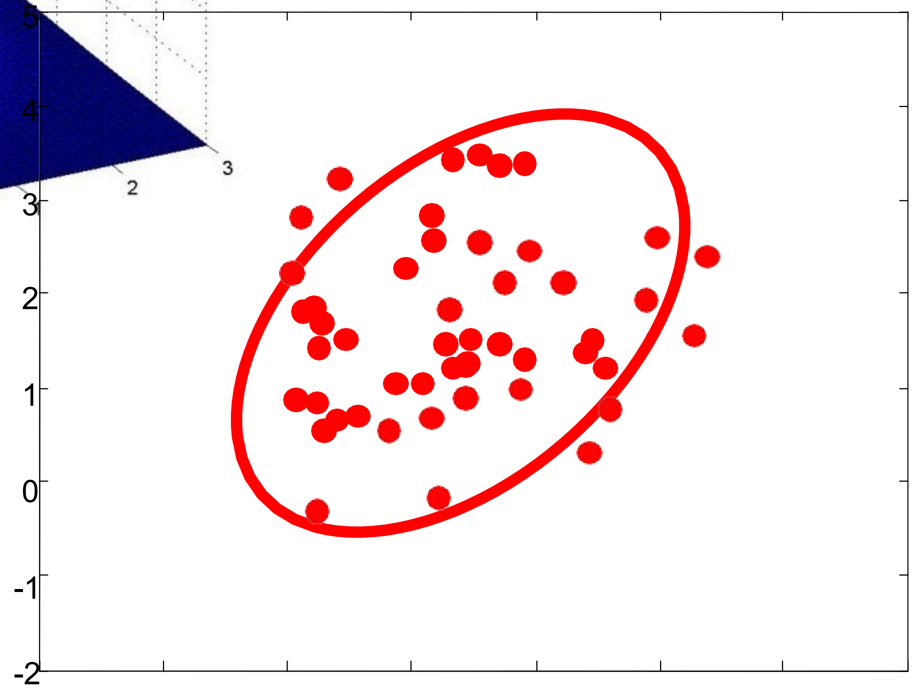


Multivariate Gaussian models

- Similar to univariate case

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





$\mu = n \times 1$ mean vector

$\Sigma = n \times n$ covariance matrix

Maximum likelihood estimate:

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

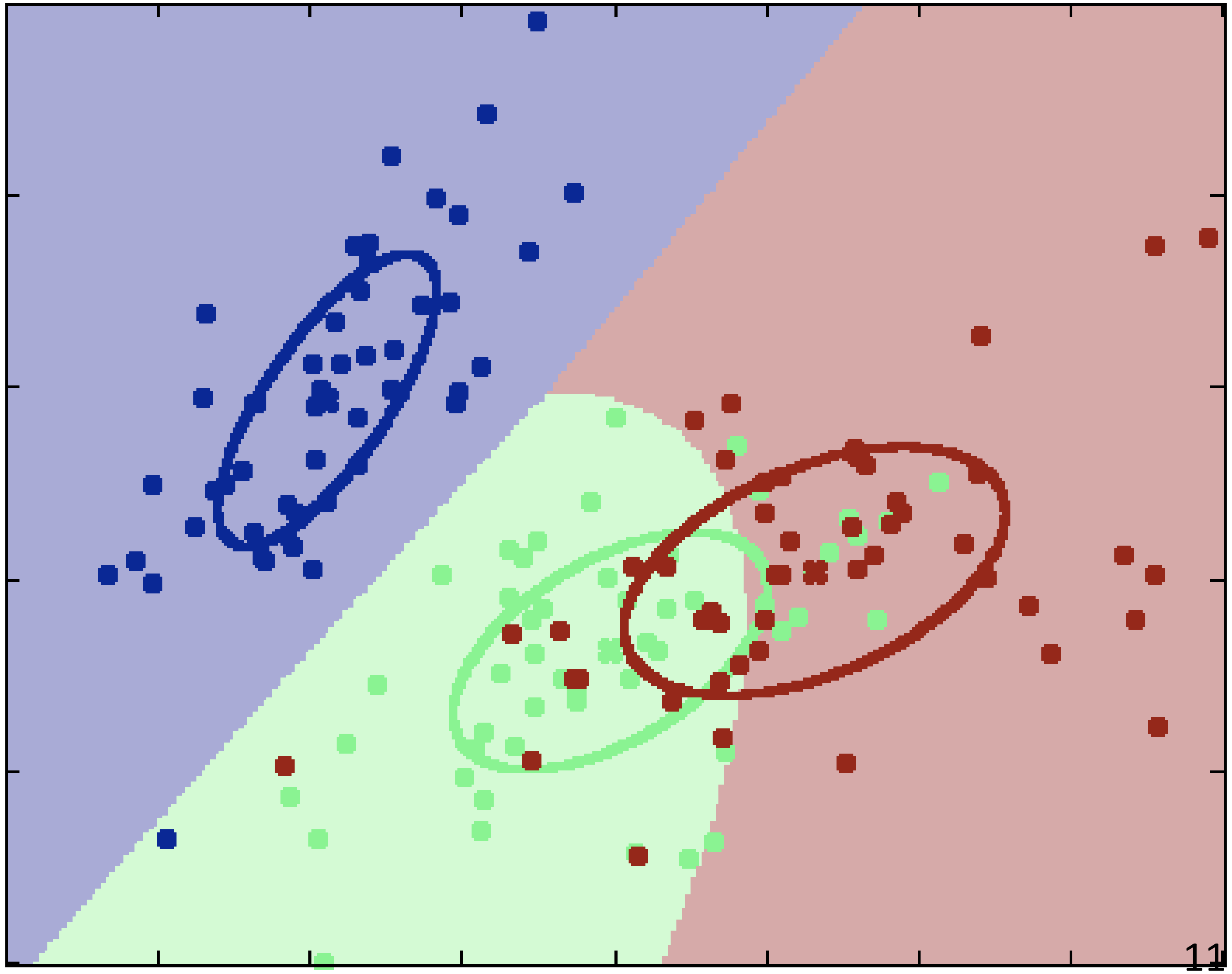
$$\hat{\Sigma} = \frac{1}{m} \sum_j (\underline{x}^{(j)} - \underline{\hat{\mu}})^T (\underline{x}^{(j)} - \underline{\hat{\mu}})$$

Example: Gaussian Bayes for Iris Data

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

$$p(y) = \text{Discrete}(\tfrac{1}{3}, \tfrac{1}{3}, \tfrac{1}{3})$$

$$p(x_1, x_2 | y = 0) = \mathcal{N}(x\,;\, \mu_0, \Sigma_0)$$
$$p(x_1, x_2 | y = 1) = \mathcal{N}(x\,;\, \mu_1, \Sigma_1)$$
$$p(x_1, x_2 | y = 2) = \mathcal{N}(x\,;\, \mu_2, \Sigma_2)$$



Contents

- Bayesian Classification
- Naïve Bayes
- Bayes Error Rates
- Gaussian Bayes Classifier

Bayes classifiers

- Estimate p(y) = [p(y=0) , p(y=1) …]
- 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?

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

p(y)	383/690	307/690

$\Rightarrow$

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$\Rightarrow$

p(y=0|x)	p(y=1|x)
.7368	.2632
.5408	.4592
.3750	.6250

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 & density estimation

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

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

Overfitting & density estimation

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

- Estimate probabilities from the data
  - E.g., how many times (what fraction) did each outcome occur?
- 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 $\hat{p}(a,b,c) \propto (M_{abc} + \alpha)$
- Normalize to make sure values sum to one…

Overfitting & density estimation

- Another option: reduce the model complexity by assuming the features are independent of one another
- Independence:
- $p(a,b) = p(a)\,p(b)$
- $p(x_1, x_2, \ldots x_N \mid y=1) =$
  $p(x_1 \mid y=1)\, p(x_2 \mid y=1) \ldots p(x_N \mid y=1)$
- 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

$\Rightarrow$

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

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

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

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

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

Prediction given some observation x?

$$\hat{p}(y=1)\hat{p}(x=11|y=1) \quad \begin{matrix} < \\ > \end{matrix} \quad \hat{p}(y=0)\hat{p}(x=11|y=0)$$

$$\frac{4}{8} \times \frac{2}{4} \times \frac{1}{4} \qquad\qquad \frac{4}{8} \times \frac{3}{4} \times \frac{2}{4}$$

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

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

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

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

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

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

$$= \frac{1}{4}$$

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

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

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

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

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

$$= 0$$

Naïve Bayes Models

- Variable y to predict, e.g. "auto accident in next year?"
- We have *many* co-observed vars $\mathbf{x}=[x_1 \ldots x_n]$
  - Age, income, education, zip code, …
- Want to learn $p(y \mid x_1 \ldots x_n)$, to predict y
  - Arbitrary distribution: $O(d^n)$ values!
- Naïve Bayes:
  - $p(y|\mathbf{x}) = p(\mathbf{x}|y)\, p(y) / p(\mathbf{x})$; $p(\mathbf{x}|y) = \Pi_t\, p(x_i|y)$
  - 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 ∈{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: $\approx 2^{270}$…

- Model words ***given*** email type as independent
- Some words more likely for spam (“lottery”)
- Some more likely for non-spam (“probabilistic”)
- Only 1000’s of parameters now…

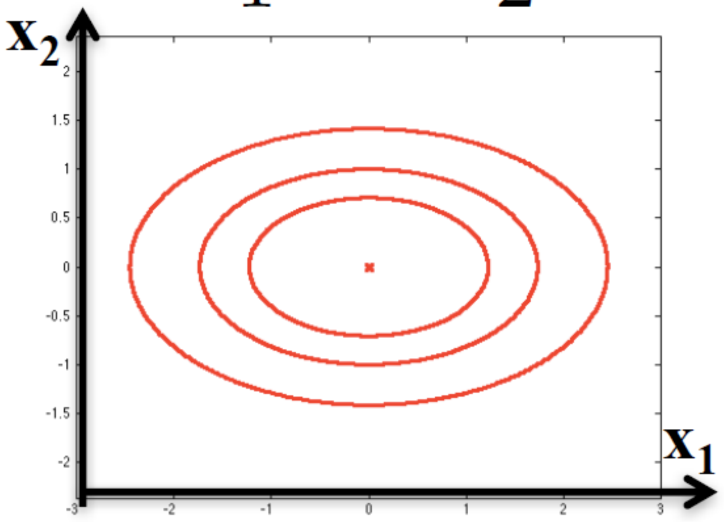
Naïve Bayes Gaussian Models

$$p(x_1) = \frac{1}{Z} \exp\left\{ -\frac{1}{2\sigma_1^2}(x_1 - \mu_1)^2 \right\} \qquad p(x_2) = \frac{1}{Z_2} \exp\left\{ -\frac{1}{2\sigma_2^2}(x_2 - \mu_2)^2 \right\}$$

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

$$\sigma_1^2 > \sigma_2^2$$

$$\underline{\mu} = [\mu_1 \;\; \mu_2]$$
$$\Sigma = \mathrm{diag}(\sigma_1^2 \;,\; \sigma_2^2)$$



Again, reduces the number of parameters of the model:

Bayes: $n^2/2$ Naïve Bayes: n

You should know…

- Bayes rule; $p(y \mid x)$
- Bayes classifiers
  - Learn $p(x \mid y=C)$, $p(y=C)$
- Naïve Bayes classifiers
  - Assume features are independent given class:
  - $p(x \mid y=C) = p(x_1 \mid y=C)\, p(x_2 \mid y=C) \ldots$

- Maximum likelihood (empirical) estimators for
  - Discrete variables
  - Gaussian variables
  - Overfitting; simplifying assumptions or regularization

Contents

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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Gets these examples wrong:

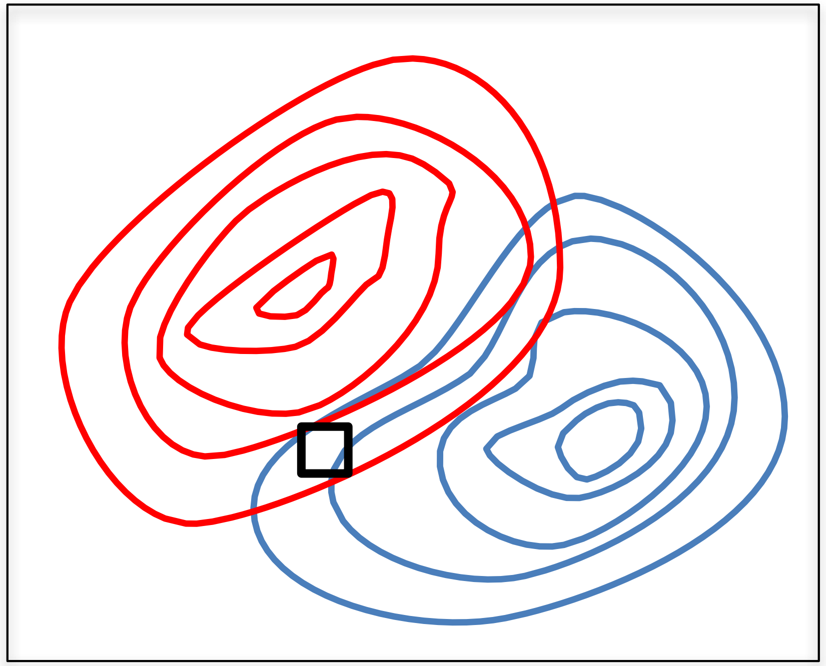
Pr[error] = (15 + 287 + 3) / (690)

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

Bayes Error Rate

- Suppose that we knew the true probabilities:

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



  – 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:

$$\mathbb{E}_{xy}[y \neq \hat{y}] = \mathbb{E}_x[1 - \max_c p(y=c|x)]$$ = "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

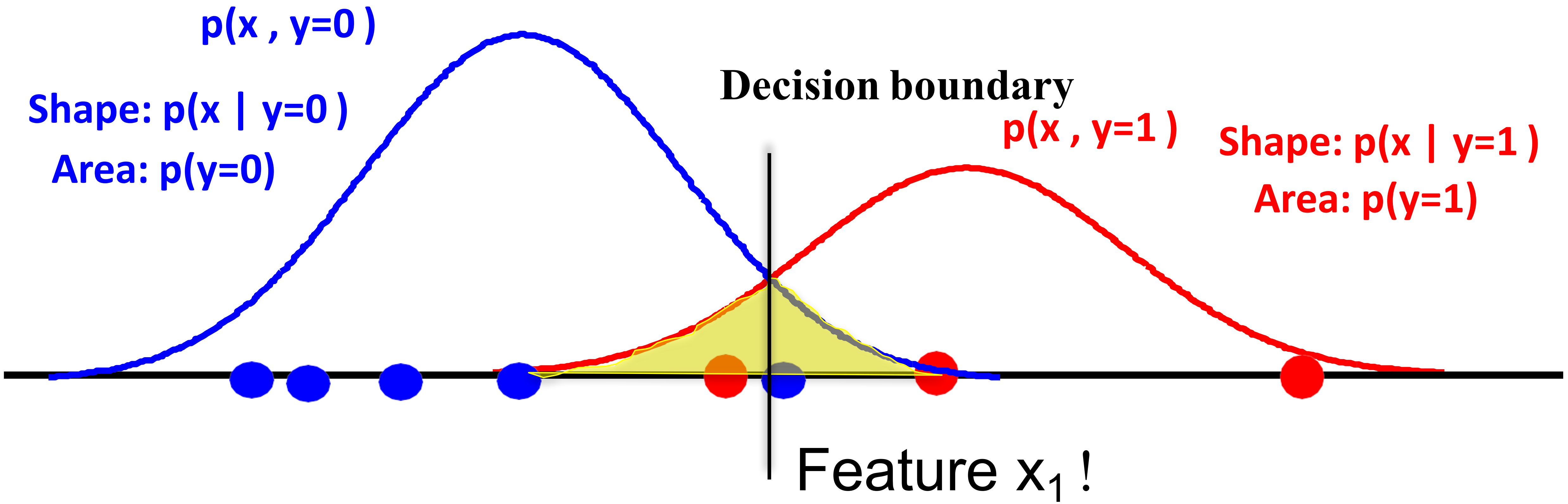
A Bayes classifier

- Bayes classification decision rule compares probabilities:

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

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

- Can visualize this nicely if x is a scalar:

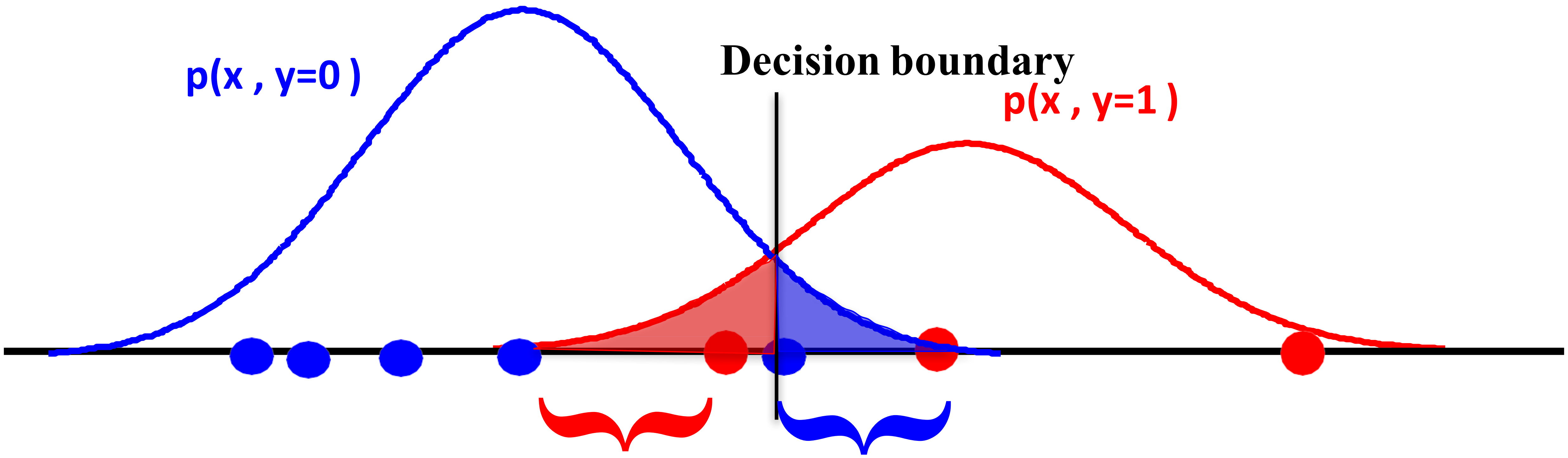


A Bayes classifier

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

Add multiplier alpha:

$$\alpha \; p(y=0,x) \;\lessgtr\; p(y=1,x)$$



Type 1 errors: false positives Type

2 errors: false negatives

False positive rate: (# y=0, ŷ=1) / (#y=0)

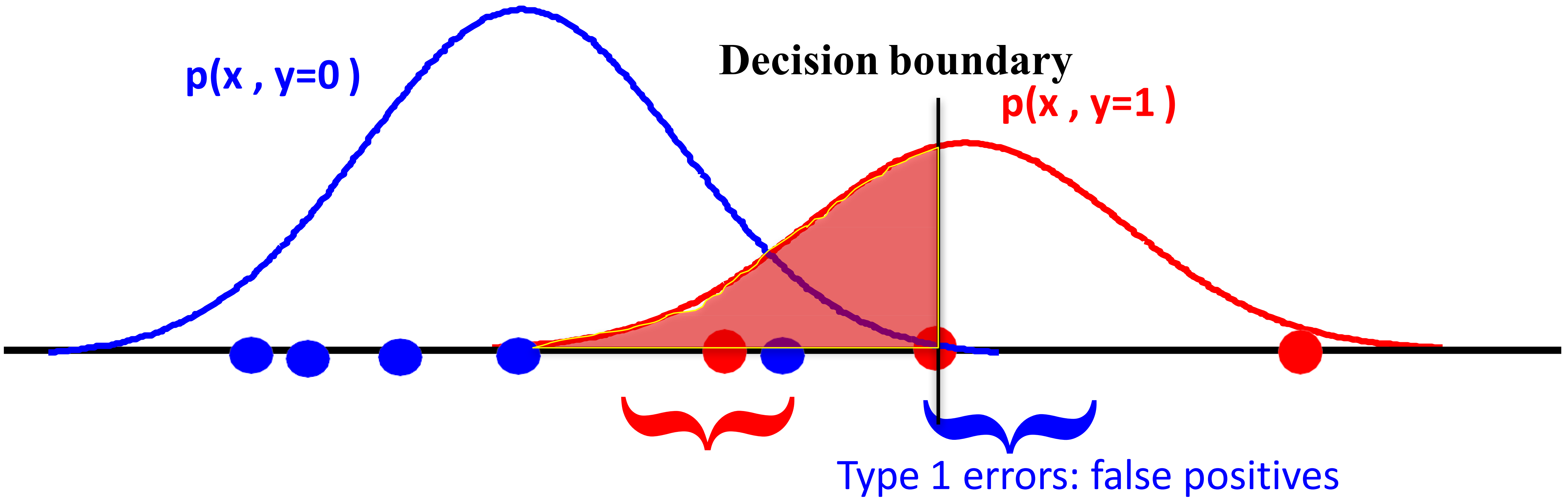
False negative rate: (# y=1, ŷ=0) / (#y=1)

A Bayes classifier

- Increase alpha: prefer class 0
- Spam detection

Add multiplier alpha:

$$\alpha \; p(y=0,x) \;\underset{>}{<}\; p(y=1,x)$$



False positive rate: (# y=0, ŷ=1) / (#y=0)

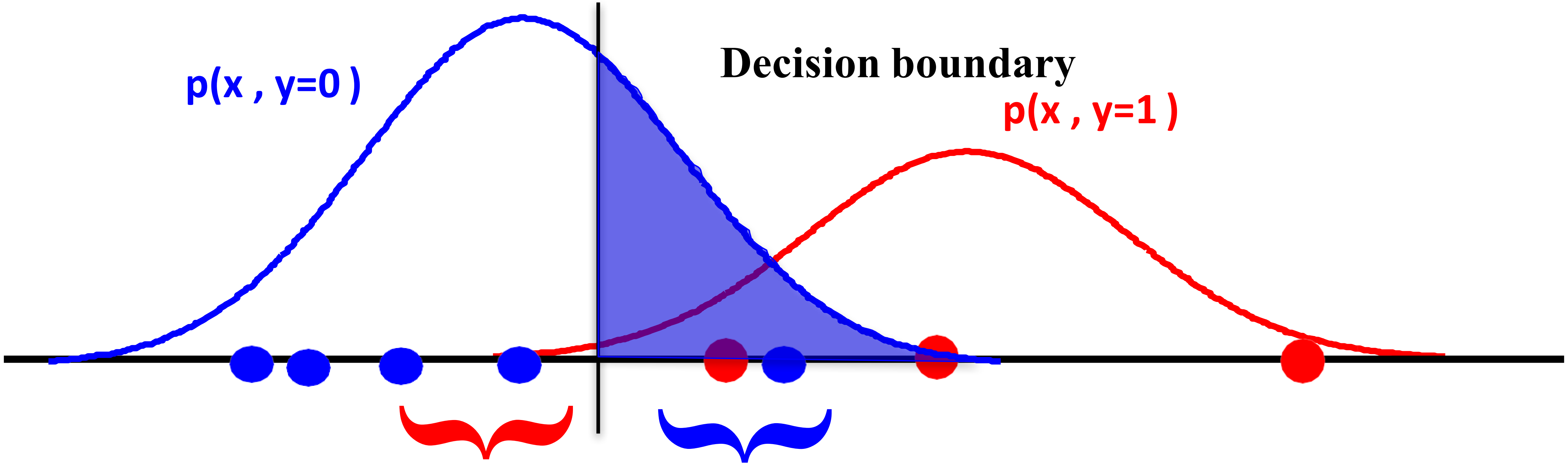
False negative rate: (# y=1, ŷ=0) / (#y=1)

A Bayes classifier

Add multiplier alpha:

$$\alpha \; p(y=0,x) \;\underset{>}{<}\; p(y=1,x)$$

- Decrease alpha: prefer class 1
- Cancer detection



Type 1 errors: false positives

Type 2 errors: false negatives

False positive rate: (# y=0, ŷ=1) / (#y=0)

False negative rate: (# y=1, ŷ=0) / (#y=1)

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:

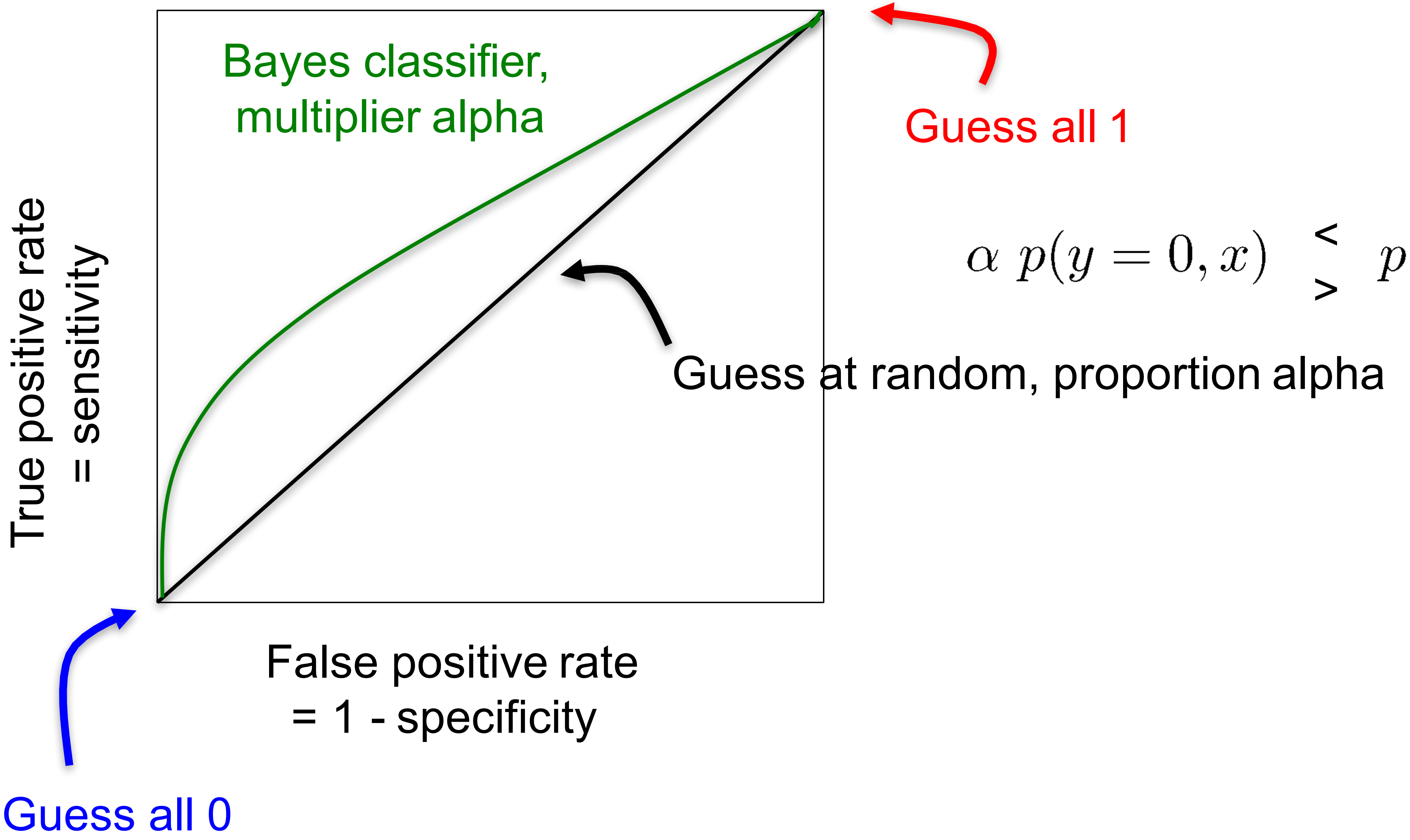
$$p(y=0,x) \;\; \begin{matrix} < \\ > \end{matrix} \;\; p(y=1,x) \quad = \quad \log \frac{p(y=0)}{p(y=1)} \;\; \begin{matrix} < \\ > \end{matrix} \;\; \log \frac{p(x|y=1)}{p(x|y=0)}$$

"log likelihood ratio"

- Likelihood ratio: relative support for observation "x" under "alternative hypothesis" y=1, compared to "null hypothesis" y=0
- Can vary the decision threshold: $\gamma \;\; \begin{matrix} < \\ > \end{matrix} \;\; \log \frac{p(x|y=1)}{p(x|y=0)}$
- 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?

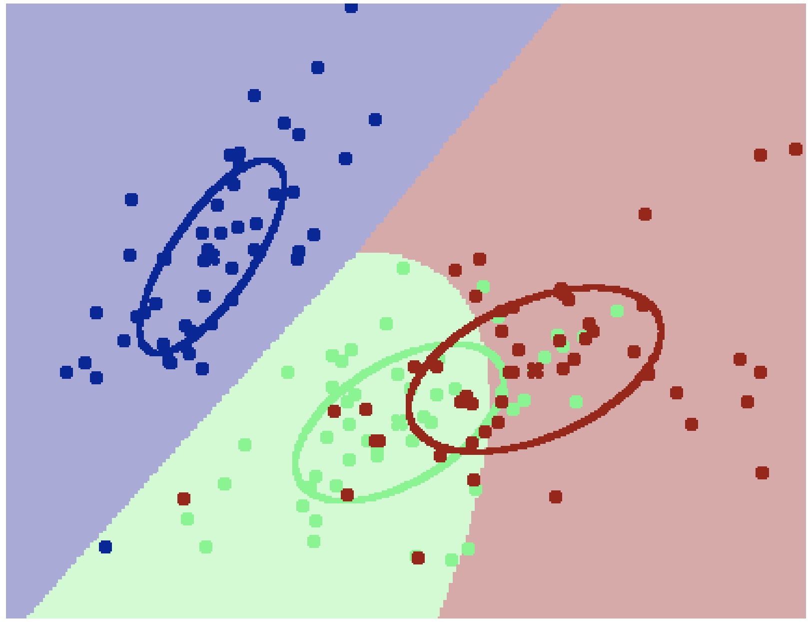
ROC Curves

- Characterize performance as we vary the decision threshold?

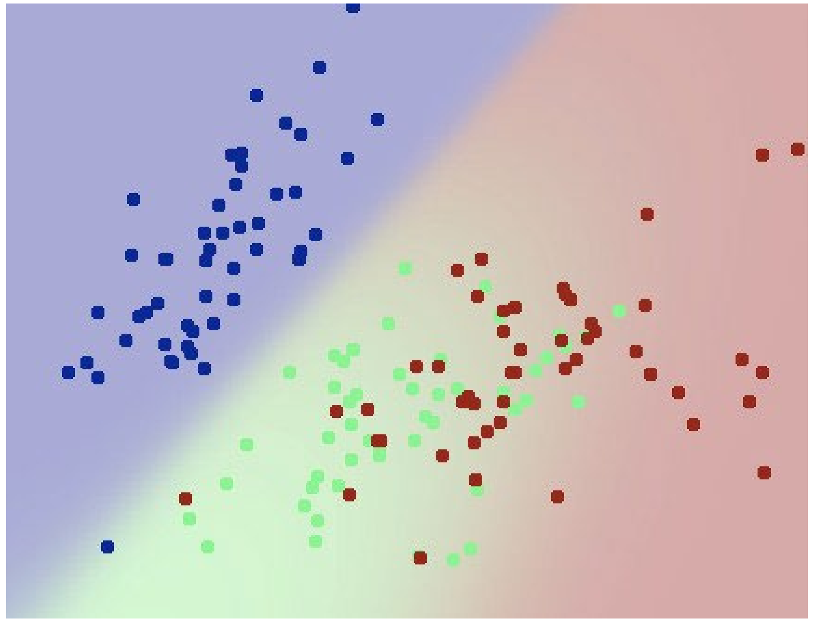


$$\alpha\ p(y=0,x) \ \underset{>}{<}\ p(y=1,x)$$

Probabilistic vs. Discriminative learning



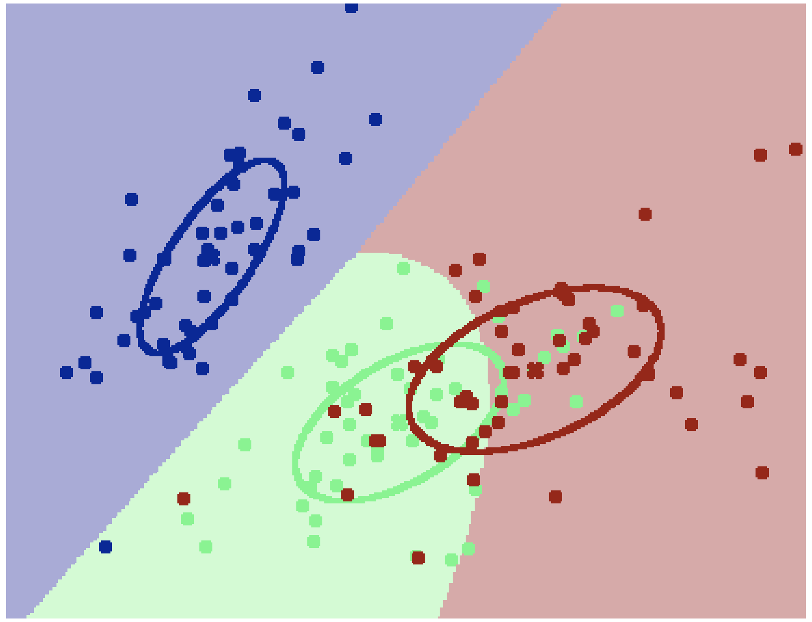
"Discriminative" learning:
Output prediction ŷ(x)

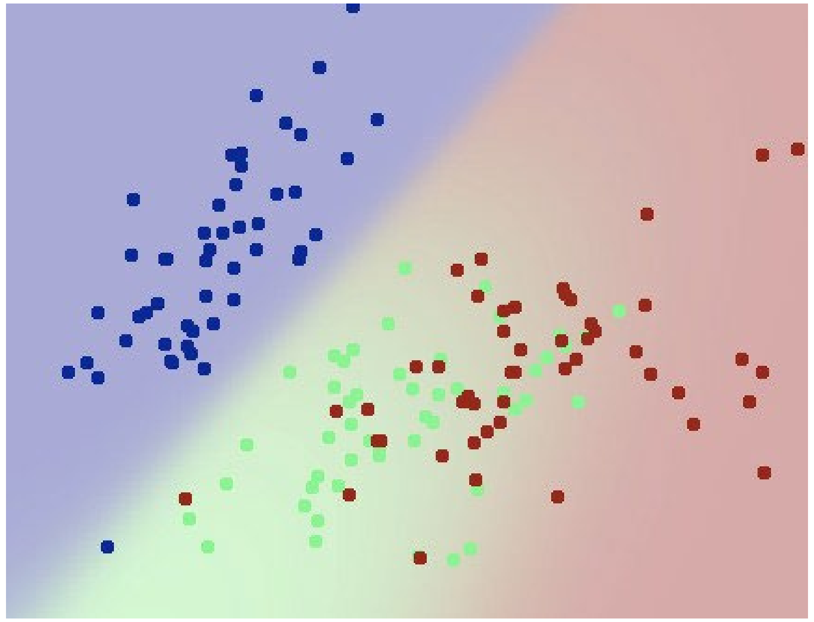


"Probabilistic" learning:
Output probability p(y|x)
(expresses confidence in outcomes)

- "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 $\hat{y}(x)$

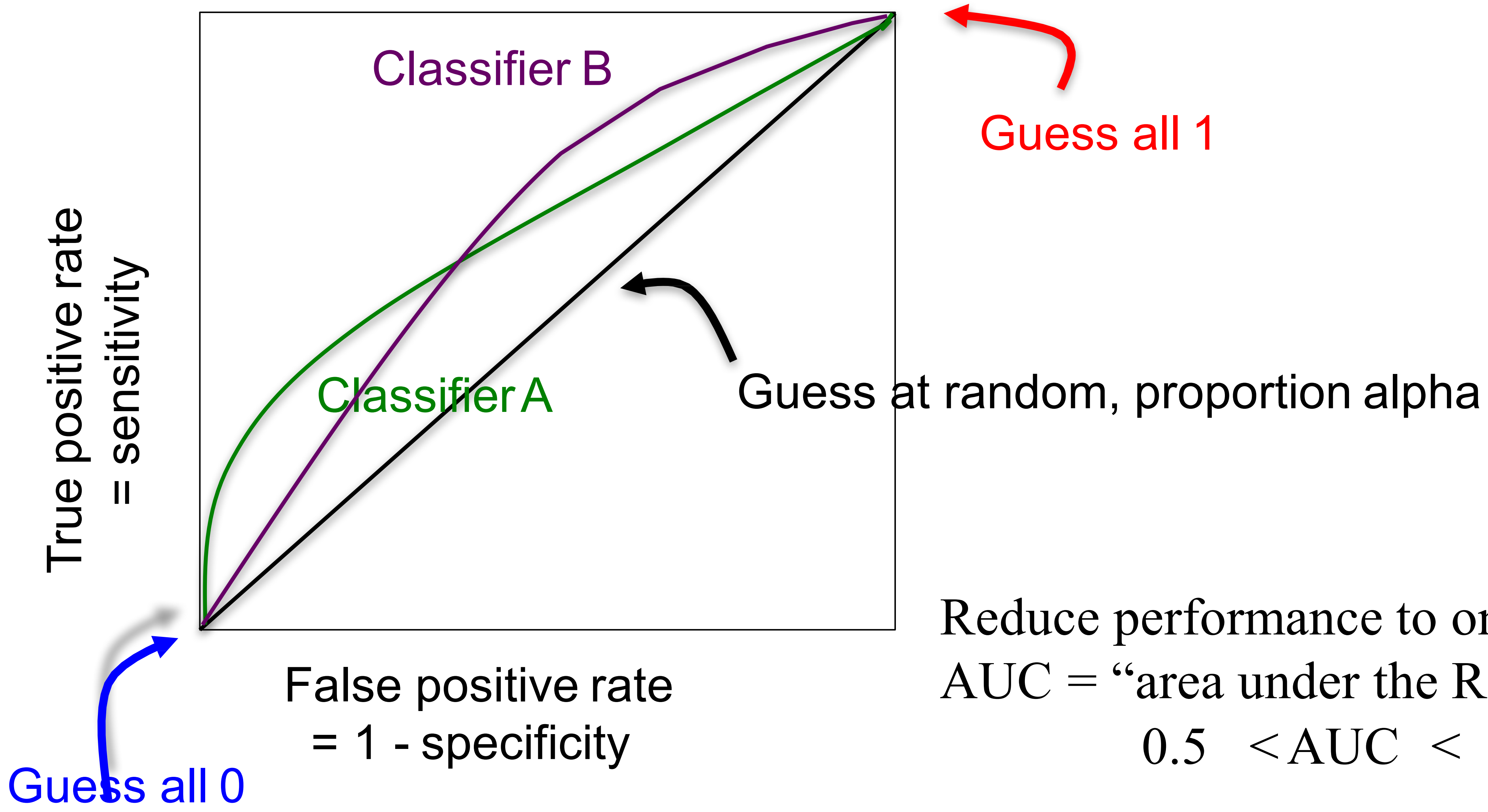
"Probabilistic" learning:
Output probability $p(y|x)$
(expresses confidence in outcomes)

- 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"
$0.5 < AUC < 1$

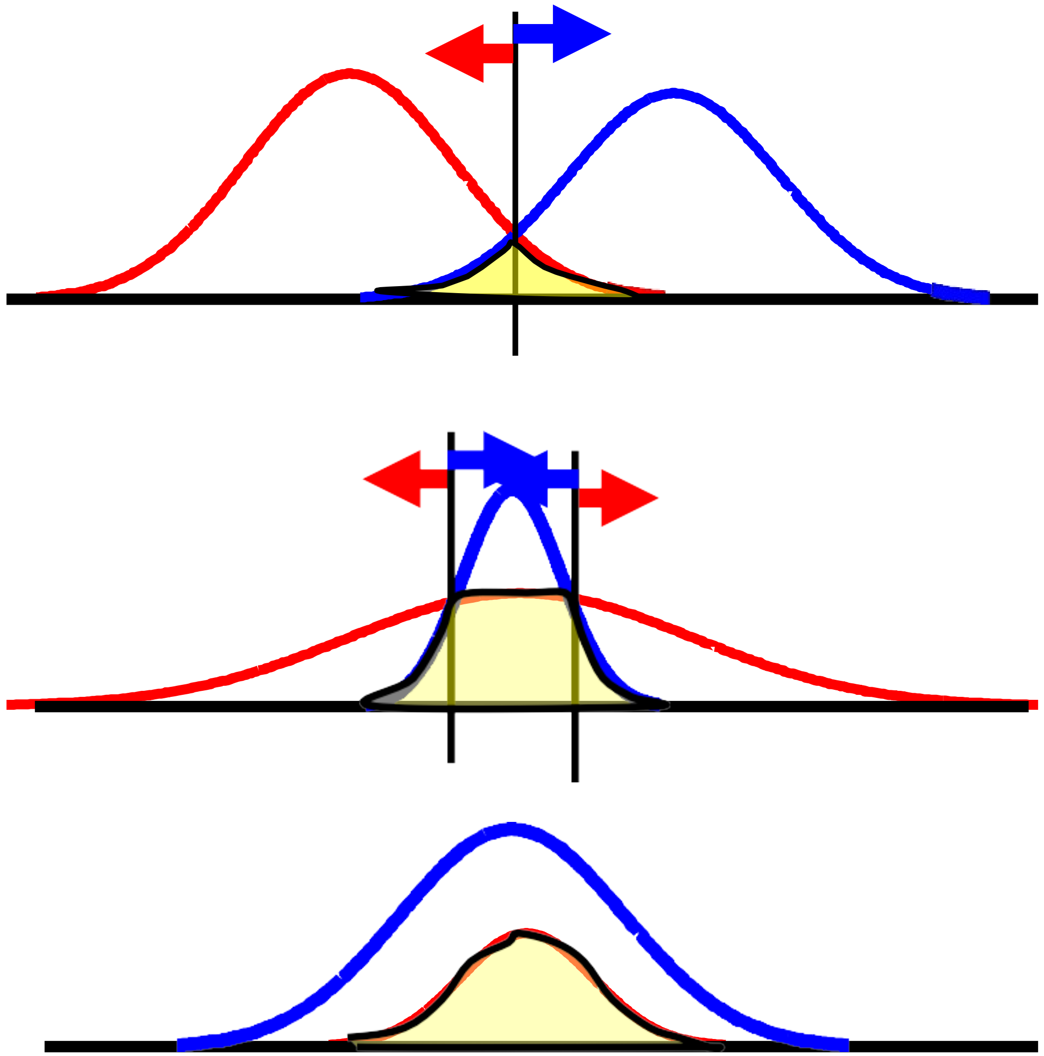
Contents

- Bayesian Classification
- Naïve Bayes
- Bayes Error Rates
- Gaussian Bayes Classifier

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

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

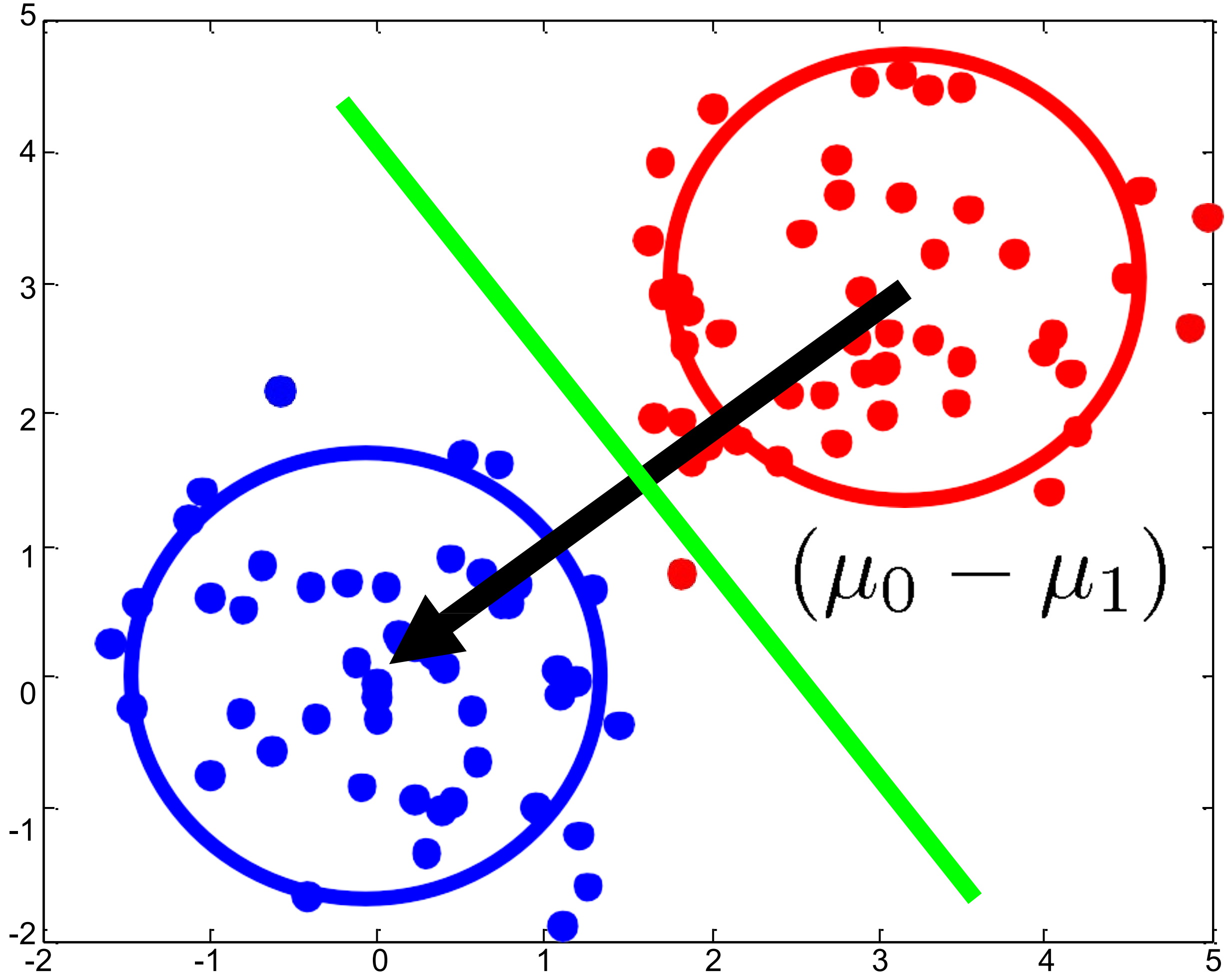
$$\begin{aligned} 0 \ \substack{<\\>}\ \log \frac{p(x|y=0)}{p(x|y=1)} \frac{p(y=0)}{p(y=1)} &= \log \frac{p(y=0)}{p(y=1)} + \\ &\quad -.5(x\Sigma^{-1}x - 2\mu_0^T\Sigma^{-1}x + \mu_0^T\Sigma^{-1}\mu_0) \\ &\quad +.5(x\Sigma^{-1}x - 2\mu_1^T\Sigma^{-1}x + \mu_1^T\Sigma^{-1}\mu_1) \\ &= (\mu_0 - \mu_1)^T\Sigma^{-1}x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

Gaussian example

- Spherical covariance: $\Sigma = \sigma^2 I$
- Decision rule

$$= (\mu_0 - \mu_1)^T \Sigma^{-1} x + constants$$

$$(\mu_0 - \mu_1)^T x \underset{>}{\overset{<}{}} C$$



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

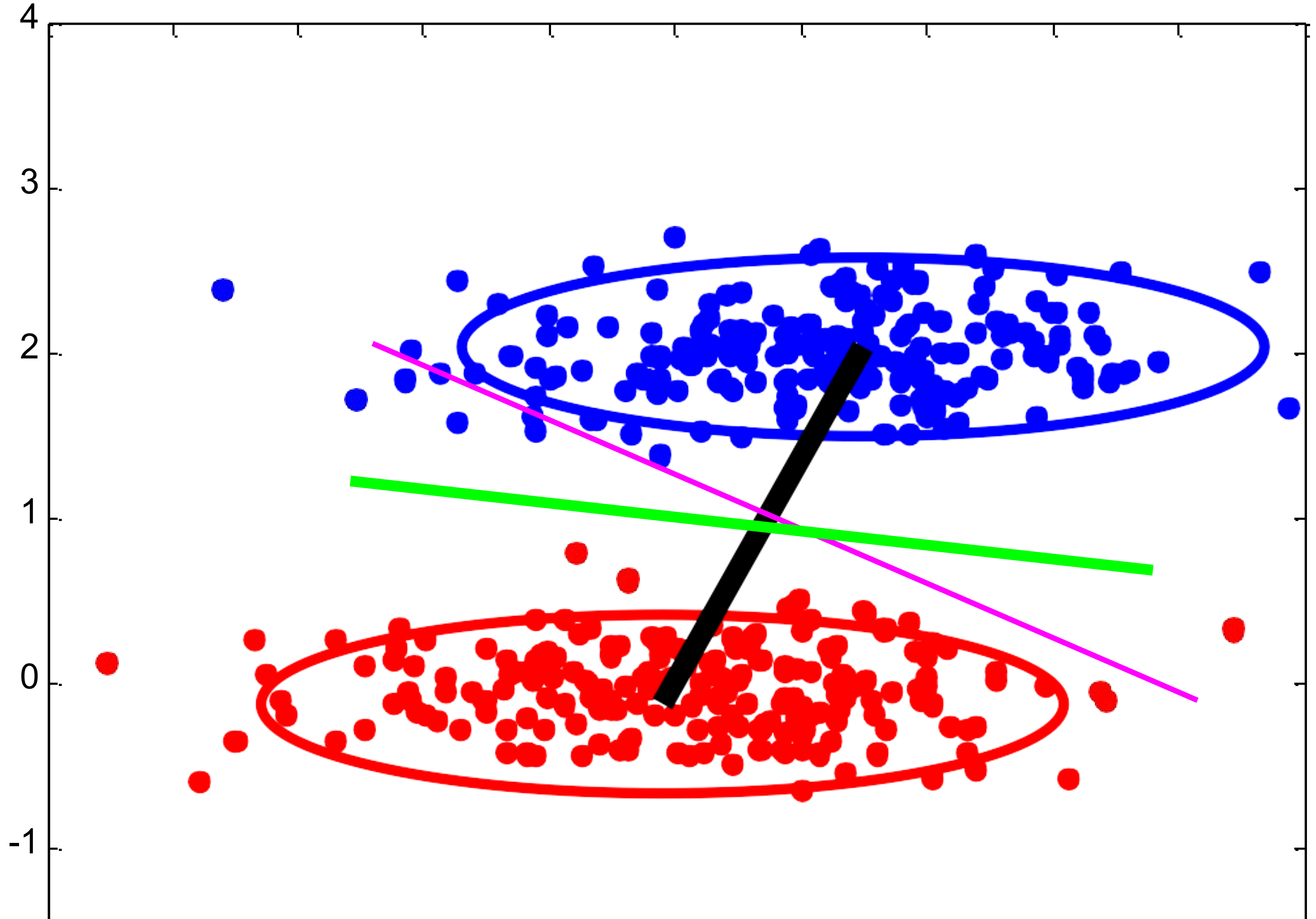
Non-spherical Gaussian distributions

- 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?

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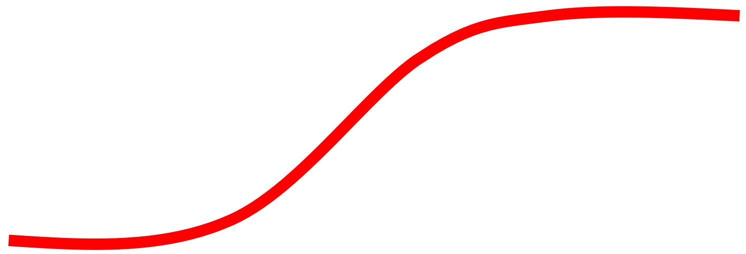
- We can compute posterior using Bayes’ rule
  - p(y=c | x) = p(x|y=c) p(y=c) / p(x)
- Compute p(x) using sum rule / law of total prob.
  - p(x) = p(x|y=0) p(y=0) + p(x|y=1)p(y=1)

Class posterior probabilities

- Consider comparing two classes
  - $p(x \mid y=0) * p(y=0)$ vs $p(x \mid y=1) * p(y=1)$
  - Write probability of each class as
  - $p(y=0 \mid x) = p(y=0, x) / p(x)$
  - $\quad = p(y=0, x) / (p(y=0,x) + p(y=1,x))$
  - $\quad = 1 / (1 + \exp(-a))$ (**)
  - $a = \log [p(x|y=0) p(y=0) / p(x|y=1) p(y=1)]$
  - (**) called the logistic function, or logistic sigmoid.



Gaussian models

- Return to Gaussian models with equal covariances

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

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

(**)

Now we also know that the probability of each class is given by:
p(y=0 | x) = Logistic(**) = Logistic($a^T x + b$)

We'll see this form again soon…

Readings

[DHS] Chap. 2

Next Lecture

Logistics Regression