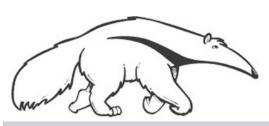
Machine Learning and Data Mining

Bayes Classifiers

Prof. Alexander Ihler







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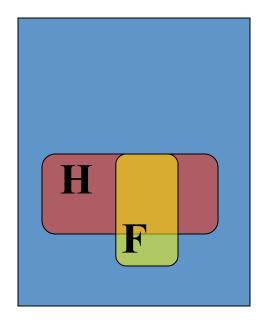
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- Ex: credit rating prediction (bad/good)
 - $X_1 = income (low/med/high)$
 - How can we make the most # of correct predictions?
 - Predict more likely outcome for each possible observation
 - Can normalize into probability:p(y=good | X=c)

_	How to generalize?	

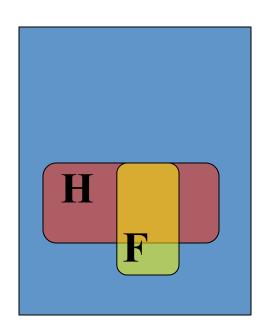
Features	# bad	# good
X=0	.7368	.2632
X=1	.5408	.4592
X=2	.3750	.6250

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

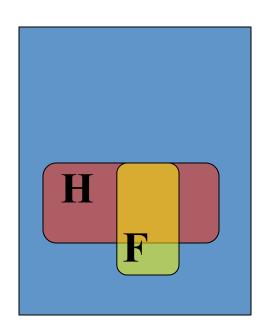


 You wake up with a headache – what is the chance that you have the flu?

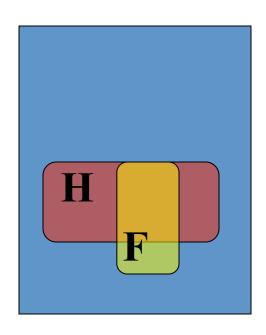
- Two events: headache, flu
- p(H) = 1/10
- p(F) = 1/40
- p(H|F) = 1/2
- P(H & F) = ?
- P(F|H) = ?



- · 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) = ?



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

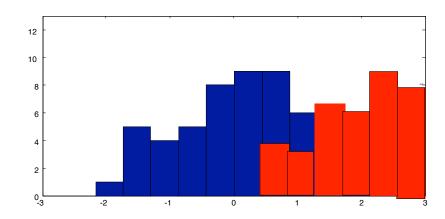
(Use the rule of total probability to calculate the denominator!)
$$= \frac{p(x|y)p(y)}{\sum_{c} p(x|y=c)p(y=c)}$$

- 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 a discrete x, this recalculates the same table...

Features	# bad	# good	p(x y=0)	p(x y=1)		p(y=0 x)	p(y=1 x)
X=0	42	15	42 / 383	15 / 307		.7368	.2632
X=1	338	287	338 / 383	287 / 307	→	.5408	.4592
X=2	3	5	3 / 383	5 / 307		.3750	.6250

p(y)	383/690	307/690
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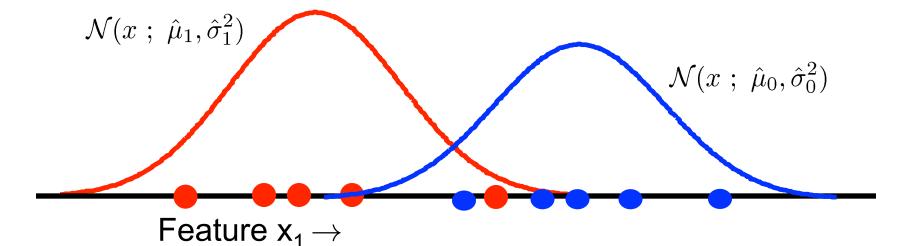
- Learn "class conditional" models
 - Estimate a probability model for each class
- Training data
 - Split by class
 - $D_c = \{ x^{(j)} : y^{(j)} = c \}$
- Estimate p(x | y=c) using D_c
- For continuous x, can use any density estimate we like
 - Histogram
 - Gaussian
 - **–** ...



Gaussian models

Estimate parameters of the Gaussians from the data

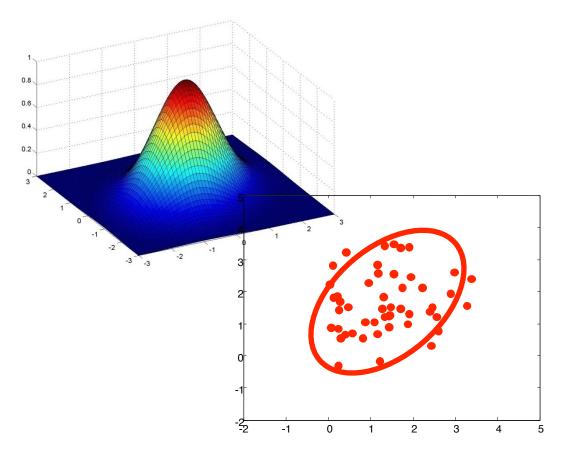
$$\alpha = \frac{m_1}{m} = \hat{p}(y = c_1)$$
 $\hat{\mu} = \frac{1}{m} \sum_j x^{(j)}$ $\hat{\sigma}^2 = \frac{1}{m} \sum_j (x^{(j)} - \mu)^2$



Multivariate Gaussian models

Similar to univariate case

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



 μ = length-d column vector Σ = d x d matrix

 $|\Sigma|$ = matrix determinant

Maximum likelihood estimate:

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

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

Example: Gaussian Bayes for Iris Data

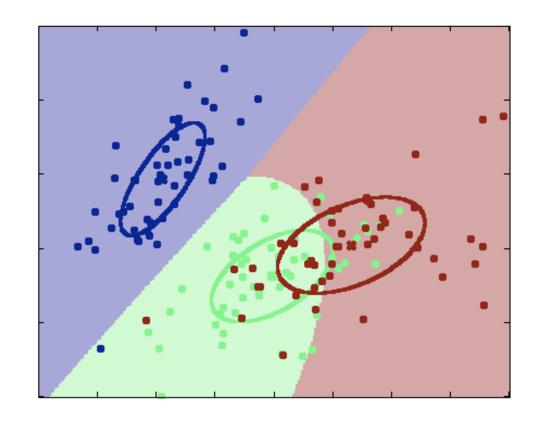
Fit Gaussian distribution to each class {0,1,2}

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

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

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

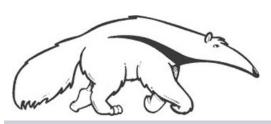
$$p(x_1, x_2 | y = 2) = \mathcal{N}(x; \mu_2, \Sigma_2)$$



Machine Learning and Data Mining

Bayes Classifiers: Naïve Bayes

Prof. Alexander Ihler







- 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		p(x y=0)	p(x y=1)		p(y=0 x)	p(y=1 x)
X=0	42	15		42 / 383	15 / 307		.7368	.2632
X=1	338	287	>	338 / 383	287 / 307	→	.5408	.4592
X=2	3	5		3 / 383	5/307		.3750	.6250

p(y)	383/690	307/690
------	---------	---------

Joint distributions

Make a truth table of all combinations of values

Α	В	С
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?

Α	В	С	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 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!

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

Overfitting and density estimation

- Estimate probabilities from the data
 - E.g., how many times (what fraction)

		U		1/10
did each outcome occur?	0	1	0	0/10
	0	1	1	0/10
M data << 2^N parameters?		0	0	1/10
ivi data < 2 in parameters:			1	2/10
	1	1	0	1/10
What about the zeros?	1	1	1	1/10

 $p(A,B,C \mid y=1)$

4/10

1/10

- - 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 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)
- $p(x_1, x_2, ... x_N | y=1) = p(x_1 | y=1) p(x_2 | y=1) ... p(x_N | y=1)$
- Only need to estimate each individually

Α	p(A y=1)
0	.4
1	.6

В	p(B y=1)
0	.7
1	.3

С	p(C y=1)	
0	.1	\Rightarrow
1	.9	,

Α	В	С	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	у
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?

$$\hat{p}(y=1)\hat{p}(x=11|y=1) \qquad \stackrel{\checkmark}{>} \qquad \hat{p}(y=0)\hat{p}(x=11|y=0)$$

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

Decide class 0

Example: Naïve Bayes

Observed Data:

X ₁	X ₂	у
1	1	0
1	0	0
1	0	1
0	0	0
0	1	1
1	1	0
0	0	1
1	0	1

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

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

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

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

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

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

Example: Joint Bayes

Observed Data:

X_1	X ₂	у
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

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

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 x=[x₁...x_n]
 - Age, income, education, zip code, ...
 - Want to learn p(y | x₁...x_n), to predict y
 - Arbitrary distribution: O(dⁿ) 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 {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: $\sim 2^{270}...$
 - 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

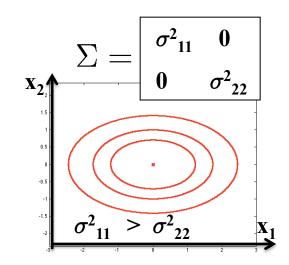
$$p(x_1) = \frac{1}{Z} \exp\left\{-\frac{1}{2\sigma_1^2}(x_1 - \mu_1)^2\right\} \qquad p(x_2) = \frac{1}{Z_2} \exp\left\{-\frac{1}{2\sigma_2^2}(x_2 - \mu_2)^2\right\}$$

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

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

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

Again, reduces the number of parameters of the model: Bayes: n²/2 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:

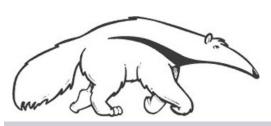
$$p(x | y=C) = p(x_1 | y=C) p(x_2 | y=C) ...$$

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

Machine Learning and Data Mining

Bayes Classifiers: Measuring Error

Prof. Alexander Ihler







- 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

- Given training data, compute p(y=c|x) and choose largest
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Features	# bad	# good
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X=1	338	287
X=2	3	5

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:

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

- Observe any x: $\Rightarrow p(y=0|x)$ (at any x) p(y=1|x)
- Optimal decision at that particular x is: $\hat{y} = f(x) = \arg\max \ p(y = c|x)$



Error rate is:

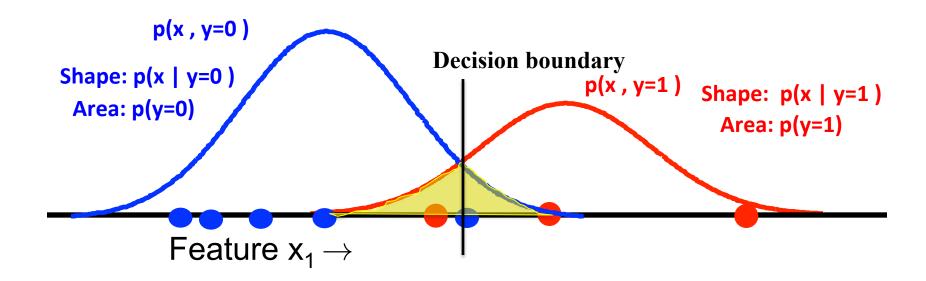
$$\mathbb{E}_{xy}[y \neq \hat{y}] = \mathbb{E}_x[1 - \max_c p(y = c|x)]$$
 = "Bayes error rate"

- 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

Can visualize this nicely if x is univariate:

$$p(y=0|x) < p(y=1|x)$$

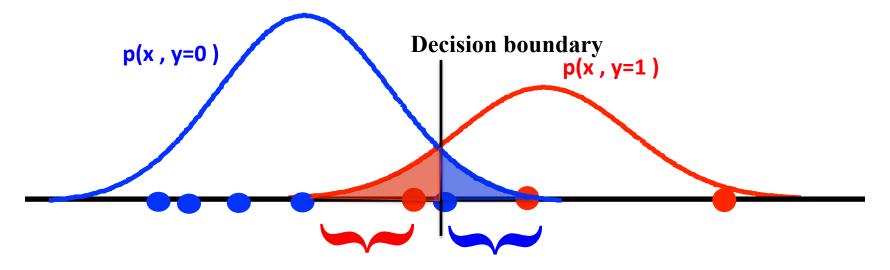
$$= p(y=0,x) < p(y=1,x)$$



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

Add multiplier alpha:

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



Type 1 errors: false positives

Type 2 errors: false negatives

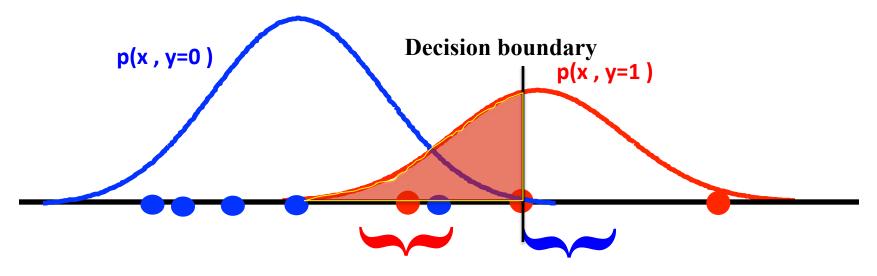
False positive rate: $(\# y=0, \hat{y}=1) / (\# y=0)$

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

- Increase alpha: prefer class 0
- Spam detection

Add multiplier alpha:

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



Type 1 errors: false positives

Type 2 errors: false negatives

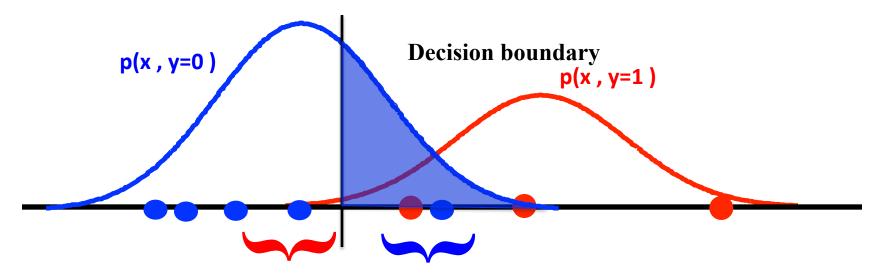
False positive rate: $(\# y=0, \hat{y}=1) / (\# y=0)$

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

- Decrease alpha: prefer class 1
- Cancer detection

Add multiplier alpha:

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



Type 1 errors: false positives

Type 2 errors: false negatives

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

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

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"

Likelihood ratio tests

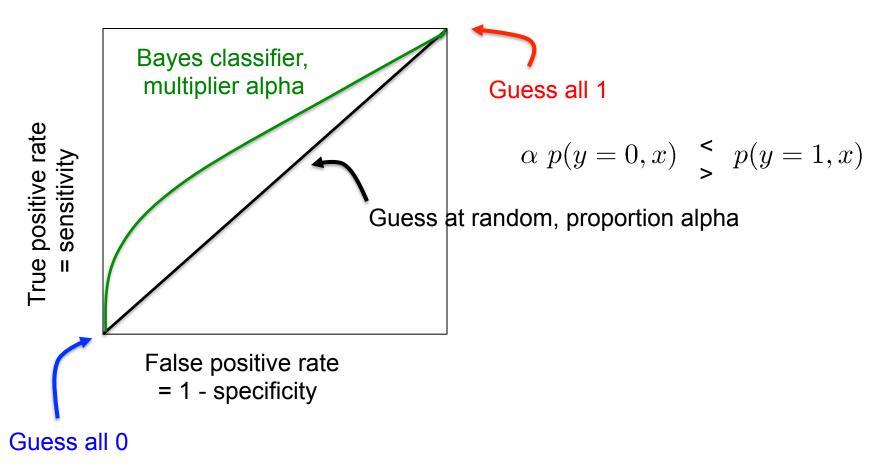
Connection to classical, statistical decision theory:

$$p(y=0,x) \leq p(y=1,x) = \log \frac{p(y=0)}{p(y=1)} \leq \log \frac{p(x|y=1)}{p(x|y=0)}$$
 "log likelihood ratio"

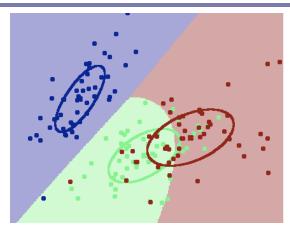
- Likelihood ratio: relative support for observation "x" under "alternative hypothesis" y=1, compared to "null hypothesis" y=0
- Can vary the decision threshold: $\gamma < \log \frac{p(x|y=1)}{p(x|y=0)}$
- Classical testing:
 - Choose gamma so that FPR is fixed ("p-value")
 - Given that y=0 is true,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

ROC Curves

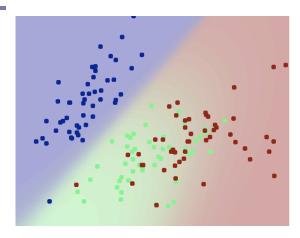
• Characterize performance as we vary the decision threshold?



Probabilistic vs. Discriminative learning



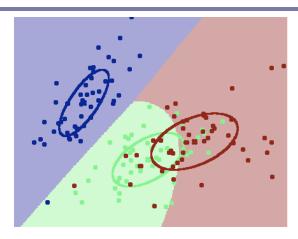
"Discriminative" learning: Output prediction $\hat{y}(x)$



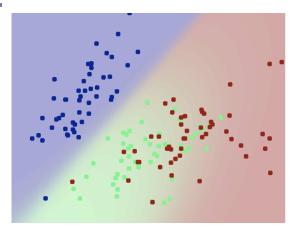
"Probabilistic" learning:
Output probability p(y|x)
(expresses confidence in outcomes)

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



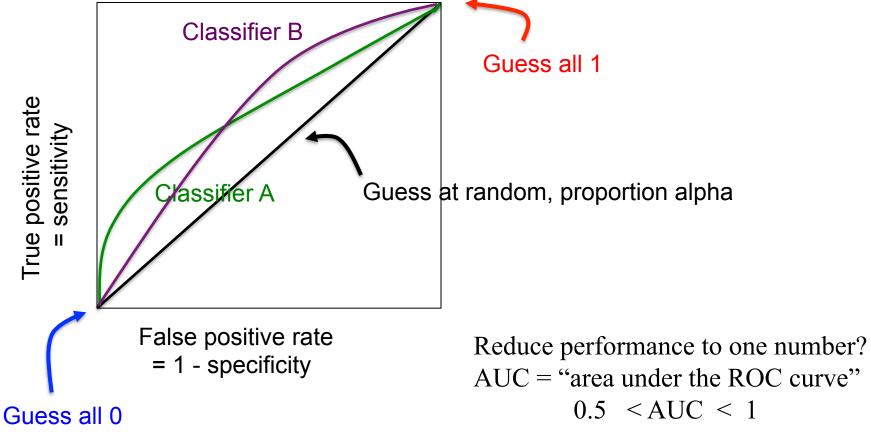
"Probabilistic" learning:
Output probability p(y|x)
(expresses confidence in outcomes)

- 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

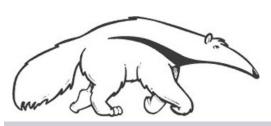
Characterize performance as we vary our confidence threshold?



Machine Learning and Data Mining

Gaussian Bayes Classifiers

Prof. Alexander Ihler

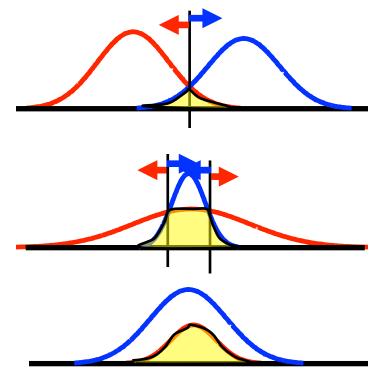






Gaussian models

- "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

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

$$0 \leq \log \frac{p(x|y=0)}{p(x|y=1)} \frac{p(y=0)}{p(y=1)} = \log \frac{p(y=0)}{p(y=1)} + \dots$$

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

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

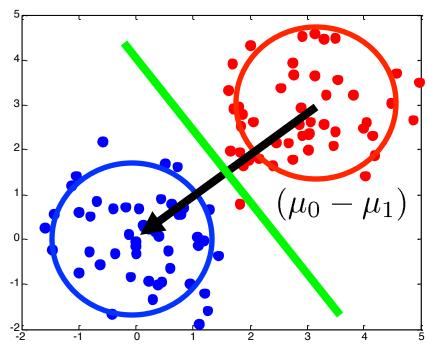
$$= (\mu_0 - \mu_1)^T \Sigma^{-1} x + constants$$

Gaussian example

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

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

$$(\mu_0 - \mu_1)^T x < C$$

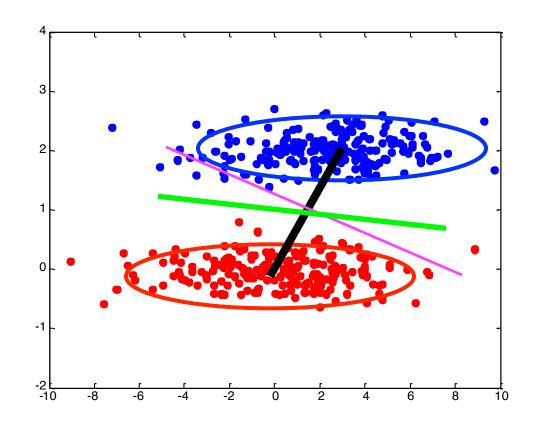


$$C = .5(\mu_0^T \Sigma^{-1} \mu_0)$$
$$- \mu_1^T \Sigma^{-1} \mu_1)$$
$$- \log \frac{p(y=0)}{p(y=1)}$$

Non-spherical Gaussian distributions

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

Ex: Variance [3 0] [0 .25]



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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 - 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

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- p(x | y=0) * p(y=0) vs p(x | y=1) * p(y=1)
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Write probability of each class as

$$- p(y=0 \mid x) = p(y=0, x) / p(x)$$

$$- p(y=0, x) / (p(y=0,x) + p(y=1,x))$$

$$- = 1 / (1 + exp(-a)) (**)$$

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

Gaussian modelsReturn to Gaussian models with equal covariances

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

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

We'll see this form again soon...