

Naïve Bayes Classifier

(Murphy book) Sections 3.2 and 3.5

Physical Address for Prof. Ilias Tagkopoulos

Computer Science:

Office: 3063 Kemper Hall

Phone: (530) 752-4821

Fax: (530) 752-4767

Instructor: Ilias Tagkopoulos

iliast@ucdavis.edu

Genome and Biomedical Sciences Facility:

Office: 5313 GBSF

Phone: (530) 752-7707

Fax: (530) 754-9658

■ A Probabilistic classification approach

- The simplest probabilistic classifier: Naïve Bayes
 - a **generative** method.
- The three main concepts here are:
 - **PRIOR probability**
 - **POSTERIOR probability**
 - **LIKELIHOOD**
- The main assumption is that given a class, any feature is **independent** of any other feature.
 - The reason the classifier is called “naïve”.
- In practice, it works quite well, even when features are not independent especially when
 - Features are not highly correlated, or their function is a complex one
 - The number of data points (training data) is modest, so more complex classifiers risk over-fitting.

Building a Bayesian classifier: Prior Probability

- Suppose that you have a **total of n classes**, i.e $y \in \{c_1, \dots, c_n\}$.
- Without having any other information, what is the ***a priori*** probability that any given object (j) belong to any given class?

$$p(y^{(j)} = c_i) = \frac{1}{n}$$

- This probability that a random object will belong to a certain class is called **prior probability**.
- What happens when classes have **different frequencies** in the dataset (population)?

$$p(y^{(j)} = c_i) = \frac{f_i}{\sum_1^n f_i}$$

- For instance, what is the prior probability for each class in the following example, given its member size?

	A	B	C	D	E
Members	100	300	5	500	95
Prior Probability	?	?	?	?	?

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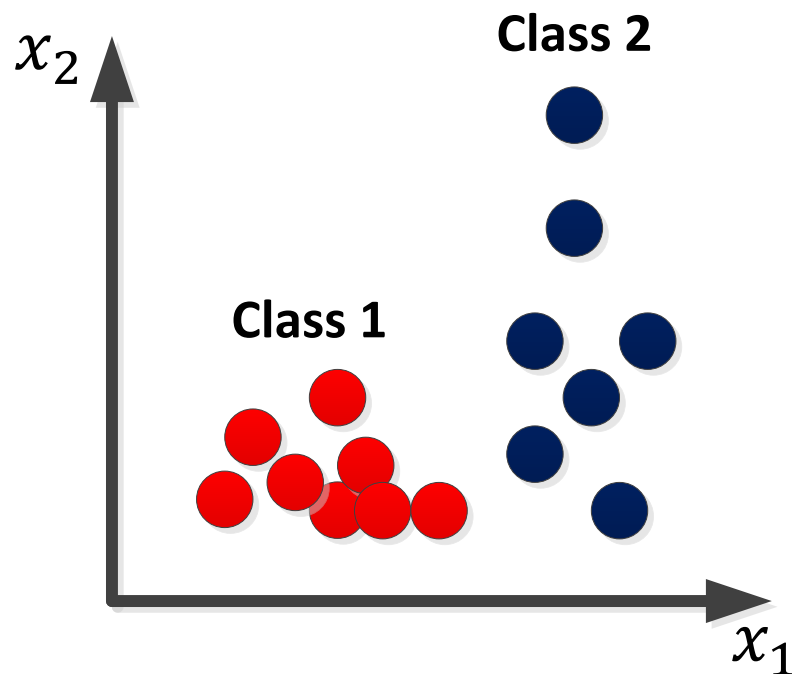
$$p(y^{(j)} = c_i) = \frac{f_i}{\sum_1^n f_i}$$

- For instance, what is the prior probability for each class in the following example, given its member size?

	A	B	C	D	E
Members	100	300	5	500	95
Prior Probability	0.1	0.3	0.005	0.5	0.095

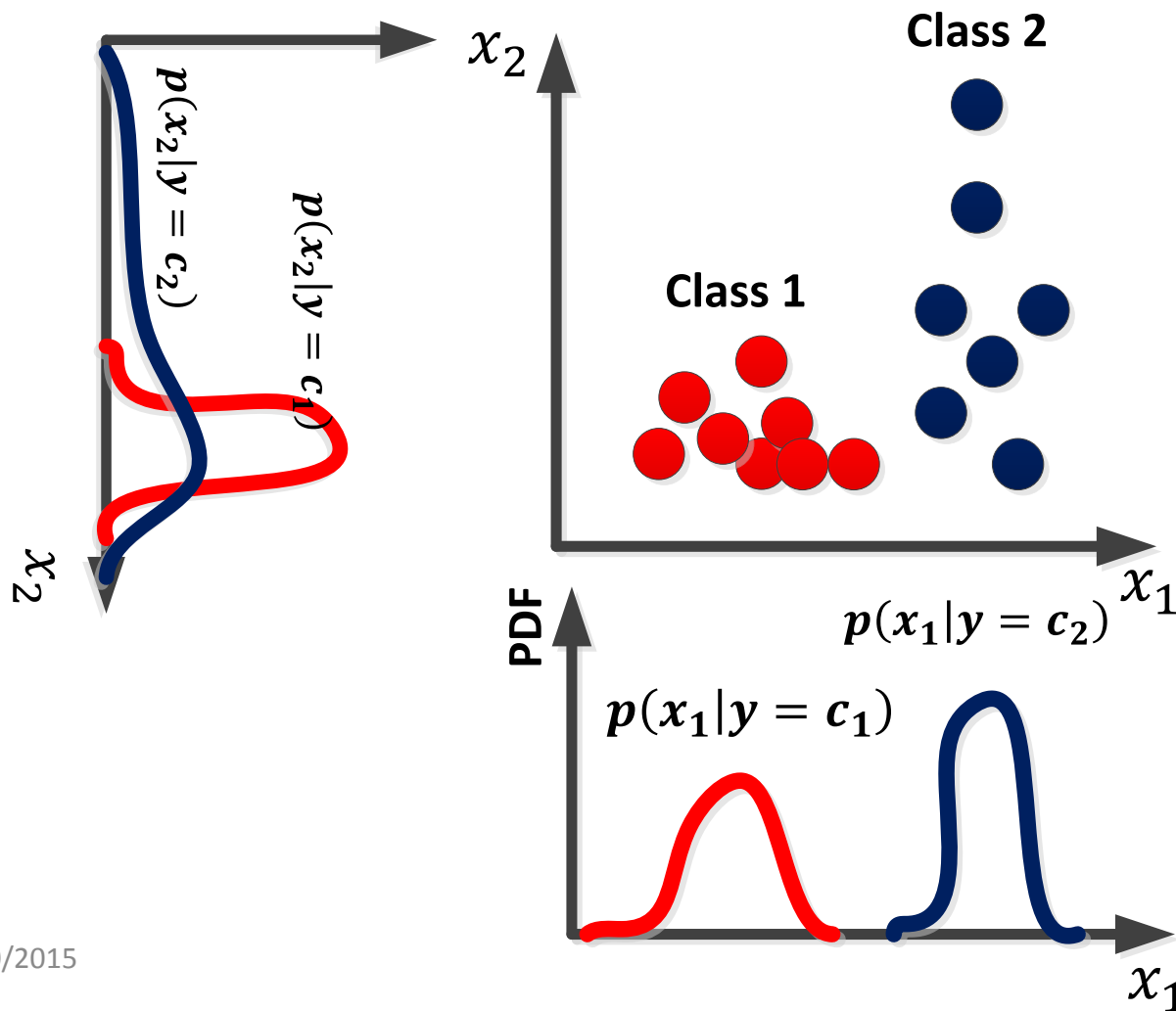
■ Building a Bayesian classifier: Likelihood

- The Likelihood $l(x|y) = p(x|y = c_i)$ can be thought as the **class-conditional probability distribution** of the feature (input) for a specific class c_i
- Example: assume two features and two classes, like in the picture. What will the $p(x|y = c_i)$ be?



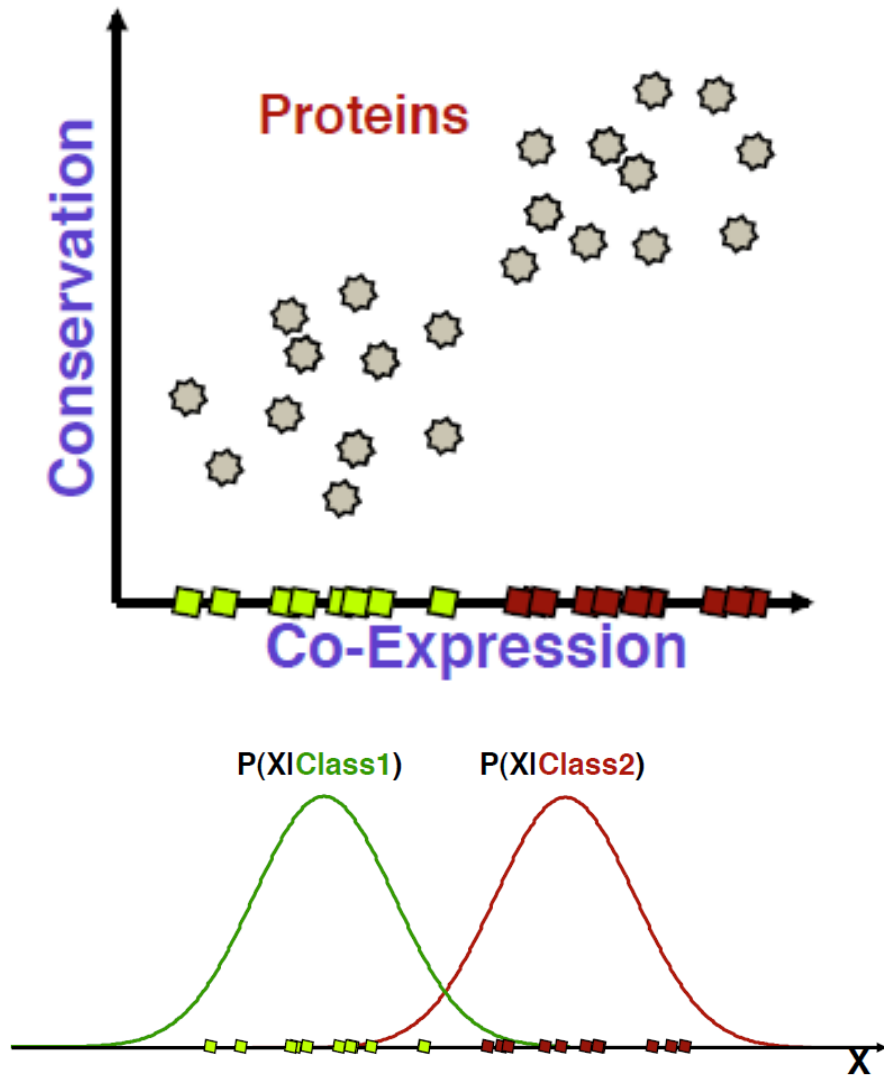
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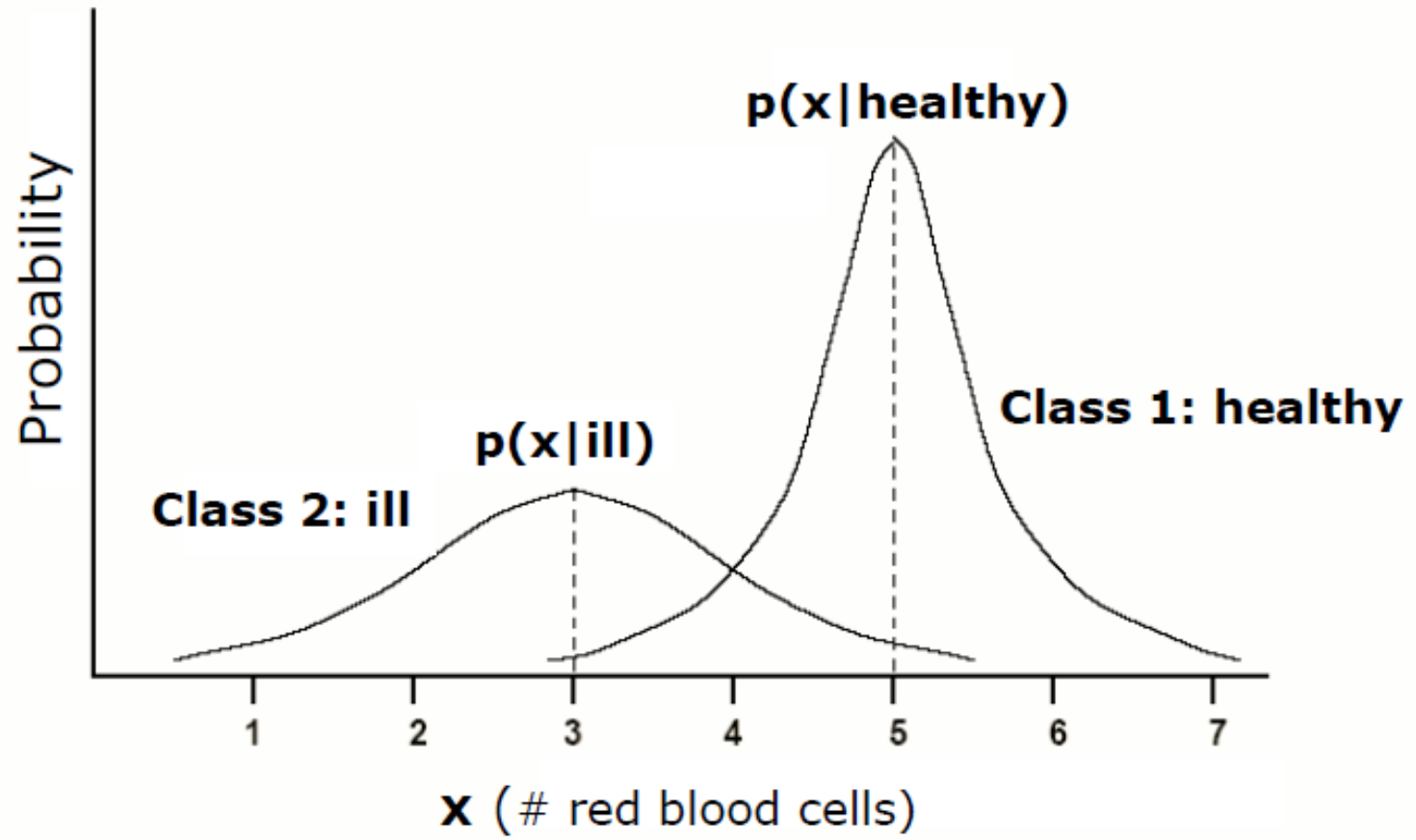
■ Building a Bayesian classifier: Likelihood

- Another example: proteins



■ Building a Bayesian classifier: Likelihood

- Another example: patients



Should we always model it as a Gaussian ? What if the features are binary?

■ Building a Bayesian classifier

- So far, we have calculated:
 - **Prior Probability:** The “default”, *a priori* probabilities for each class
 - **Likelihood:** The probability of a feature(s) having a specific value(s), given a certain class (also called class-conditional probabilities)
- What we want to calculate, however is the **posterior probability**: the probability of a sample being in a specific class given the feature values
- How can we link all these ?

Bayes Theorem

Bayes Theorem



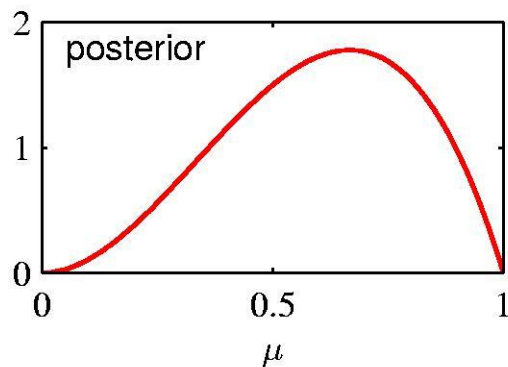
$$P(\textit{Class} \mid \textit{Feature}) = \frac{P(\textit{Feature} \mid \textit{Class}) \cdot P(\textit{Class})}{P(\textit{Feature})}$$



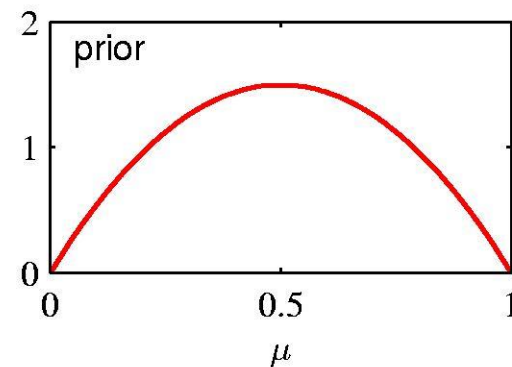
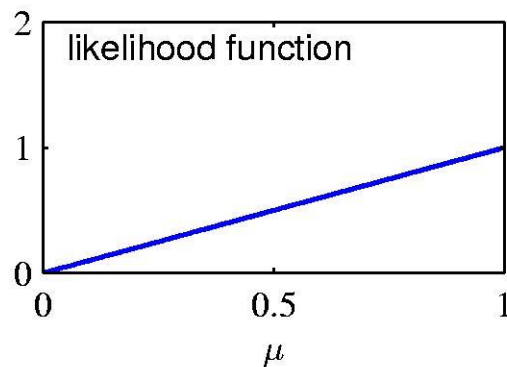
From Bayes Theorem:

Posterior probability is proportional to
Likelihood times the Prior Probability

$$\text{Posterior} \sim \text{Likelihood} \times \text{Prior}$$



\sim



■ Building a Bayesian classifier: How to assign classes

- We can now calculate the probability of a sample belonging to a class (**posterior**), for any given class, assuming that we know the **prior**, **evidence** and the **likelihood**
- One way to build a classifier: **calculate all posterior probabilities** for the sample and **assign it to the class that is has the highest probability.**
- Another way to build a classifier: **Create a discriminant function. Assign to the first class when:**

$$P(\text{Feature } X | \text{Class1}) \cdot P(\text{Class1}) > P(\text{Feature } X | \text{Class2}) \cdot P(\text{Class2})$$

- Or equivalently if **$G(X) > 0$** , where $G(X)$ is given by

$$G(X) = \log \frac{P(\text{Feature } X | \text{Class1}) \cdot P(\text{Class1})}{P(\text{Feature } X | \text{Class2}) \cdot P(\text{Class2})}$$

■ Building a classifier: Multiple features

- Which one is better? Having a **discriminant function doesn't need** the calculation of the **evidence**
- Until now we focused on **a single feature X**. What happens when we have **multiple features**?
- In that case, our discriminant function becomes:

$$G(X) = \log \frac{P(\text{Feature } X_1, \text{Feature } X_2, \dots \text{Feature } X_n | \text{Class1}) \cdot P(\text{Class1})}{P(\text{Feature } X_1, \text{Feature } X_2, \dots \text{Feature } X_n | \text{Class2}) \cdot P(\text{Class2})}$$

- We can build a table with the probability for each feature.
 - Good luck with that! Assume that each feature can take k values, what is the **complexity** of your problem?

■ Naïve Bayes Classifier

- Assumes that all features are **INDEPENDENT**

- With the assumption of independence, our likelihood is given by:

$$\begin{aligned} P(\text{Feature } X_1, \text{Feature } X_2, \dots, \text{Feature } X_n | \text{Class1}) &= P(\text{Feature } X_1 | \text{Class1}) P(\text{Feature } X_2 | \text{Class1}) \dots P(\text{Feature } X_n | \text{Class1}) \\ &= \prod_i P(\text{Feature } X_i | \text{Class1}) \end{aligned}$$

- And hence our discriminant function becomes:

$$G(X_1, \dots, X_n) = \log \frac{\prod_i P(\text{Feature } X_i | \text{Class1}) \cdot P(\text{Class1})}{\prod_i P(\text{Feature } X_i | \text{Class2}) \cdot P(\text{Class2})}$$

Bayesian classification: an example

- How do **we find the parameters** for Naïve Bayes?
 - From your book:

Algorithm 3.1: Fitting a naive Bayes classifier to binary features

```
1  $N_c = 0, N_{jc} = 0;$ 
2 for  $i = 1 : N$  do
3    $c = y_i$  // Class label of  $i$ 'th example;
4    $N_c := N_c + 1$  ;
5   for  $j = 1 : D$  do
6     if  $x_{ij} = 1$  then
7        $N_{jc} := N_{jc} + 1$ 
8  $\hat{\pi}_c = \frac{N_c}{N}, \hat{\theta}_{jc} = \frac{N_{jc}}{N}$ 
```

Bayesian classification: an example

- Some proteins are more expressed in cancerous vs. healthy tissues and thus they can be used as **features** to classify patients
- Assume two **classes/categories/labels**:
 - Class 1: Cancer
 - Class 2: Healthy
- Assume that we have measured the concentration of protein [X] in various people with and without cancer. We use 0 if the protein is expressed in low concentrations, 1 otherwise.

Class conditional probabilities for X

X (Protein)	Class A (Cancer)	Class B (Healthy)
0	0.9	0.2
1	0.1	0.8

- Additionally it is known that **only 1% of the population is found to have cancer when a screening is performed.**
- A new patient with **high levels of protein X** wants to know how probable it is for him to have cancer.

An example of Naïve Bayes classification

■ PRIOR Probability

- $P(\text{Cancer}) = 0.01$

■ LIKELIHOOD

- $P(X=1 | \text{Cancer}) = 0.1$

X (Protein)	Class A (Cancer)	Class B (Healthy)
0	0.9	0.2
1	0.1	0.8

■ EVIDENCE

- $P(X=1) = 0.1 * 0.01 + 0.8 * 0.99 = 0.793$

■ POSTERIOR Probability

- $P(\text{Cancer} | X=1) = 0.1 * 0.01 / 0.793 = \mathbf{0.00126}$

- $P(\text{Healthy} | X=1) = 0.8 * 0.99 / 0.793 = 0.99873$

Example: Building the classifier

- Now we would like to **build a classifier** that can tell whether a patient is likely to have cancer or not based on a protein X concentration.

- Build a discriminative function:**

$$G(X) = \log \frac{P(\text{Feature } X | \text{Class1}) \cdot P(\text{Class1})}{P(\text{Feature } X | \text{Class2}) \cdot P(\text{Class2})}$$

X (Protein)	Class A (Cancer)	Class B (Healthy)
0	0.9	0.2
1	0.1	0.8

- When **$G(X) > 0$** then patient is more likely to have cancer (Class 1) and vice versa.
- Example: $G(X=1) = \log(0.1 \cdot 0.01 / 0.8 \cdot 0.99) = -2.89$
- Example: $G(X=0) = \log(0.9 \cdot 0.01 / 0.2 \cdot 0.99) = 2.64$

Example: Adding more features

- Now assume that we measure protein Y too, which has the following pattern:

Y	Class A (Cancer)	Class B (Healthy)
0	0.9	0.5
1	0.1	0.5

- How can we add it as a feature?
- Assume a new patient with [X] high and [Y] low, what is his probability of cancer?

Feature independence

- Discriminative function **for multiple features**:

$$G(X) = \log \frac{P(\text{Feature } X_1, \text{Feature } X_2, \dots \text{Feature } X_n | \text{Class1}) \cdot P(\text{Class1})}{P(\text{Feature } X_1, \text{Feature } X_2, \dots \text{Feature } X_n | \text{Class2}) \cdot P(\text{Class2})}$$

- But if we assume **independence** (naïve bayes)

$$G(X_1, \dots, X_n) = \log \frac{\prod P(\text{Feature } X_i | \text{Class1}) \cdot P(\text{Class1})}{\prod P(\text{Feature } X_i | \text{Class2}) \cdot P(\text{Class2})}$$

- So here:

$$G(X, Y) = \log \frac{P(X = 1 | \text{Cancer}) \cdot P(Y = 0 | \text{Cancer}) \cdot P(\text{Cancer})}{P(X = 1 | \text{Healthy}) \cdot P(Y = 0 | \text{Healthy}) \cdot P(\text{Healthy})}$$

Naïve Bayes example

X (Protein)	Class A (Cancer)	Class B (Healthy)
0	0.9	0.2
1	0.1	0.8

Y	Class A (Cancer)	Class B (Healthy)
0	0.9	0.5
1	0.1	0.5

$$\log[(0.1*0.9*0.01)/(0.8*0.5*0.99)] = \\ = -2.64$$

again he will be categorized as healthy, but we are now less certain (-2.64 vs -2.89) as low [Y] associates with more with cancer cases than healthy cases (0.9 vs. 0.5)

Measuring classification performance

Sections 5.7.2

■ Measuring classification performance

- Cross-validation
- Binary classification errors



	Really True	Really False
Predicted True	True Positive (TP)	False Positive (FP)
Predicted False	False Negative (FN)	True Negative (TN)

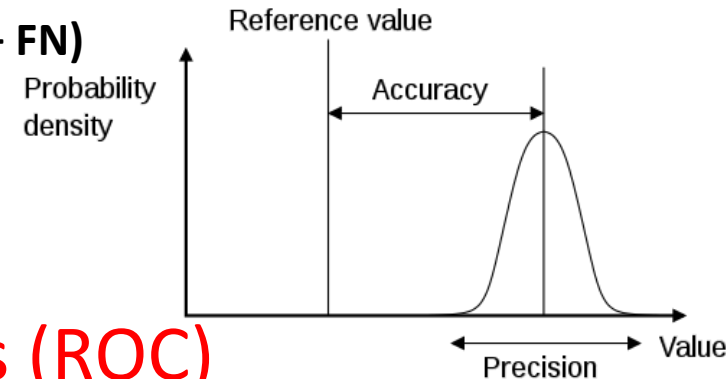
- Statistical measures :

True Positive Rate (TPR) = Recall = Sensitivity = $TP / (TP + FN)$

1- False Positive Rate (FPR) = Specificity = $TN / (TN + FP)$

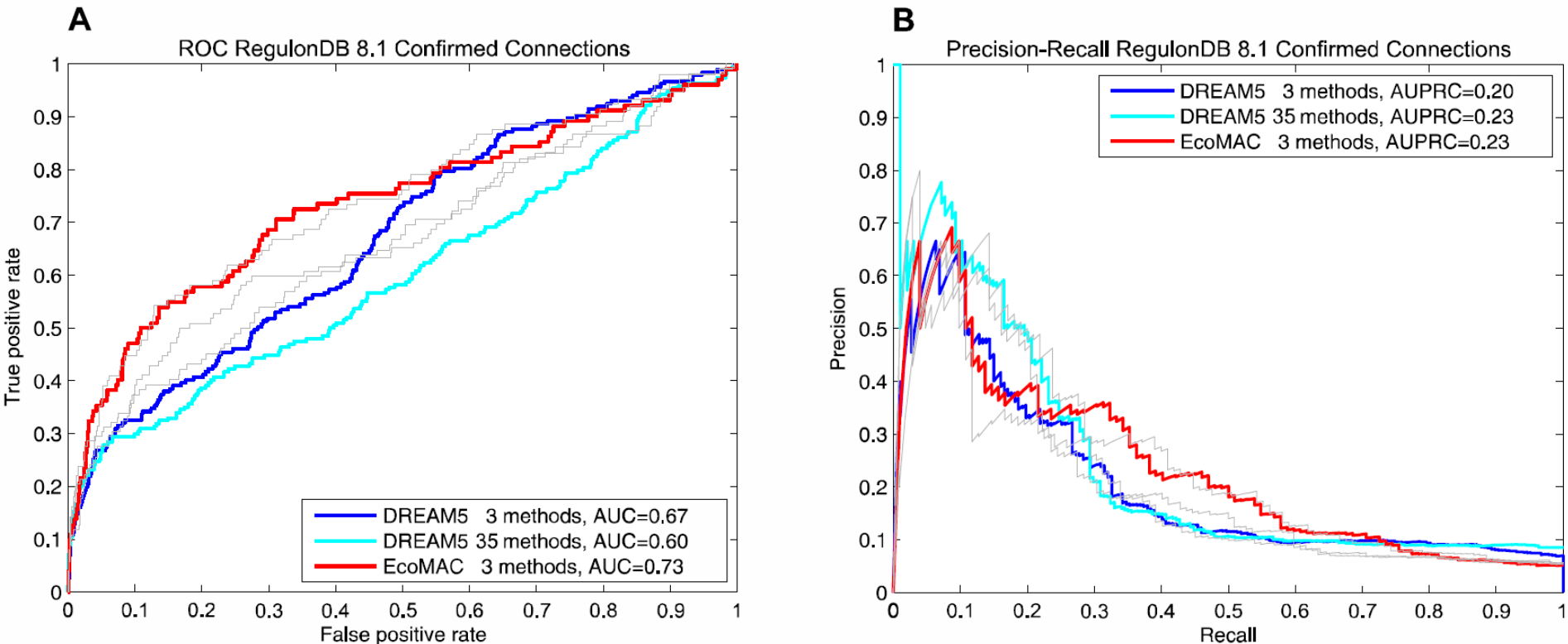
Accuracy = $(TP + TN) / (P + N)$

Precision = $1 - \text{False Discovery Rate} = TP / (TP + FP)$



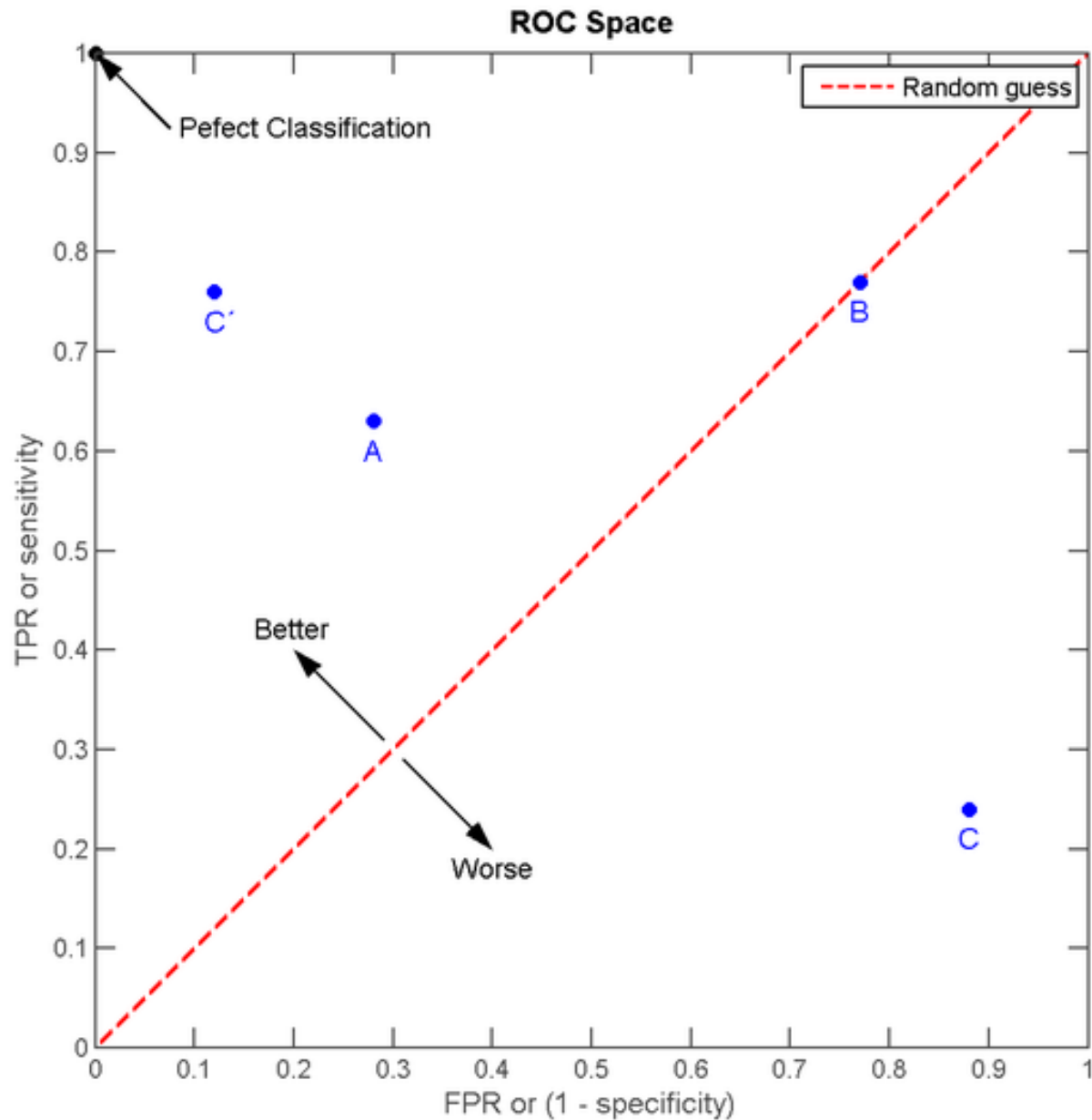
- Receiver Operating Characteristics (ROC)

Receiver Operating Characteristics (ROC curves) and Precision–Recall Curves



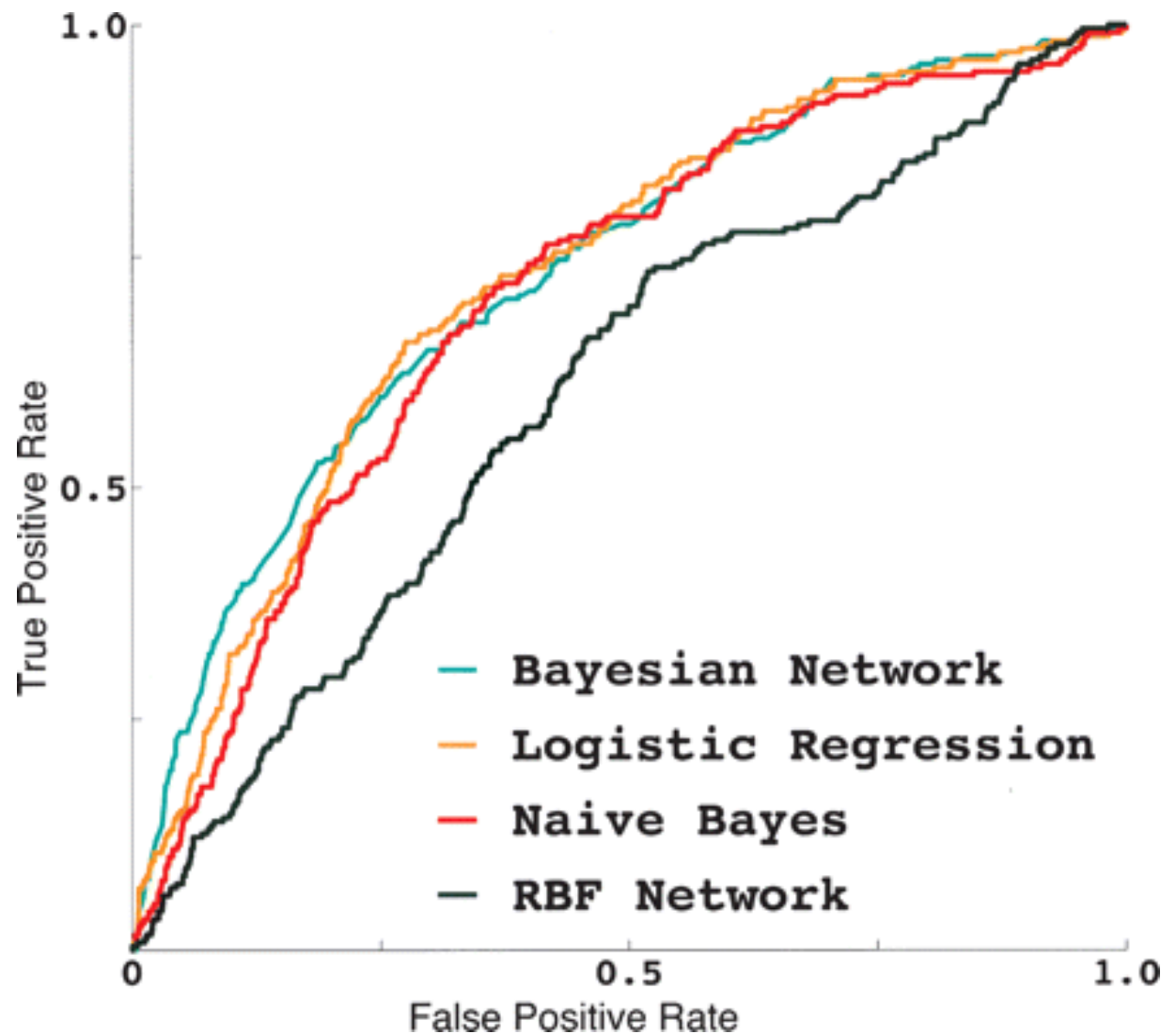
Carrera, R. Estrela, J. Luo, N. Rai, A. Tsoukalas, I. Tagkopoulos, "An integrative, multi-layer, genome-scale model reveals the phenotypic landscape of *Escherichia coli*", *Molecular Systems Biology*, 10(7):735, 2014

Receiver operating characteristic (ROC)

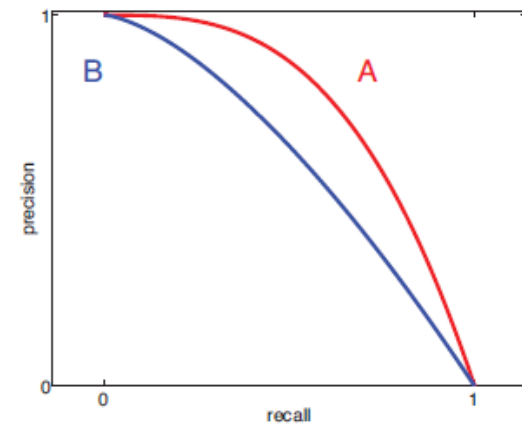
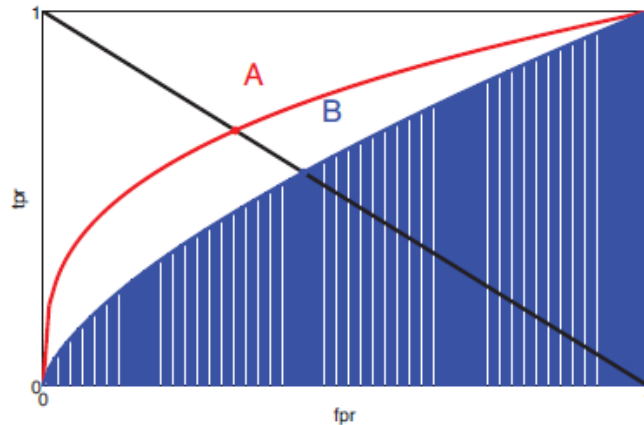


■ Receiver operating characteristic (ROC)

Quantitative systems-level
determinants of human
genes targeted
by successful drugs
L. Yao and A. Rzhetsky
Genome Res. 18:206 (2008)



■ Receiver operating characteristic (ROC)



Which classifier is better? A or B?

Can we represent both precision and recall with one measure?

- Area under the curve (AUC)
- F-score

■ Putting everything together

- Now we have everything we need to design, build and evaluate any classifier. Assume that you are presented with a dataset with **m sample data, each with n features and one label.**
 - **Step 1: Select your model.** Neural Networks, Support Vector Machines, Logistic Regression, Bayesian classifiers. Which one will it be?
 - **Step 2: Select your features.** If n is small and m large, then your classifier can disregard irrelevant features without the risk of over-fitting. In most cases, however, you need to have a feature selection or extraction method to select the most informative features. Additionally, you might need to pre-process features (scaling, missing values, etc.).
 - **Step 3: Evaluate the classifier.** The classifier should always be trained in a training set and evaluated in a mutual exclusive testing set. You can either split the original dataset in any reasonable fraction (2/3-1/3, 70-30%, 80-20%) to form these two sets, or you can use K-fold cross-validation (preferred). Report generalization error, ROC/PR curves, AUC/AUPRC.
 - **Step 4: Train your classifier.** The final classifier should be trained with the complete dataset that was provided.

End of Lecture 9