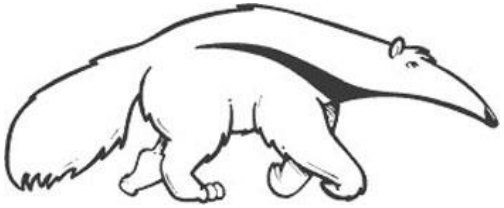
Machine Learning and Data Mining

2 : Bayes Classifiers

Kalev Kask



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

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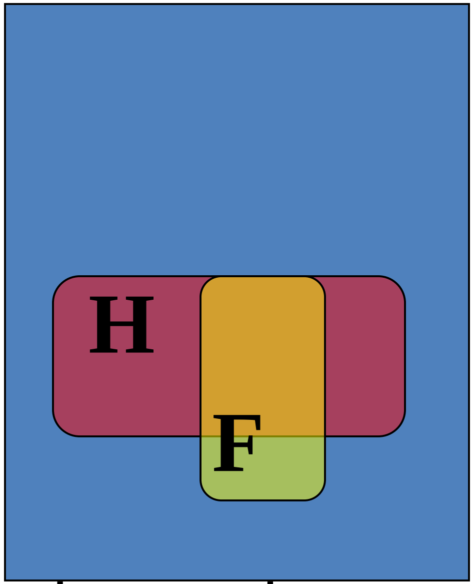
- Ex: credit rating prediction (bad/good)
  - X_1 = income (low/med/high)
  - How can we make the most # of correct predictions?
  - Predict more likely outcome
    for each possible observation
  - Can normalize into probability:
    $p(y=good \mid X=c)$
  - How to generalize?

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?

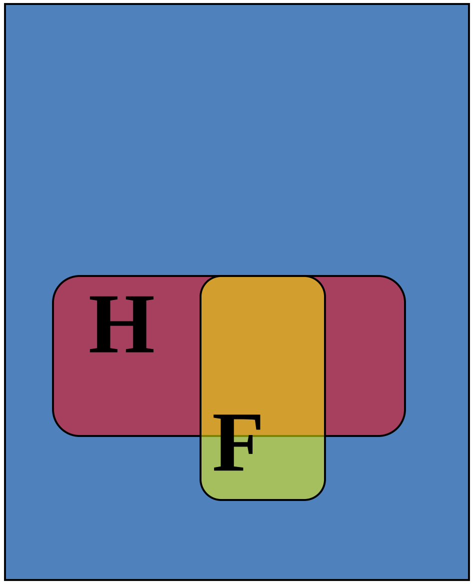
Example from Andrew Moore's slides

Bayes Rule

- Two events: headache, flu
- p(H) = 1/10
- p(F) = 1/40
- p(H|F) = 1/2

- P(H & F) = ?

- P(F|H) = ?



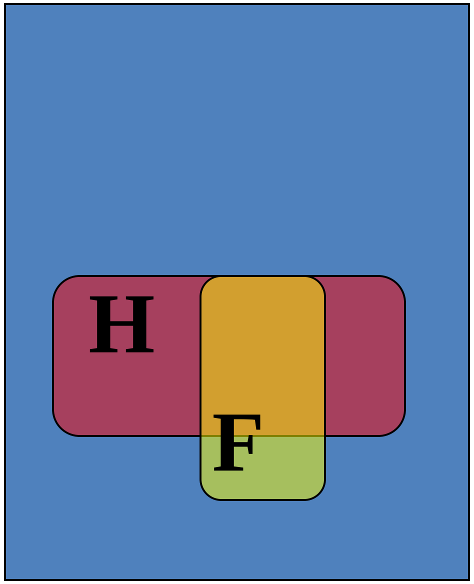
Example from Andrew Moore's slides

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) = ?

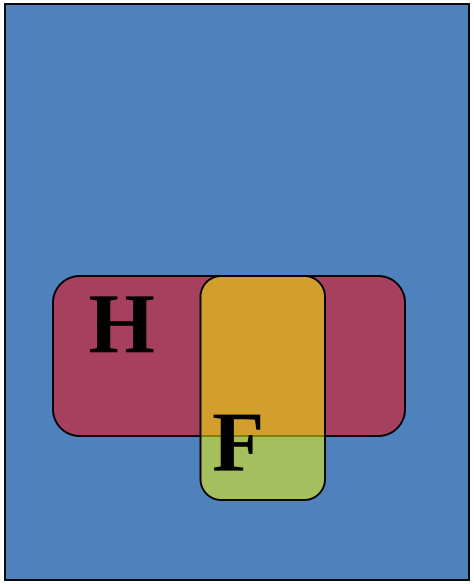


Example from Andrew Moore's slides

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



Example from Andrew Moore's slides

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:

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Posterior = ( Likelihood * Prior ) /  Evidence
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$$\Rightarrow \quad p(y|x) = p(x|y)p(y)/p(x)$$

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

(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
.3750	.6250

Bayes classifiers

- Learn "class conditional" models
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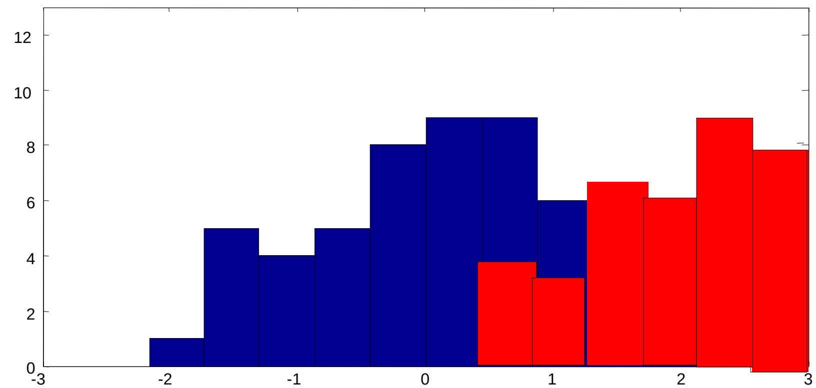
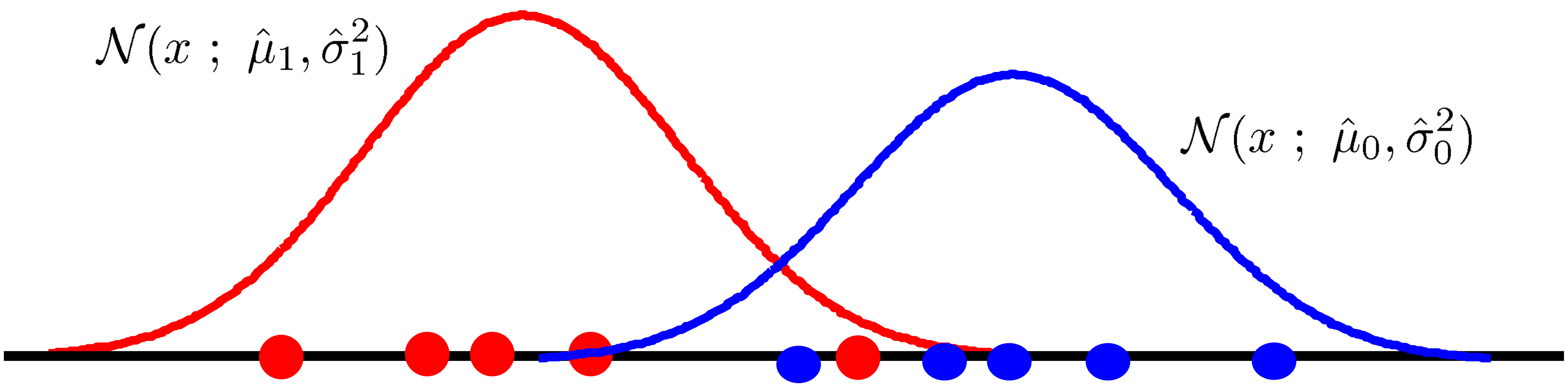
- For continuous x, can use any density estimate we like
  - Histogram
  - Gaussian
  - …



Gaussian models

- Estimate parameters of the Gaussians from the data

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



Feature x_1 !

Multivariate Gaussian models

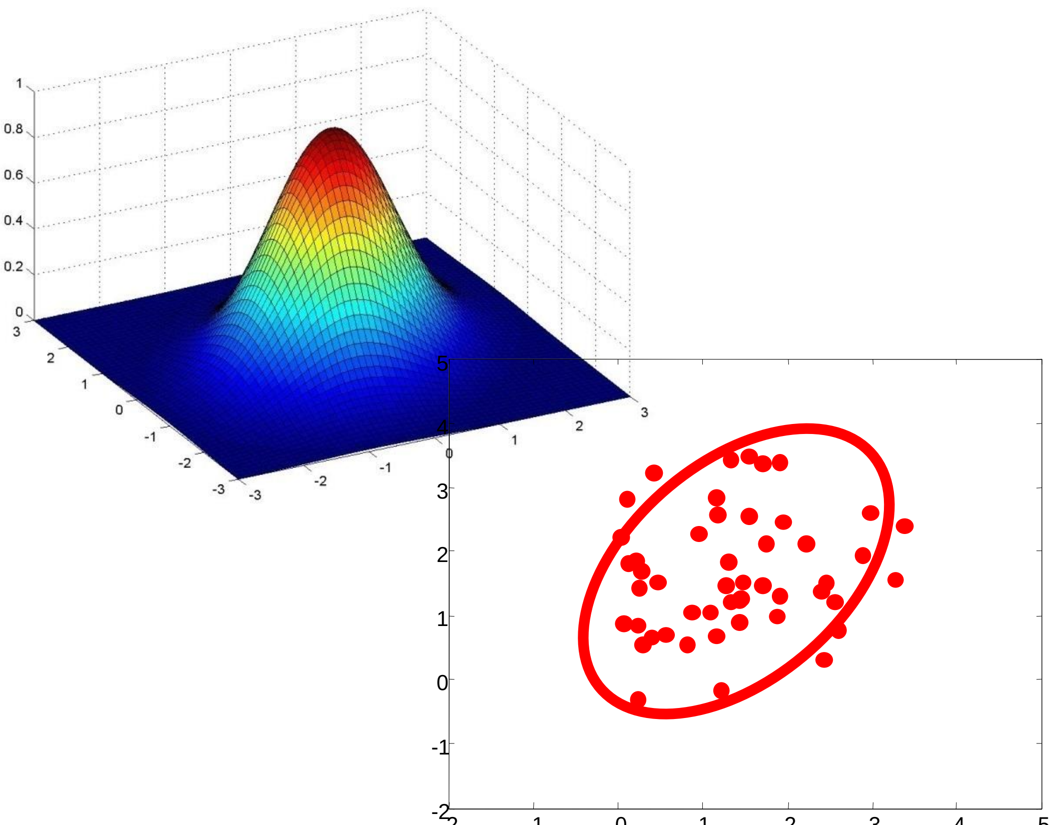
- Similar to univariate case

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

¹ = length-d column vector

§ = d x d matrix

| § | = matrix determinant



Maximum likelihood estimate:

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

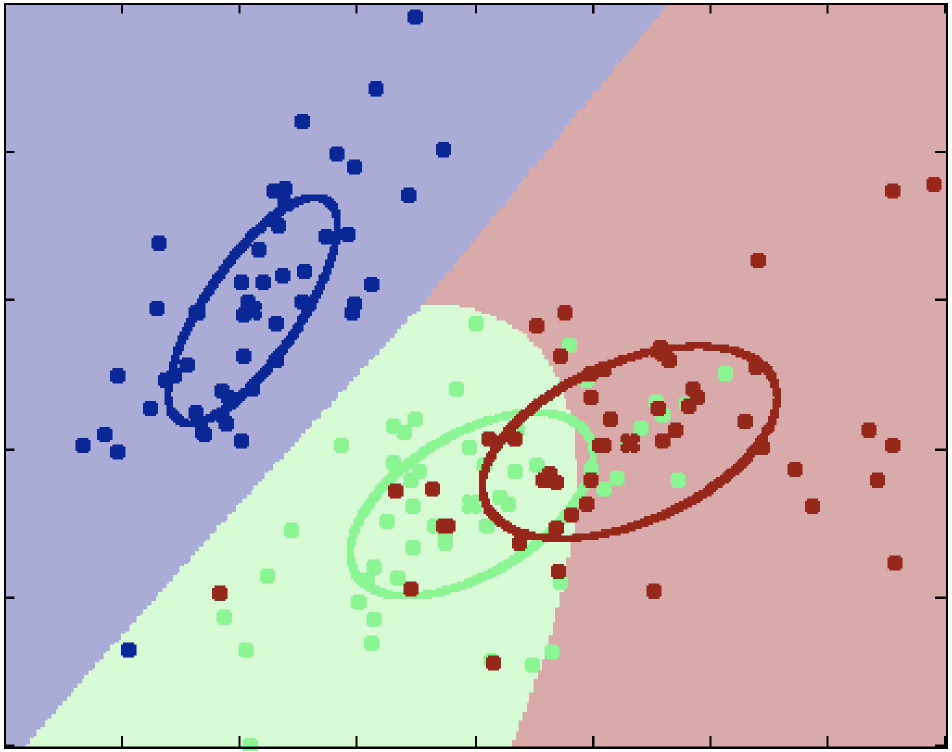
$$\hat{\Sigma} = \frac{1}{m} \sum_j (\underline{x}^{(j)} - \hat{\underline{\mu}})^T (\underline{x}^{(j)} - \hat{\underline{\mu}})$$

Example: Gaussian Bayes for Iris Data

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

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

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



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
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p(y)	383/690	307/690

$\Rightarrow$

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

$\Rightarrow$

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

- 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
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

- M data << 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 << 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
  - E.g., assume that 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

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

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

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

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

Prediction given some observation x?

$$\hat{p}(y=1)\hat{p}(x=11|y=1) \quad \lessgtr \quad \hat{p}(y=0)\hat{p}(x=11|y=0)$$

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

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
0	0	1
1	0	1

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

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

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

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

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

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

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

$$= 0$$

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:
  - $p(y|\mathbf{x}) = p(\mathbf{x}|y)\, p(y) / p(\mathbf{x})$; $p(\mathbf{x}|y) = \prod_i p(x_i|y)$
  - 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 2 {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…

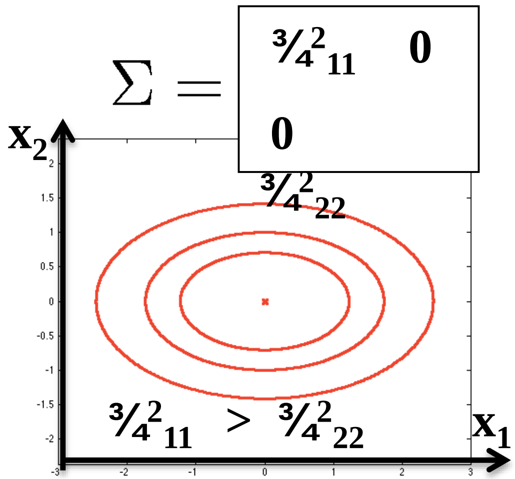
Naïve Bayes Gaussian Models

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

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

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

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



Again, reduces the number of parameters of the model:
Bayes: $n^2/2$ Naïve Bayes: n

You should know…

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

$$p(x \mid y=C) \quad = \quad p(x_1 \mid y=C) \, p(x_2 \mid y=C) \ldots$$

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
X=1	338	287
X=2	3	5

A Bayes classifier

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

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Gets these examples wrong:

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

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

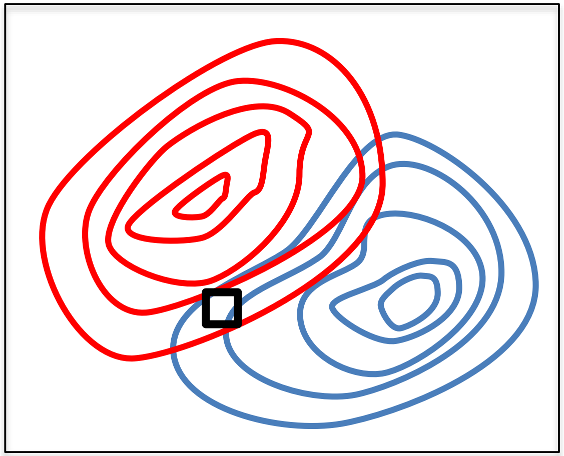
Bayes Error Rate

- 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: $\quad \Rightarrow \quad p(y=0|x)$ (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

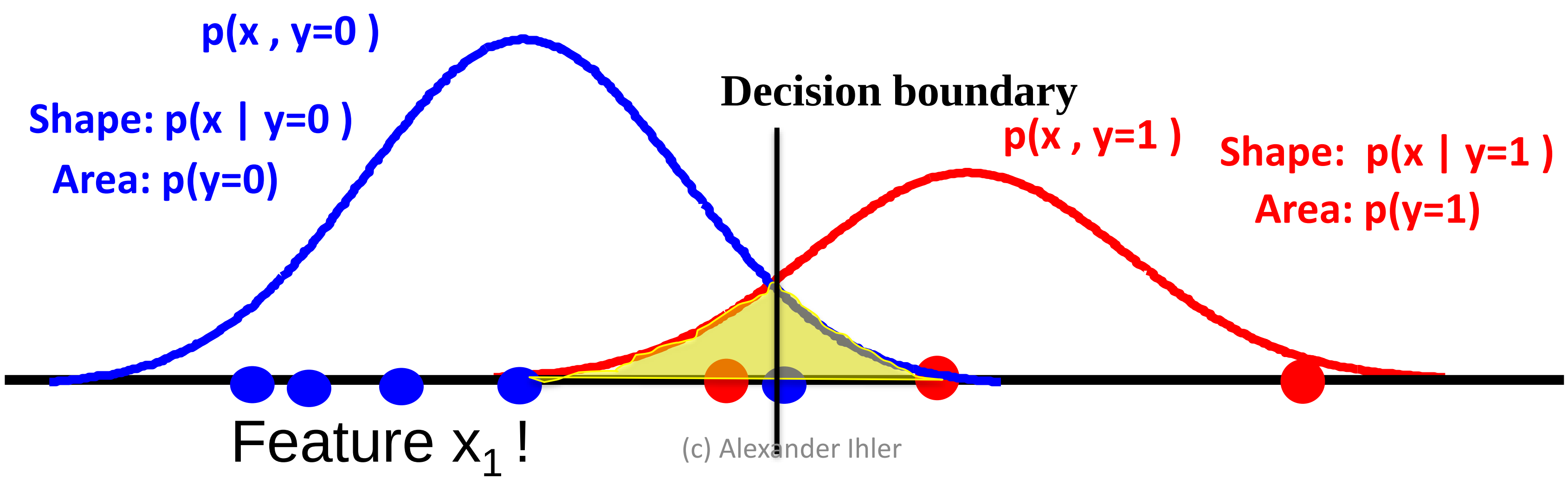
A Bayes classifier

- Bayes classification decision rule compares probabilities:

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

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

- Can visualize this nicely if x is a scalar:

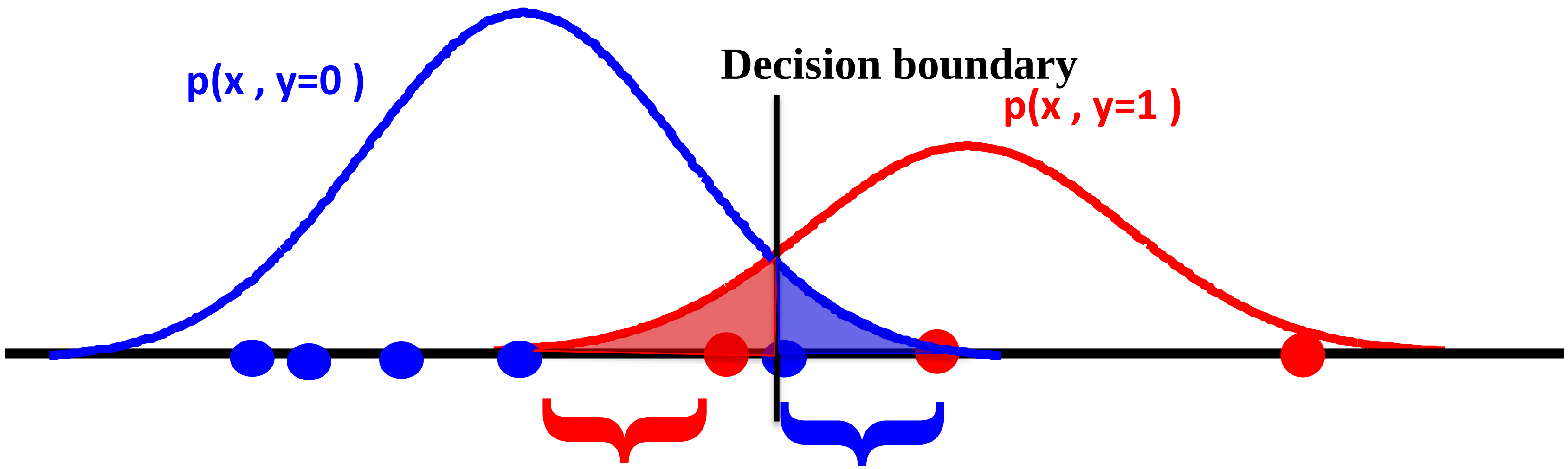


A Bayes classifier

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

Add multiplier alpha:

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



Type 1 errors: false positives

Type 2 errors: false negatives

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

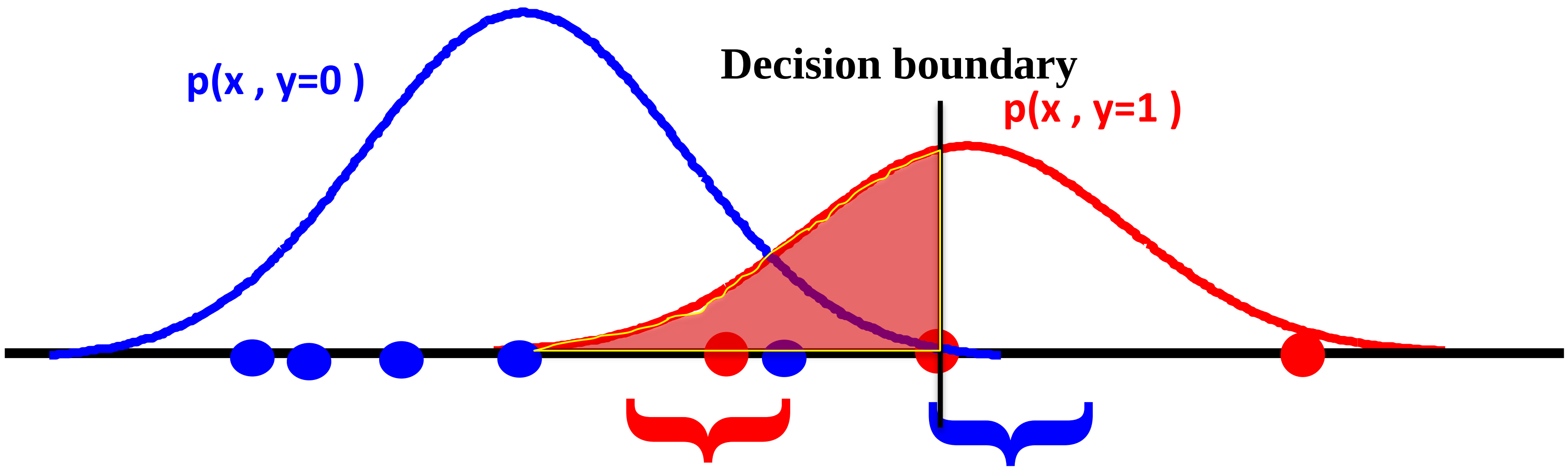
False negative rate: (# y=1, ŷ=0) / (#y=1)

A Bayes classifier

- Increase alpha: prefer class 0
- Spam detection

Add multiplier alpha:

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



Type 1 errors: false positives

Type 2 errors: false negatives

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

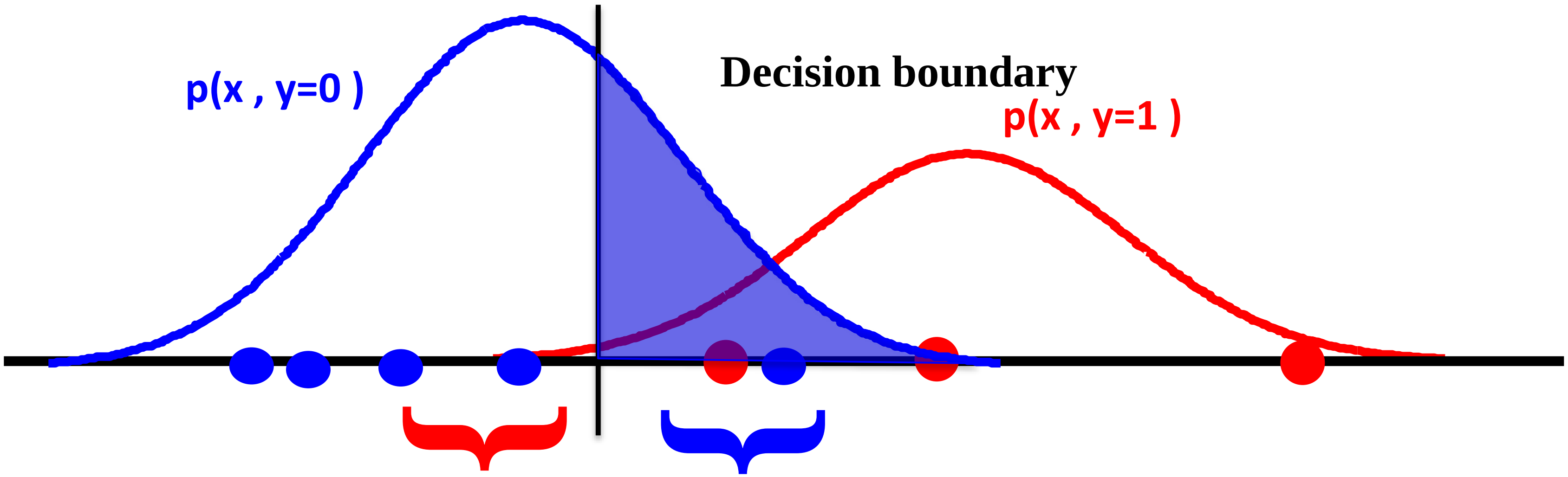
False negative rate: (# y=1, ŷ=0) / (#y=1)

A Bayes classifier

- Decrease alpha: prefer class 1
- Cancer detection

Add multiplier alpha:

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



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)

Measuring errors

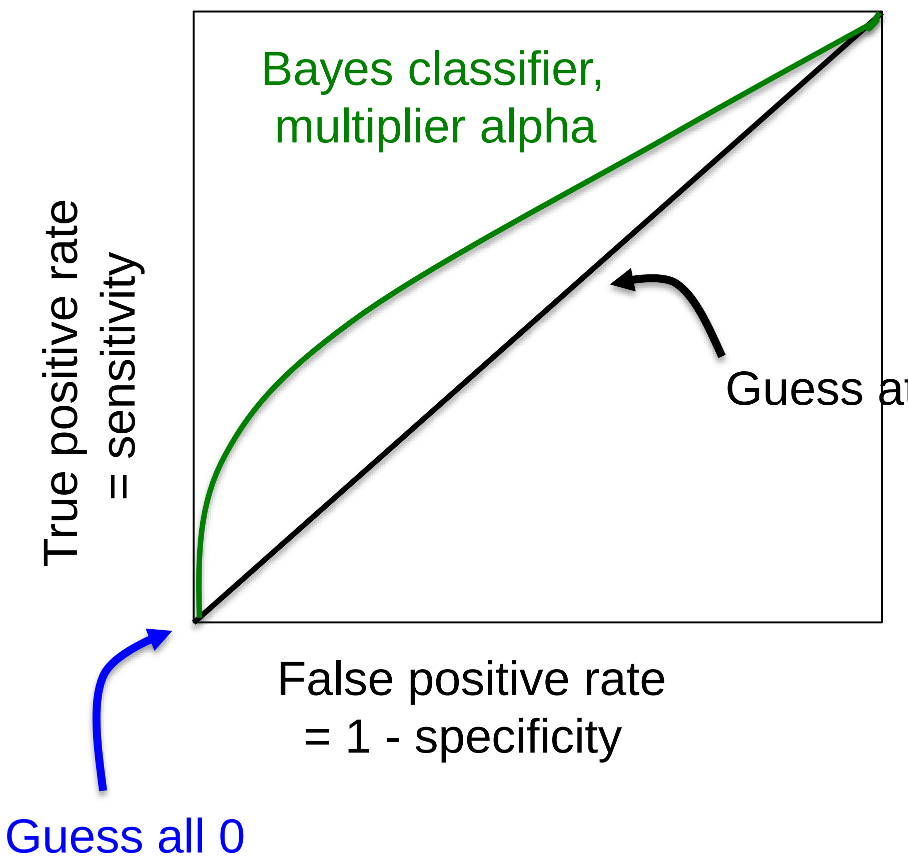
- Confusion matrix
- Can extend to more classes

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

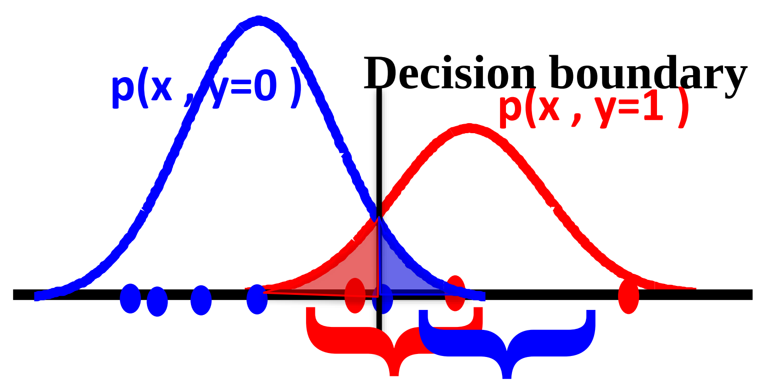
- True positive rate: #(y=1 , ŷ=1) / #(y=1) -- “sensitivity”
- False negative rate: #(y=1 , ŷ=0) / #(y=1)
- False positive rate: #(y=0 , ŷ=1) / #(y=0)
- True negative rate: #(y=0 , ŷ=0) / #(y=0) -- “specificity”

ROC Curves

- Characterize performance as we vary the decision threshold?

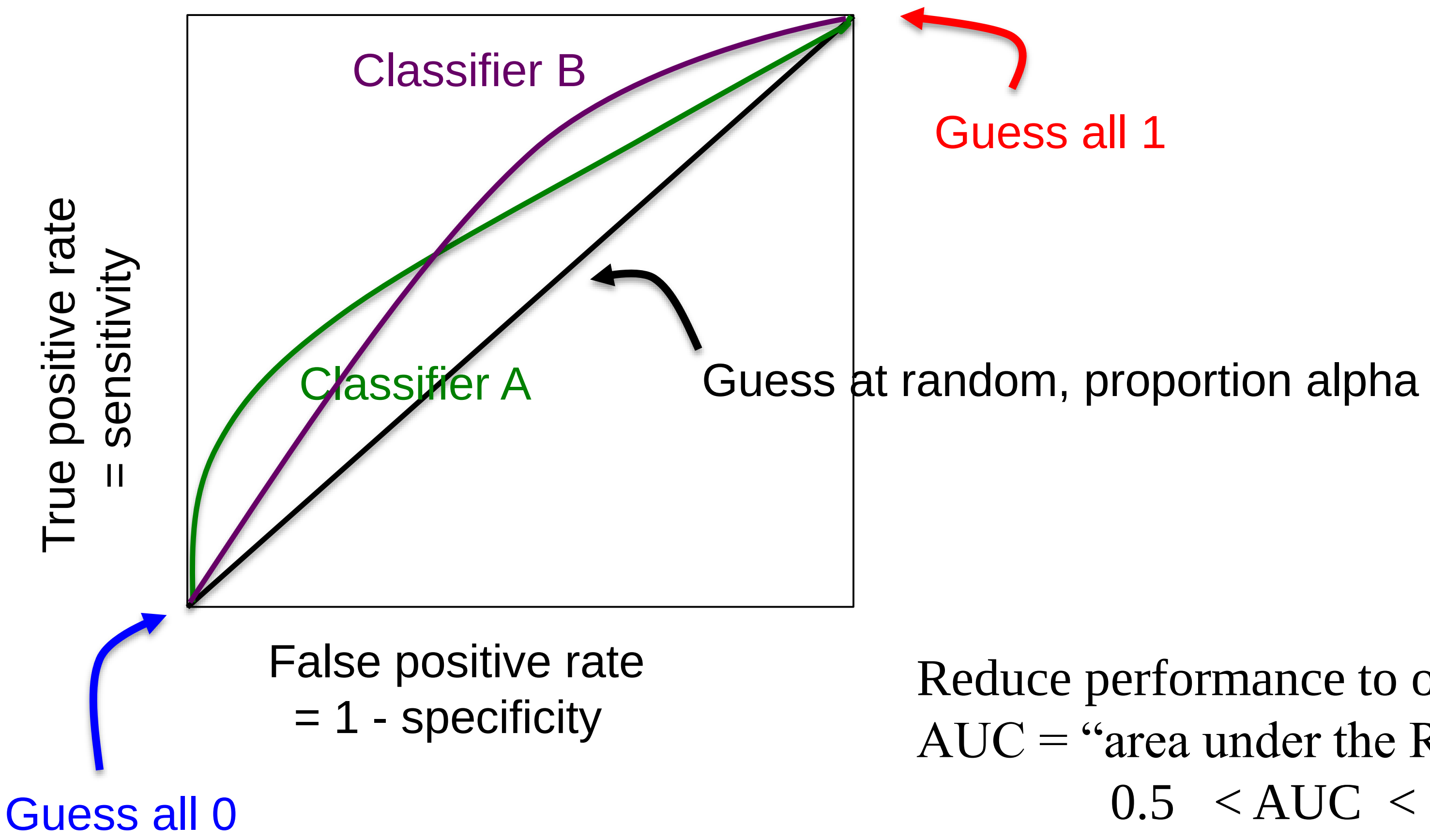


$$\alpha\ p(y=0,x) \lessgtr p(y=1,x)$$



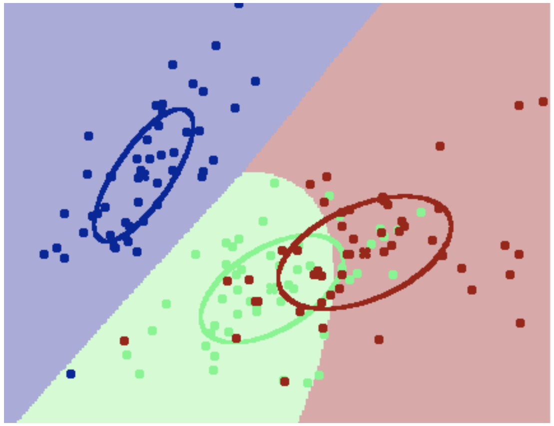
ROC Curves

- Characterize performance as we vary our confidence threshold?

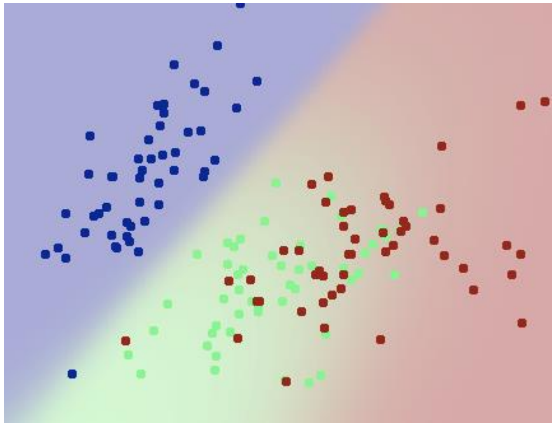


Reduce performance to one number?
AUC = “area under the ROC curve”
$0.5 < AUC < 1$

Probabilistic vs. Discriminative learning



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



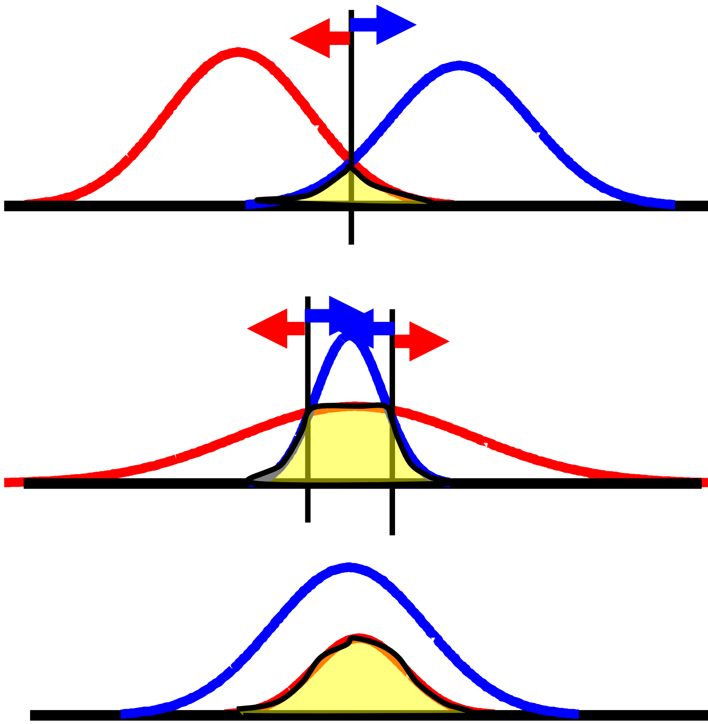
"Probabilistic" learning:
Output probability $p(y|x)$
(expresses confidence in outcomes)

- "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

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

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

$$0 \begin{array}{c} < \\ > \end{array} \log \frac{p(x|y=0)}{p(x|y=1)} \frac{p(y=0)}{p(y=1)} = \log \frac{p(y=0)}{p(y=1)} +$$

$$-.5(x\Sigma^{-1}x - 2\mu_0^T \Sigma^{-1} x + \mu_0^T \Sigma^{-1} \mu_0)$$

$$+.5(x\Sigma^{-1}x - 2\mu_1^T \Sigma^{-1} x + \mu_1^T \Sigma^{-1} \mu_1)$$

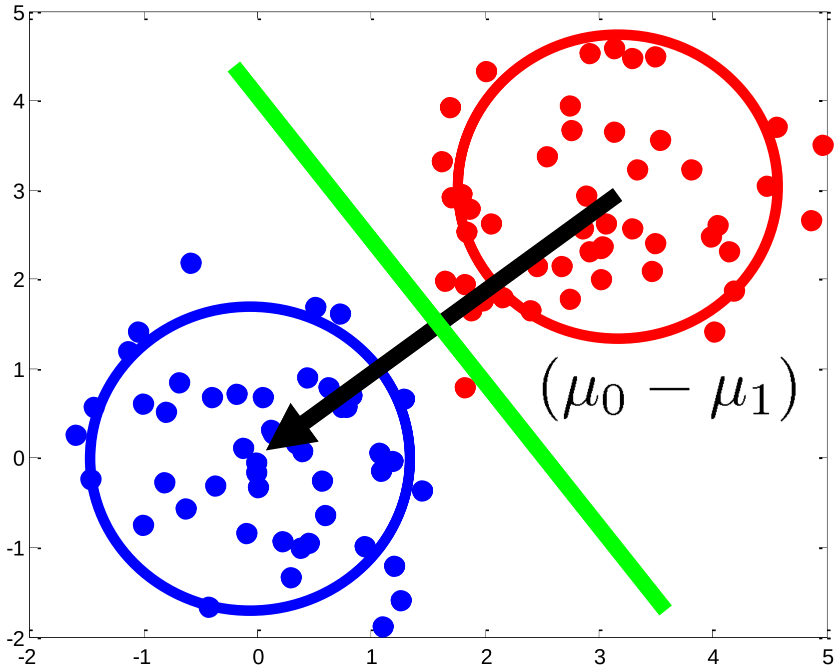
$$= (\mu_0 - \mu_1)^T \Sigma^{-1} x + constants$$

Gaussian example

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

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

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



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

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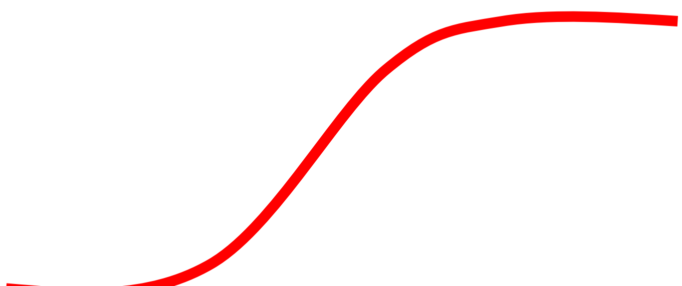
- We can compute posterior using Bayes' rule
  - p(y=c | x) = p(x|y=c) p(y=c) / p(x)
- Compute p(x) using sum rule / law of total prob.
  - p(x) = p(x|y=0) p(y=0) + p(x|y=1)p(y=1)
  - = p(y=0,x) + p(y=1,x)

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
  - $p(y=0 \mid x) = p(y=0, x) / p(x)$
  - $\qquad = p(y=0, x) / (p(y=0,x) + p(y=1,x))$
  - Divide by $p(y=0, x)$, we get
  - $\quad = 1 / (1 + \exp(-a)) \qquad (**)$
  - Where
  - $a = \log [p(x|y=0) p(y=0) / p(x|y=1) p(y=1)]$
  - (**) 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…