Other Classification Methods

Lecture 10

Classifiers

Covered so far

- K-Nearest Neighbors
- Perceptron
- Logistic Regression
- Fisher's Linear Discriminant
- Linear Discriminant Analysis
- Quadratic Discriminant Analysis
- Naïve Bayes

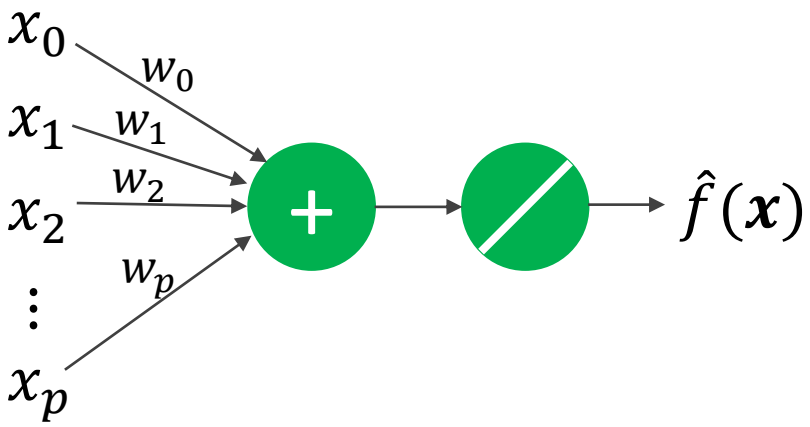
Along the way…

Projections from higher dimensions
Revisiting Bayes' Rule
Multivariate normal distributions

Remember linear models?

Linear Regression

$$\hat{f}(\boldsymbol{x}) = \sum_{i=0}^{p} w_i x_i$$

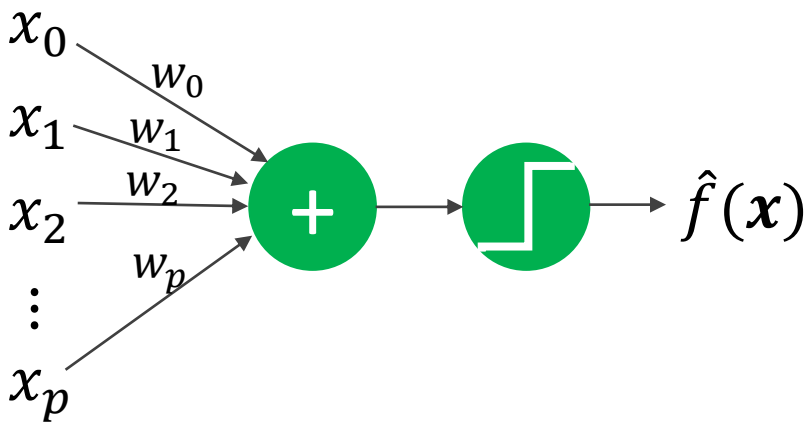


Linear Classification

Perceptron

$$\hat{f}(\boldsymbol{x}) = sign\left(\sum_{i=0}^{p} w_i x_i\right)$$

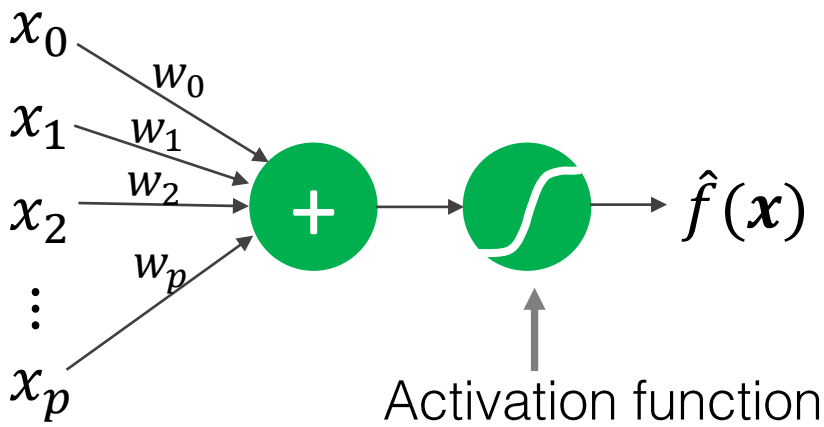
$$sign(x) = \begin{cases} 1 & x > 0 \\ -1 & \text{else} \end{cases}$$



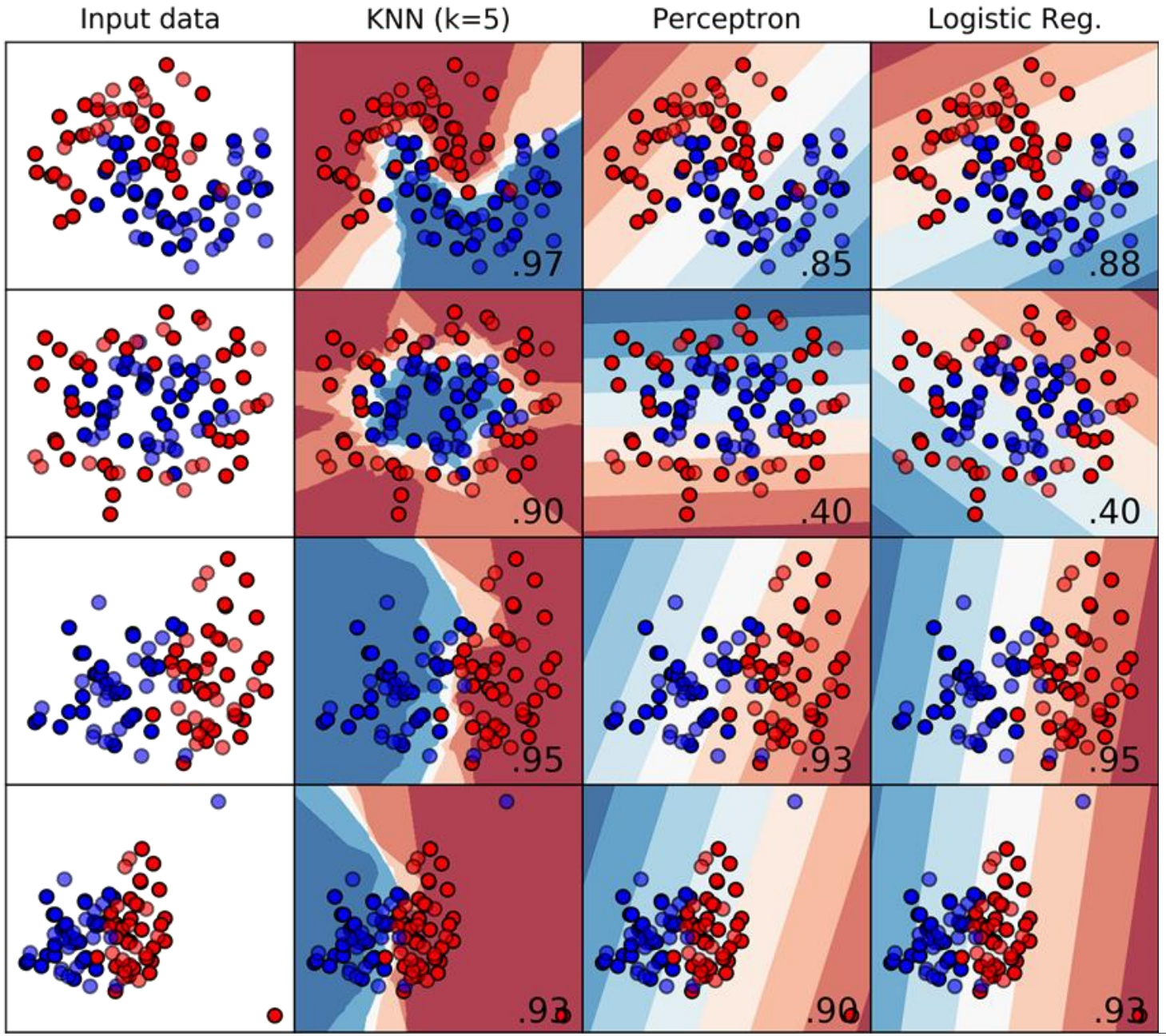
Logistic Regression

$$\hat{f}(\boldsymbol{x}) = \sigma\left(\sum_{i=0}^{p} w_i x_i\right)$$

$$\sigma(x) = \frac{1}{1 + e^{-x}}$$



Source: Abu-Mostafa, Learning from Data, Caltech



Comparison of classifiers we've seen so far

Projections

$$\mathbf{u}^T\mathbf{z} = \begin{bmatrix} u_1 & u_2 \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \end{bmatrix}$$

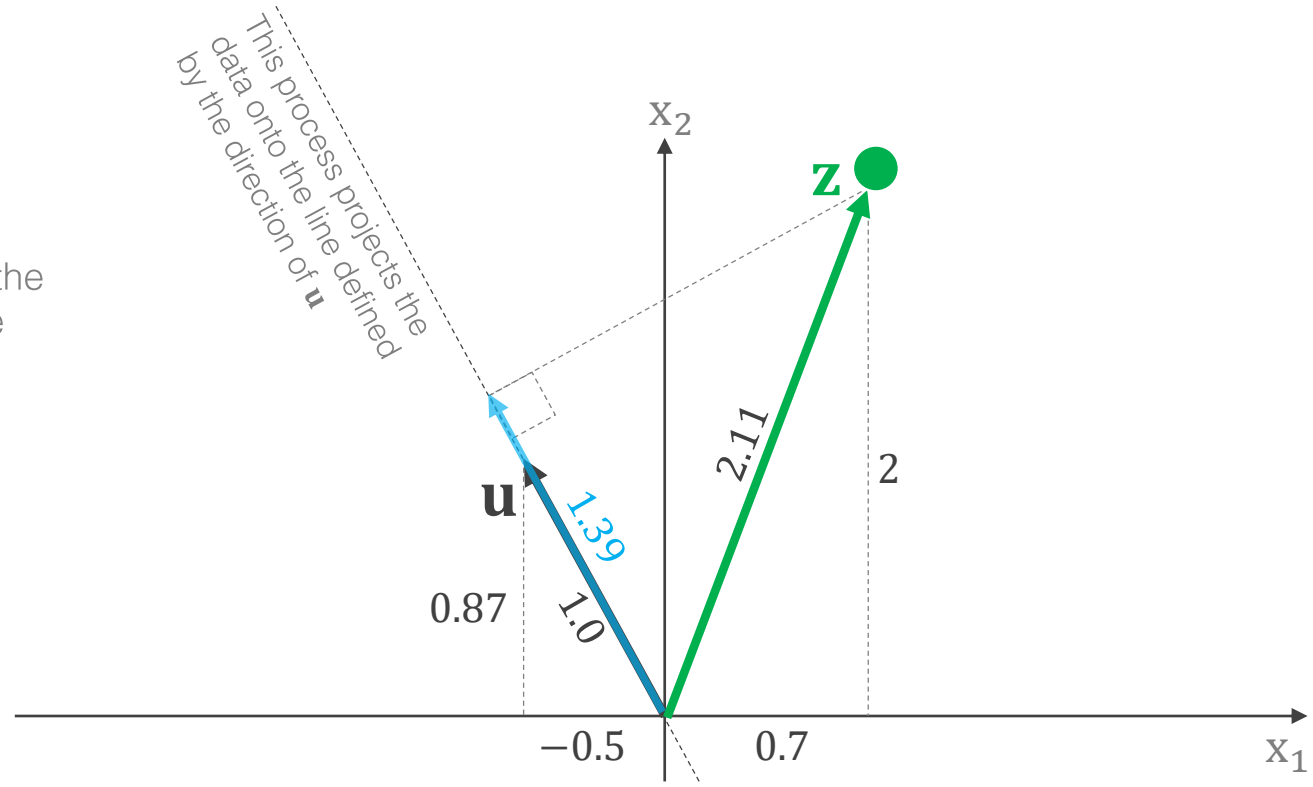
This is an inner product, but assuming $\mathbf{u}$ is a unit vector computes this as the magnitude (length) of the projection of $\mathbf{z}$ onto $\mathbf{u}$

$$= u_1 z_1 + u_2 z_2$$

$$= (-0.5)(0.7) + (0.87)(2)$$

$$= 1.39$$

Length (magnitude) of the projection of $\mathbf{z}$ onto $\mathbf{u}$



This is valid because $\mathbf{u}$ is a unit vector (length is 1: $\|\mathbf{u}\|_2 = \sqrt{u_1^2 + u_2^2} = \sqrt{(-0.5)^2 + (0.87)^2} \cong 1$)

Notes on projections:

If $\mathbf{u}$ was NOT a unit vector, the magnitude (length) of the projection of $\boldsymbol{z}$ onto $\mathbf{u}$ would be calculated by normalizing the result by the length of $\mathbf{u}$:

$$\frac{\mathbf{u}^T\mathbf{z}}{\mathbf{u}^T\mathbf{u}}$$

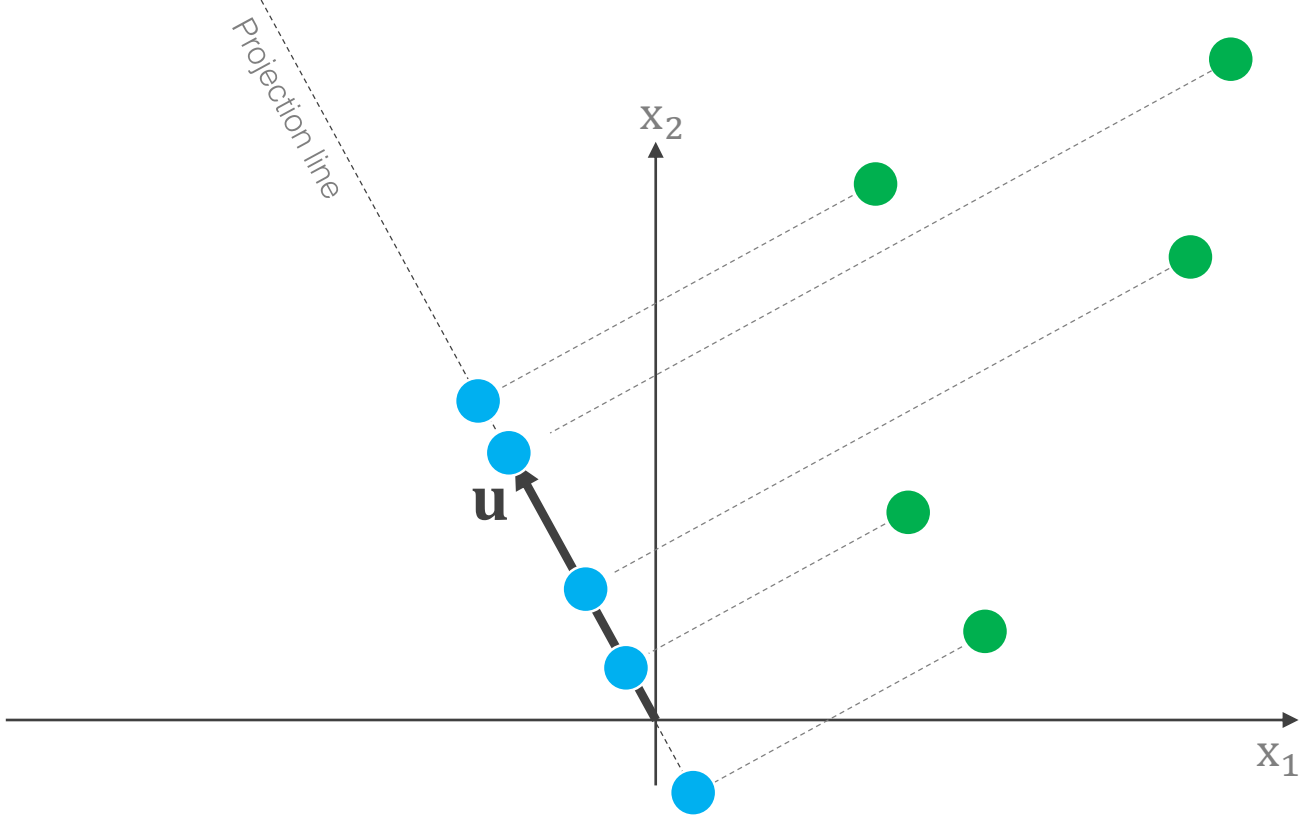
In our case above, $\mathbf{u}^T\mathbf{u} = 1$

The vector projection of $\boldsymbol{z}$ onto $\mathbf{u}$ would multiply the length by the direction of $\mathbf{u}$:

$$\text{proj}_{\mathbf{u}}(\boldsymbol{z}) = \left(\frac{\mathbf{u}^T\mathbf{z}}{\mathbf{u}^T\mathbf{u}}\right)\frac{\mathbf{u}}{\mathbf{u}^T\mathbf{u}}$$

Projections

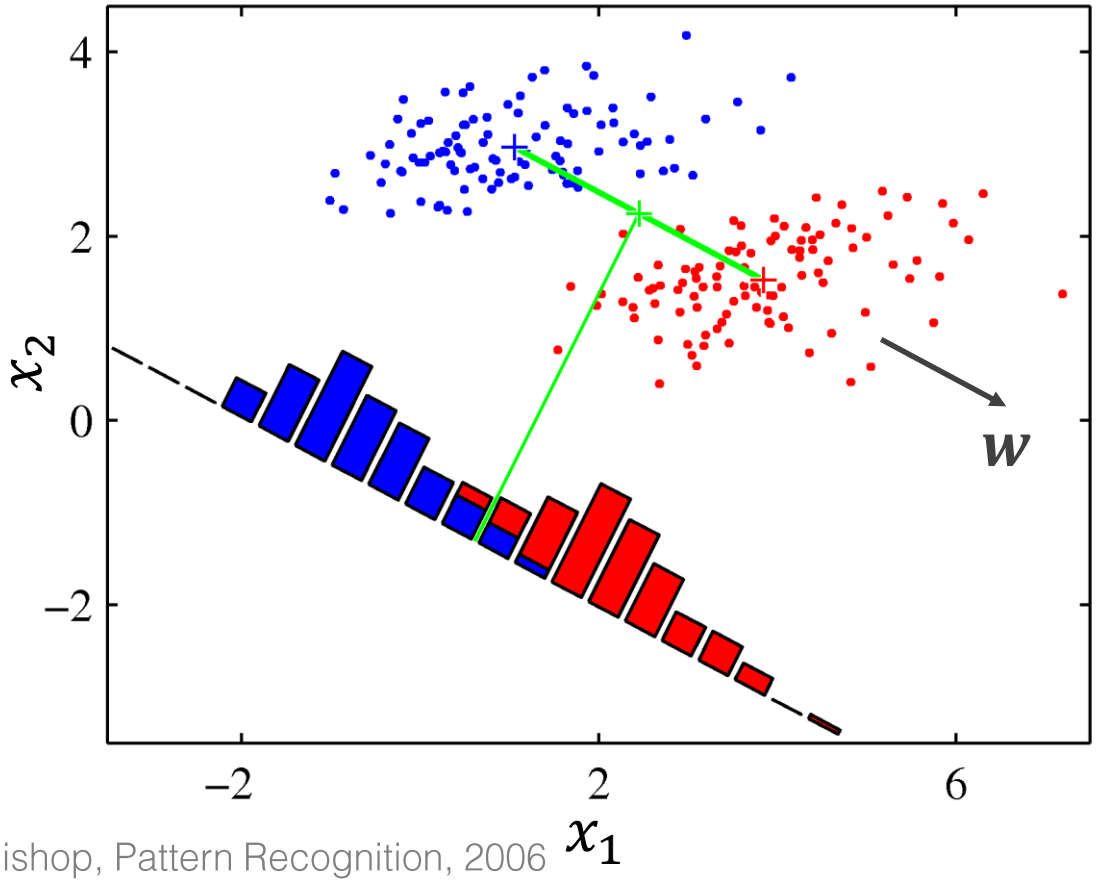
We could project any points in this space onto the line defined by the direction of unit vector $\mathbf{u}$



Fisher's Linear Discriminant

Looks for the projection into the one dimension that "best" separates the classes

Projection onto line connecting the means

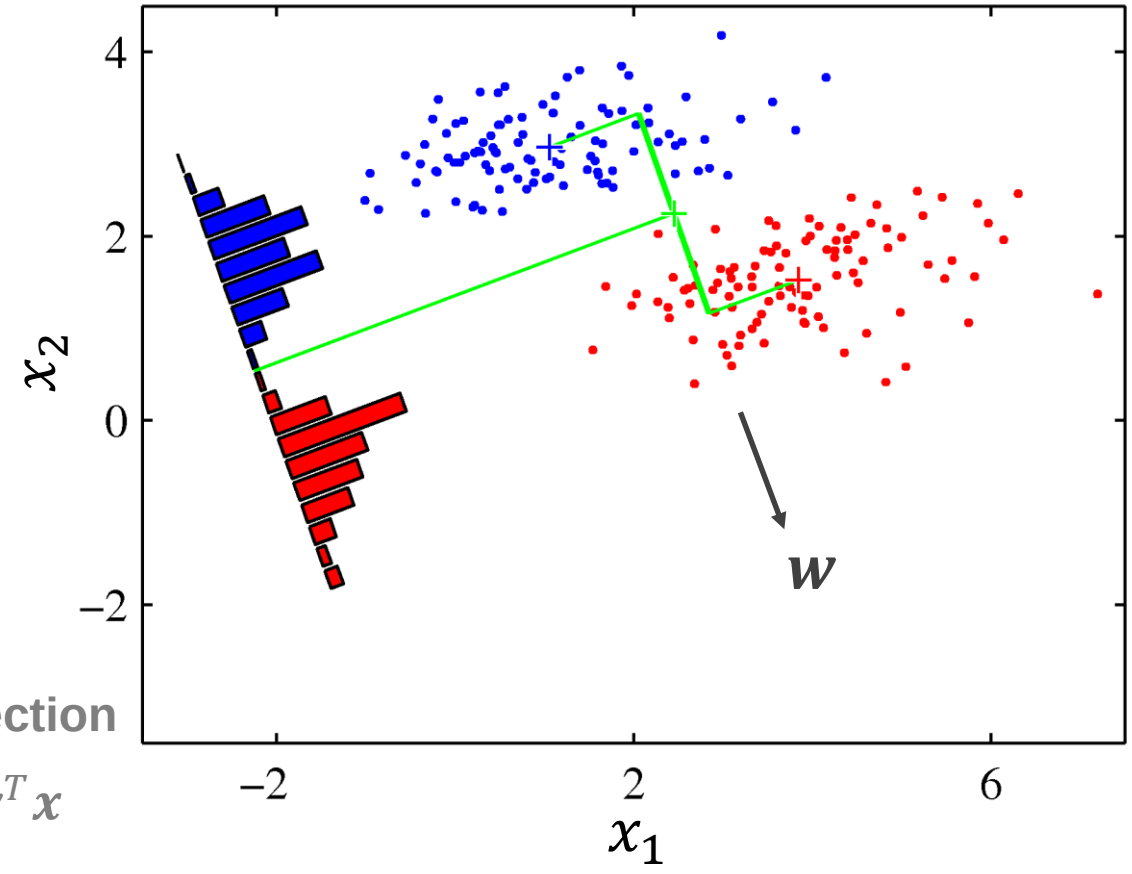


Bishop, Pattern Recognition, 2006

Linear projection

$$\hat{f}(x) = w^T x$$

Projection onto a line providing improved class separation



Fisher's Linear Discriminant (FLD)

1. Finds a projection into a lower dimension that "best" separates the classes

$$\hat{f}(\boldsymbol{x}) = \boldsymbol{w}^T \boldsymbol{x}$$

Consider $\boldsymbol{w}$ is a unit vector of parameters

2. We then classify the data in this space

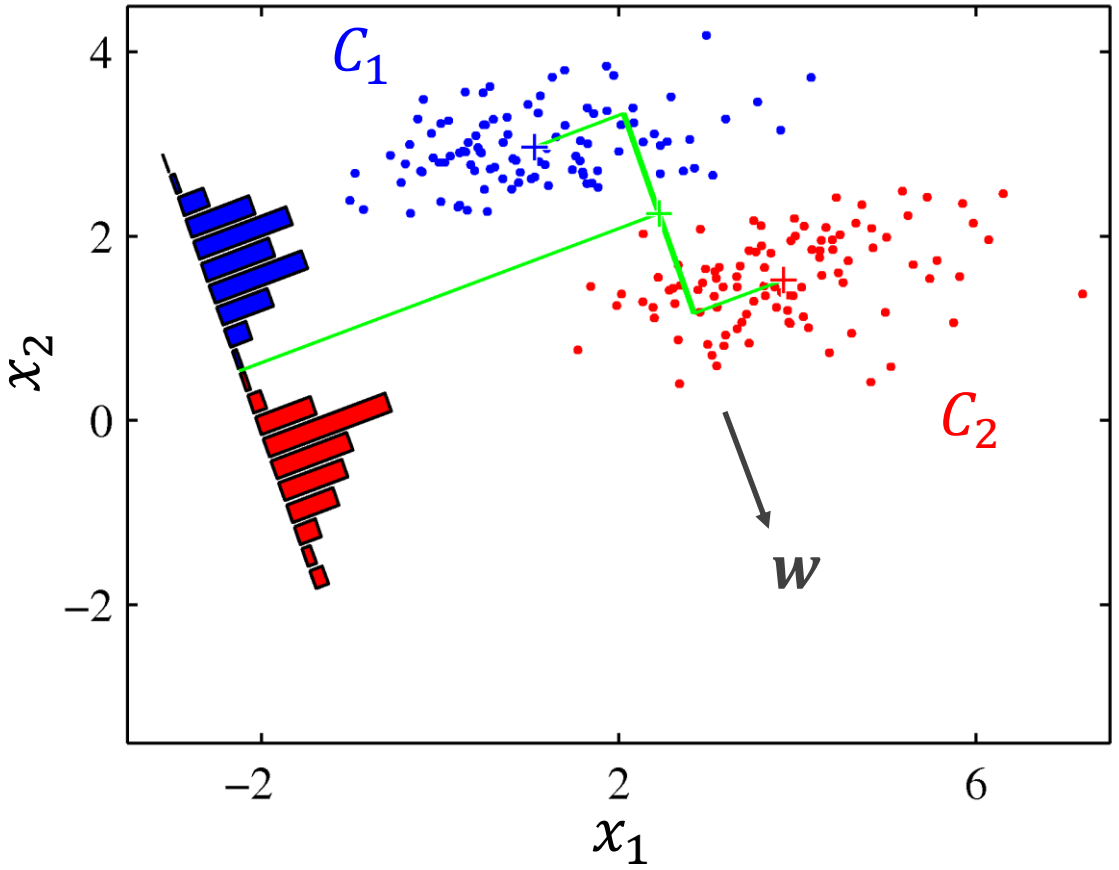
Similar to PCA, but accounts for class separability

Our decision rule becomes:

$$\text{if} \quad \hat{f}(\boldsymbol{x}) = \boldsymbol{w}^T \boldsymbol{x} > \lambda_{thresh} \qquad \text{Class 1}$$

$$\text{else} \qquad \text{Class 2}$$

FLD: how do we choose the vector w?

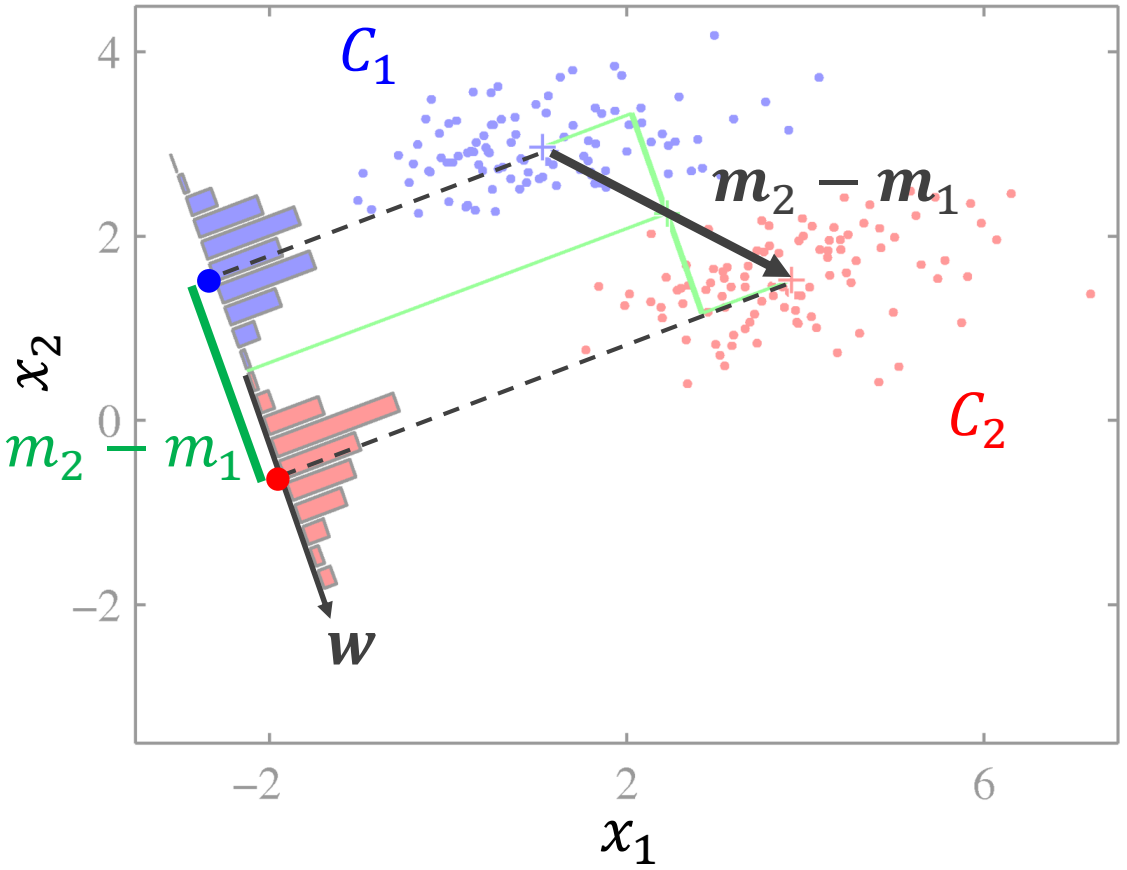


$$y = \hat{f}(\boldsymbol{x}) = \boldsymbol{w}^T \boldsymbol{x}$$

Increase the distance between the **means**

Decrease the **variance** within each class

FLD: how do we choose the vector w?



$$y = \hat{f}(\boldsymbol{x}) = \boldsymbol{w}^T \boldsymbol{x}$$

Increase the distance between the **means**

$$\boldsymbol{m}_1 = \frac{1}{N_1} \sum_{i \in C_1} \boldsymbol{x}_i$$

mean of class 1

$$\boldsymbol{m}_2 = \frac{1}{N_2} \sum_{i \in C_2} \boldsymbol{x}_i$$

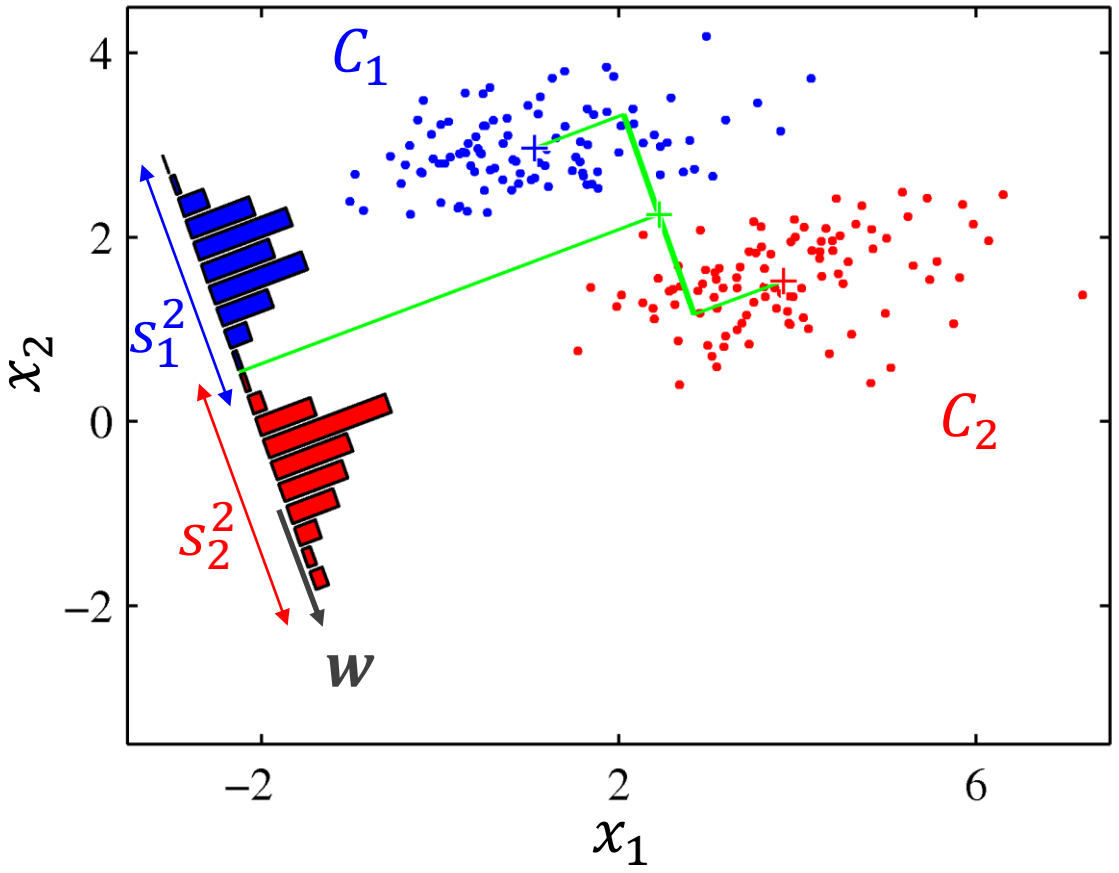
mean of class 2

The means projected onto $\boldsymbol{w}$: $m_k = \boldsymbol{w}^T \boldsymbol{m}_k$

The distance between the means:

$$m_2 - m_1 = \boldsymbol{w}^T (\boldsymbol{m}_2 - \boldsymbol{m}_1)$$

FLD: how do we choose the vector w?



$$y = \hat{f}(\boldsymbol{x}) = \boldsymbol{w}^T \boldsymbol{x}$$

Decrease the **variance** within each class

The "scatter" of the **projected** data:

$$s_k^2 = \sum_{i \in C_k} (y_i - m_k)^2$$

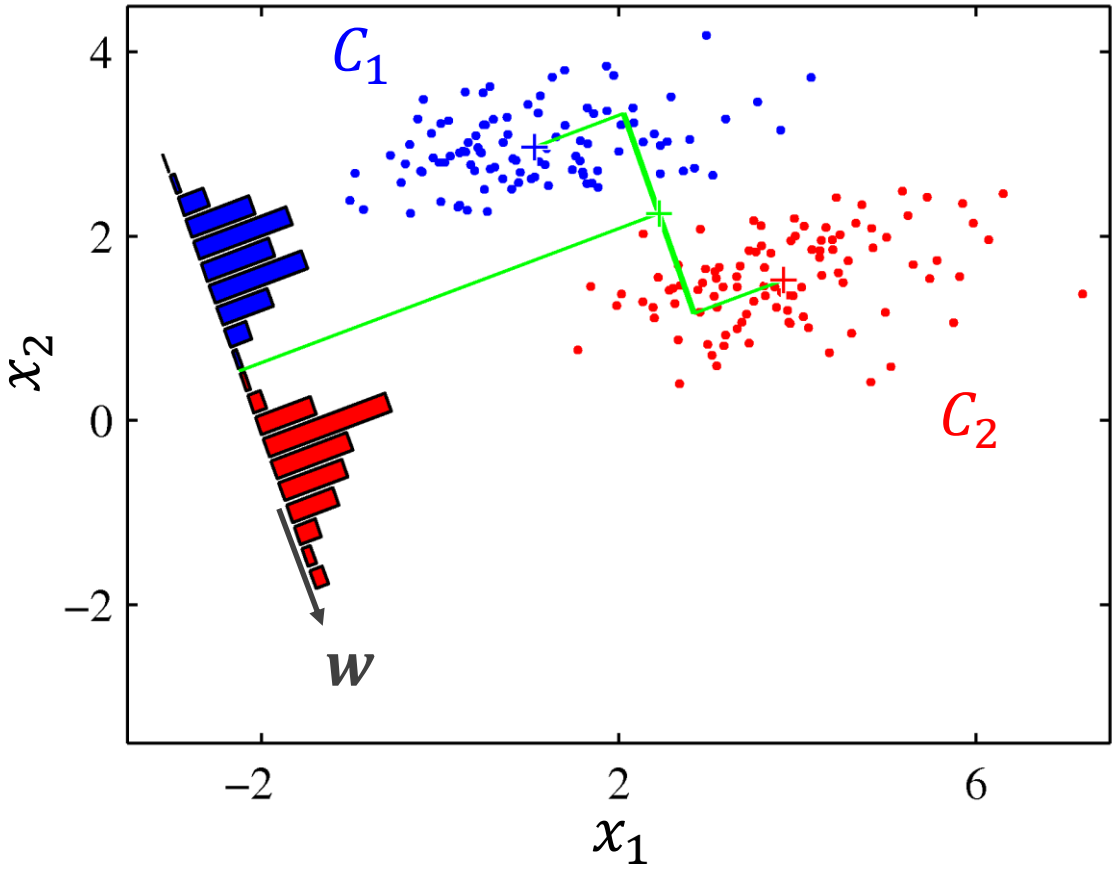
where $m_k = \boldsymbol{w}^T \boldsymbol{m}_k$

$y_i = \boldsymbol{w}^T \boldsymbol{x}_i$

Therefore the total within-class scatter:

$$S = s_1^2 + s_2^2$$

FLD: how do we choose the vector w?



$$y = \hat{f}(\boldsymbol{x}) = \boldsymbol{w}^T \boldsymbol{x}$$

Increase the distance between the **means**

$$m_2 - m_1 = \boldsymbol{w}^T(\boldsymbol{m}_2 - \boldsymbol{m}_1)$$

Decrease the **variance** within each class

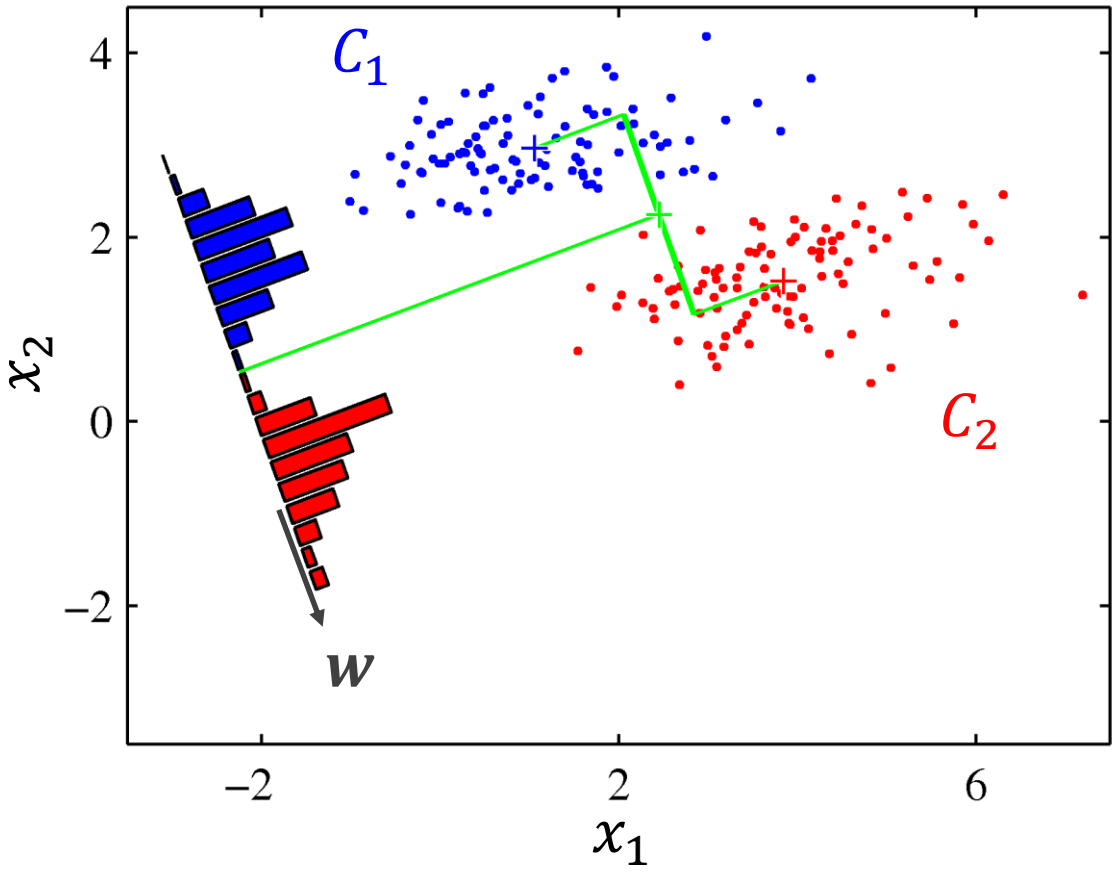
$$S = s_1^2 + s_2^2$$

The Fisher criterion is then:

$$J(\boldsymbol{w}) = \frac{(m_2 - m_1)^2}{s_1^2 + s_2^2}$$

We want to maximize this and solve for $\boldsymbol{w}$

FLD: how do we choose the vector $\boldsymbol{w}$?



$$y = \hat{f}(\boldsymbol{x}) = \boldsymbol{w}^T \boldsymbol{x}$$

We want to maximize this and solve for $\boldsymbol{w}$

$$J(\boldsymbol{w}) = \frac{(m_2 - m_1)^2}{s_1^2 + s_2^2}$$

$$= \frac{\boldsymbol{w}^T \boldsymbol{S}_B \boldsymbol{w}}{\boldsymbol{w}^T \boldsymbol{S}_W \boldsymbol{w}}$$

(see appendix slides for full derivation)

Take the derivative (gradient), set it equal to zero, solve for $\boldsymbol{w}$

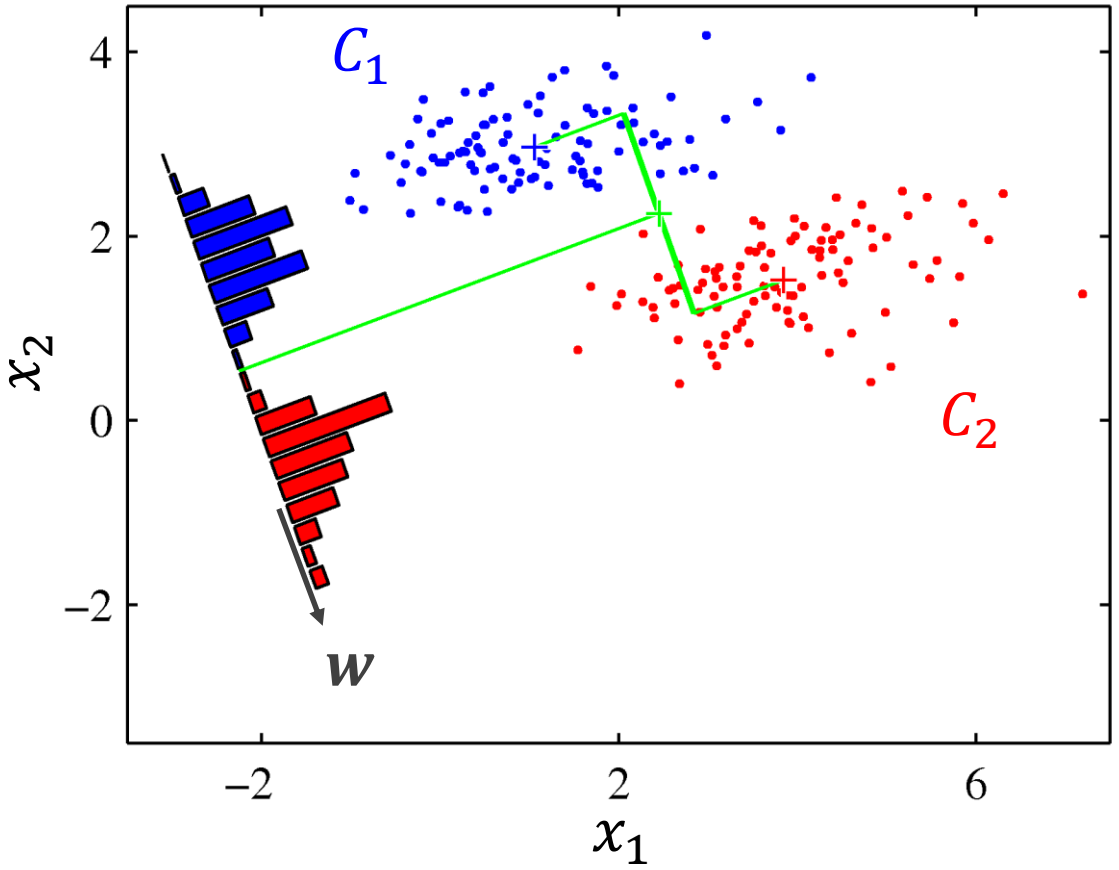
(see appendix slides for full derivation)

$$\boldsymbol{w} \propto \boldsymbol{S}_W^{-1}(\boldsymbol{m}_2 - \boldsymbol{m}_1)$$

$$\boldsymbol{w} \propto (\boldsymbol{\Sigma}_1 + \boldsymbol{\Sigma}_2)^{-1}(\boldsymbol{m}_2 - \boldsymbol{m}_1)$$

We use this to project the features into one dimension for classification, $\boldsymbol{w}^T \boldsymbol{x}$

Fisher's Linear Discriminant



$$y = \hat{f}(\boldsymbol{x}) = \boldsymbol{w}^T \boldsymbol{x}$$

No assumptions about the distribution of the data and allows for different covariance matrices for each class

Only applicable for 2 classes

This is a **projection** into one dimension that can be used to construct a discriminant (a classifier)

$$\boldsymbol{w} \propto \boldsymbol{S}_W^{-1}(\boldsymbol{m}_2 - \boldsymbol{m}_1)$$

$$\boldsymbol{w} \propto (\Sigma_1 + \Sigma_2)^{-1}(\boldsymbol{m}_2 - \boldsymbol{m}_1)$$

Bayes rule in the context of classification

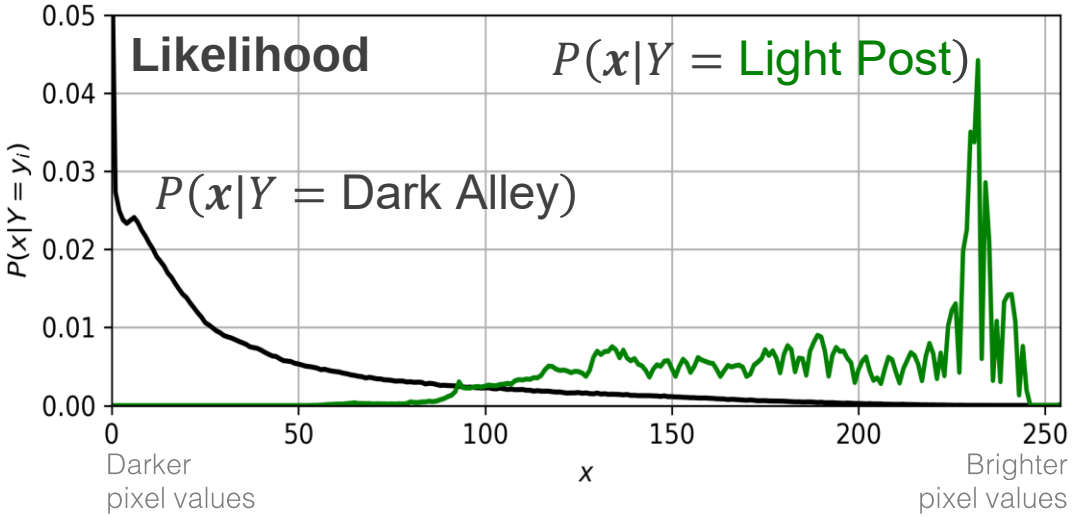
Class 1: Light Post

Class 0: Dark Alley

Randomly draw a pixel from either of the images: $x_i = 149$

Darker pixel values are lower numbers (closer to 0), brighter pixels are higher numbers (closer to 255)

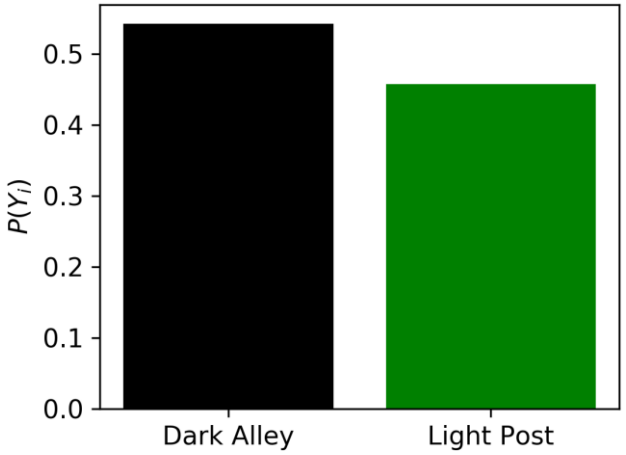
How do we determine which image it was most likely to have come from?



Class 1: Light Post y_1

Class 0: Dark Alley y_0

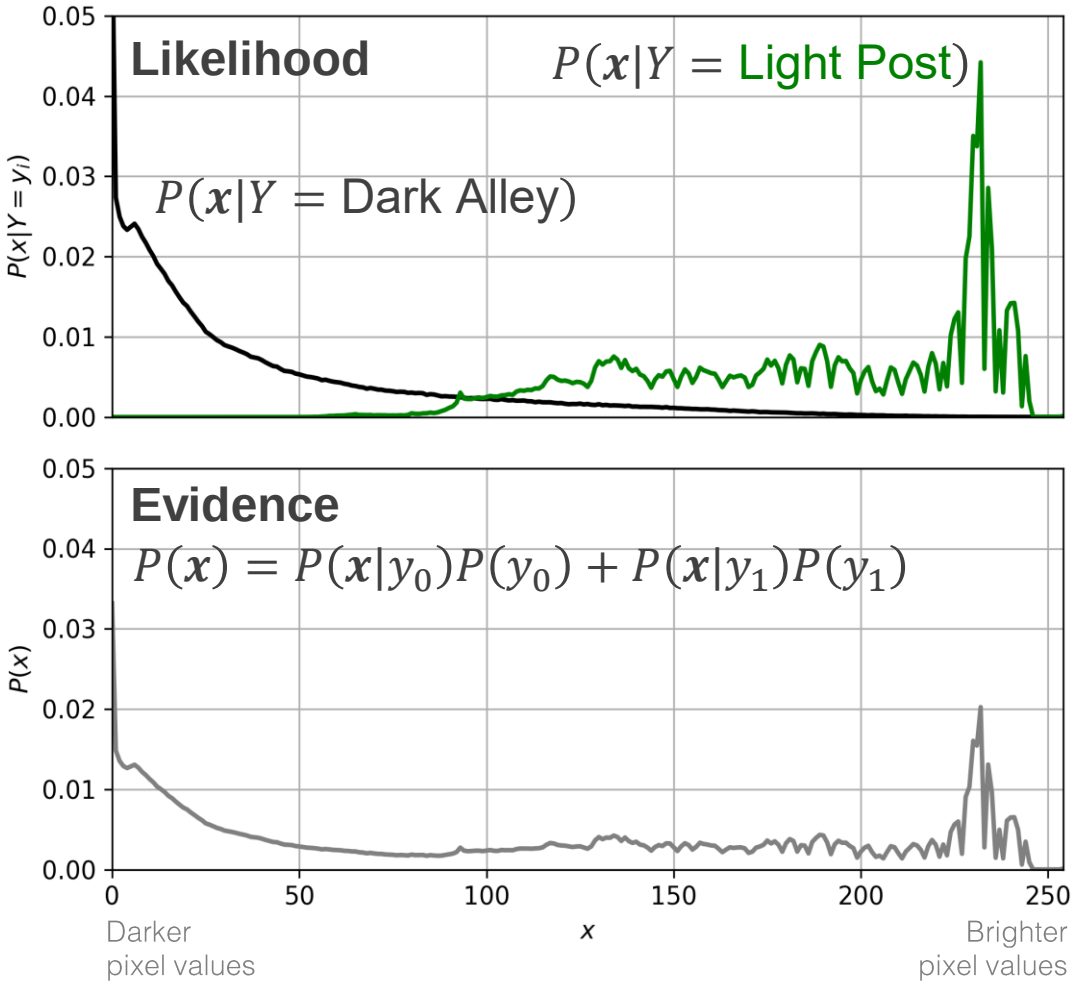
Prior: $P(Y = y_i)$



Bayes' Rule

$$P(Y = y_i|\boldsymbol{x}) = \frac{P(\boldsymbol{x}|Y = y_i)P(Y = y_i)}{P(\boldsymbol{x})}$$

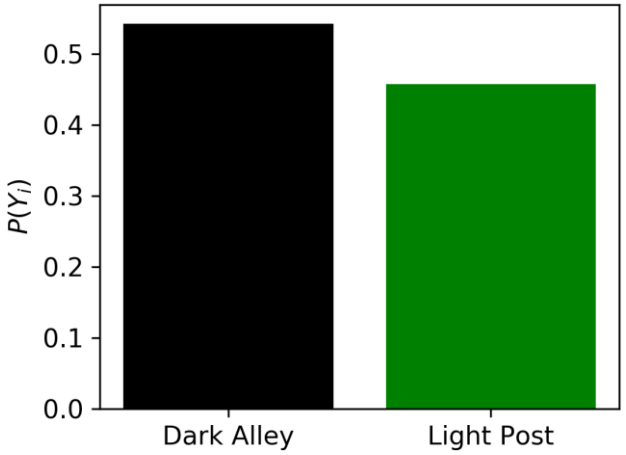
Posterior: $P(Y = y_i|\boldsymbol{x})$ — Likelihood: $P(\boldsymbol{x}|Y = y_i)$ — Prior: $P(Y = y_i)$ — Evidence: $P(\boldsymbol{x})$



Class 1: Light Post y_1

Class 0: Dark Alley y_0

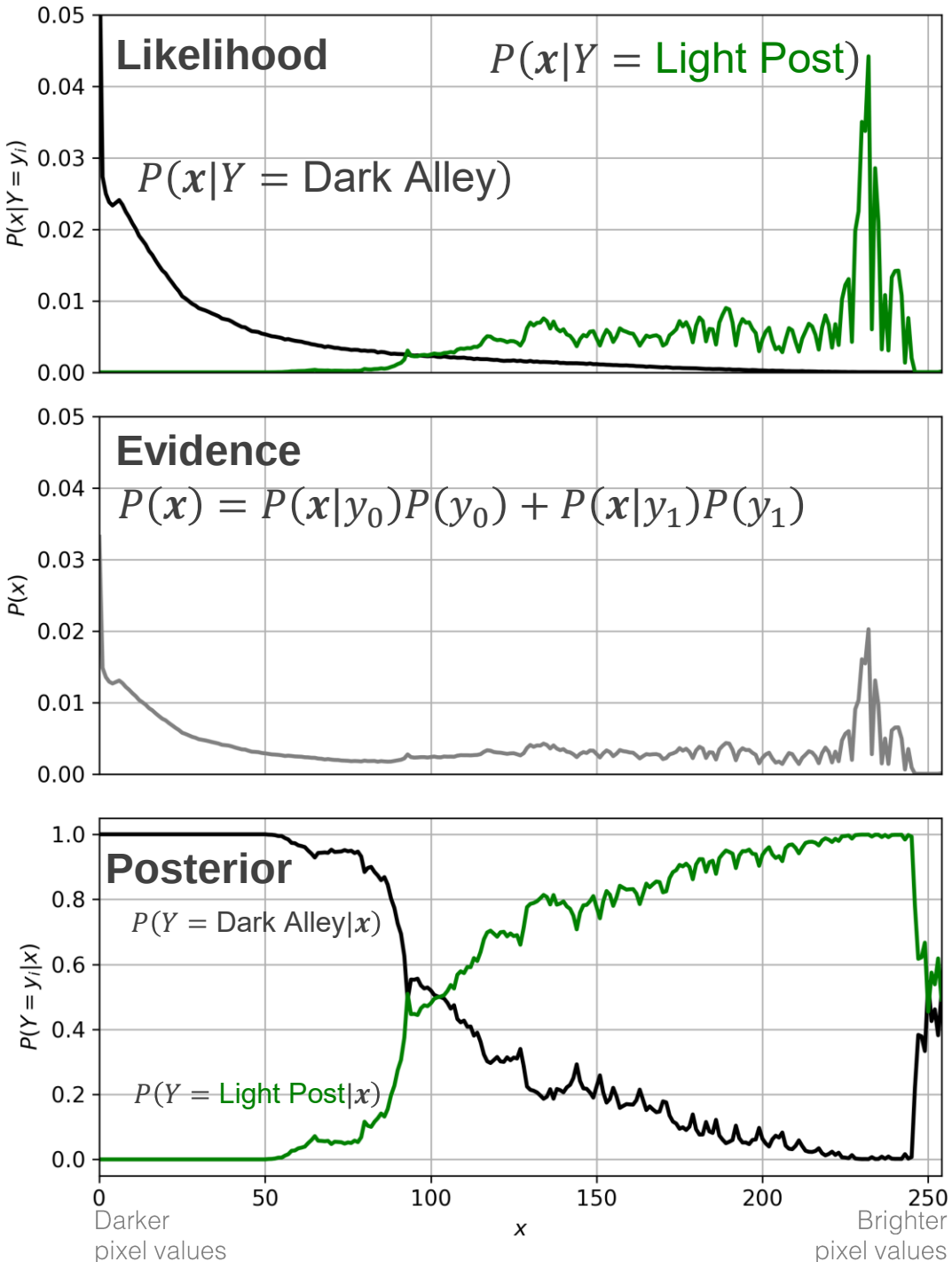
Prior: $P(Y = y_i)$



Bayes' Rule

$$P(Y = y_i|\boldsymbol{x}) = \frac{P(\boldsymbol{x}|Y = y_i)P(Y = y_i)}{P(\boldsymbol{x})}$$

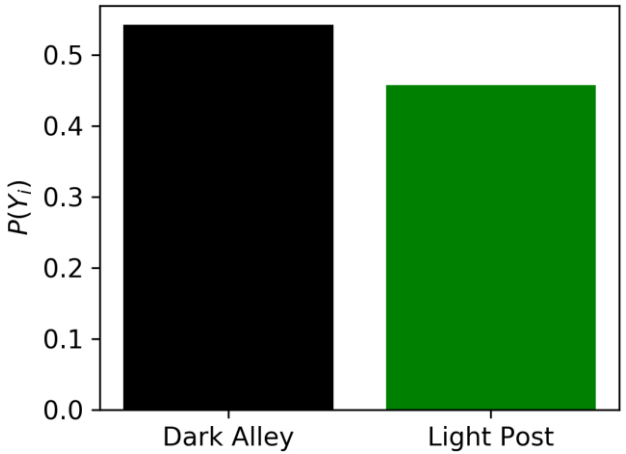
Posterior: $P(Y = y_i|\boldsymbol{x})$; Likelihood: $P(\boldsymbol{x}|Y = y_i)$; Prior: $P(Y = y_i)$; Evidence: $P(\boldsymbol{x})$



Class 1: Light Post y_1

Class 0: Dark Alley y_0

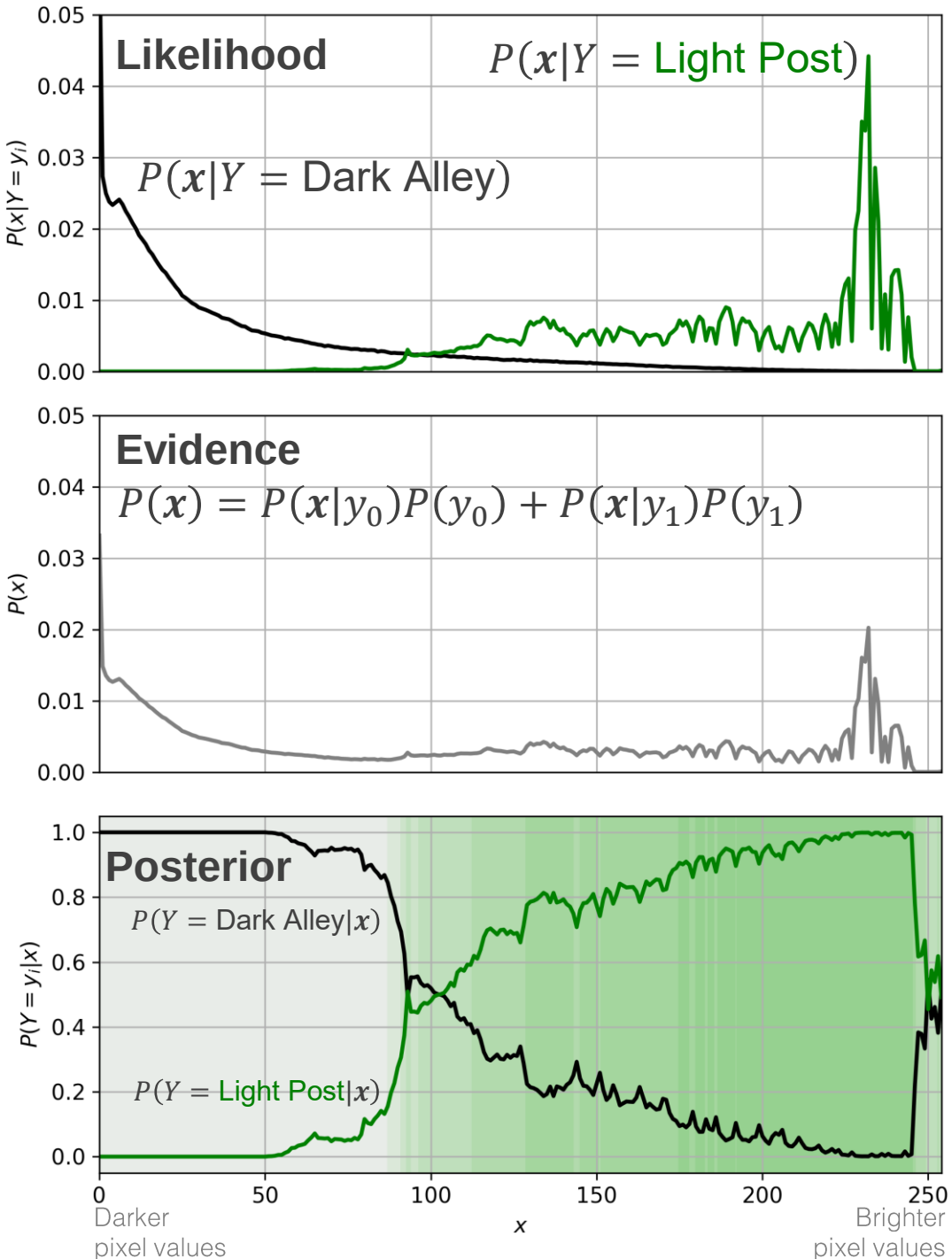
Prior: $P(Y = y_i)$



Bayes' Rule

$$P(Y = y_i|\boldsymbol{x}) = \frac{\overbrace{P(\boldsymbol{x}|Y = y_i)}^{\text{Likelihood}}\overbrace{P(Y = y_i)}^{\text{Prior}}}{\underbrace{P(\boldsymbol{x})}_{\text{Evidence}}}$$

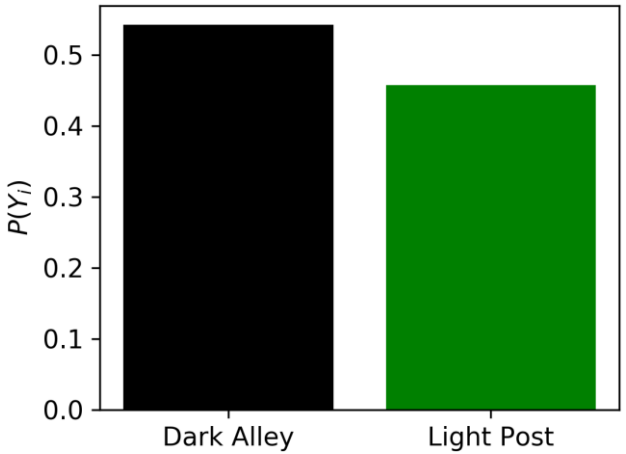
Posterior



Class 1: Light Post y_1

Class 0: Dark Alley y_0

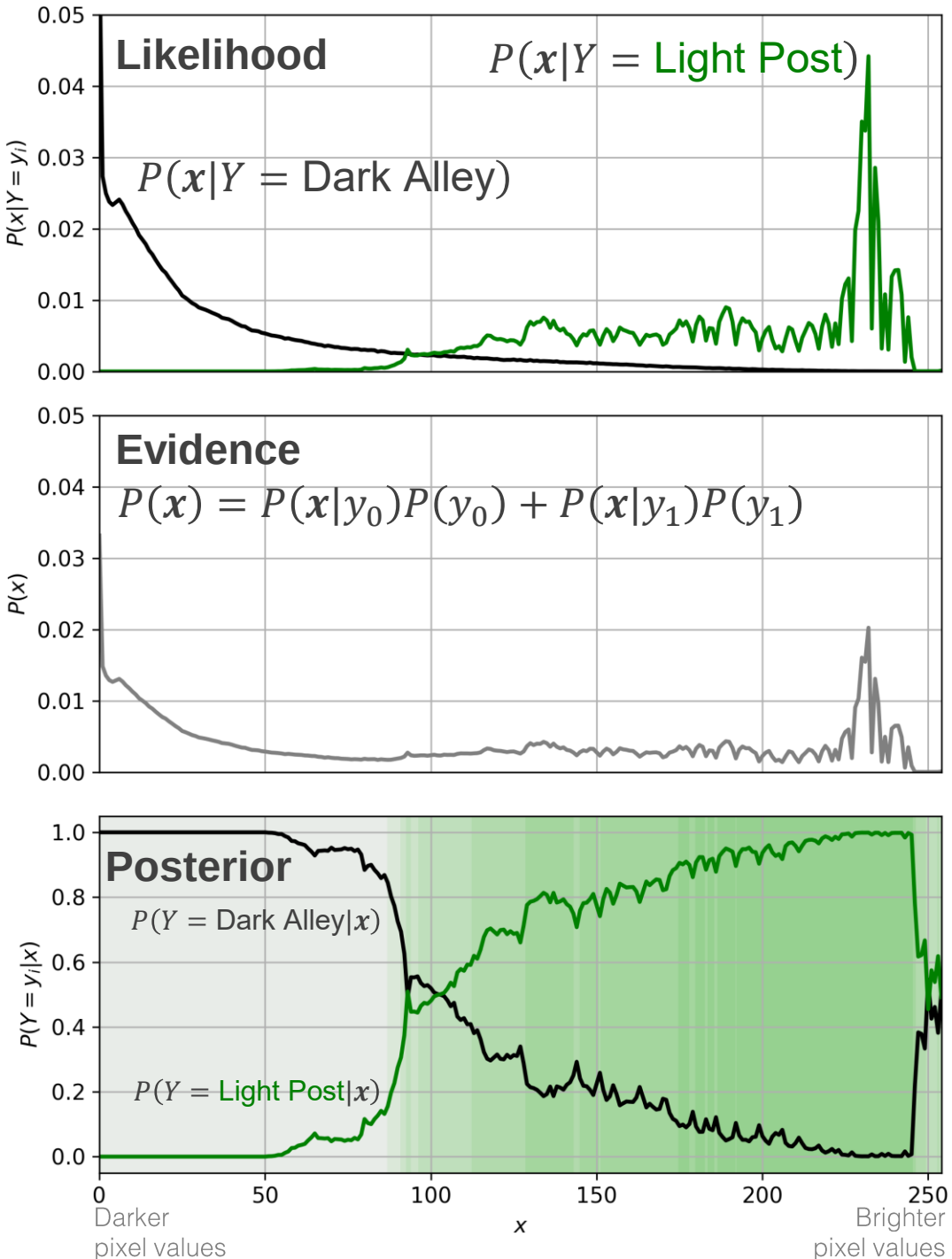
Prior: $P(Y = y_i)$



Decision rule:

If $P(Y = \text{Light Post}|x) > P(Y = \text{Dark Alley}|x)$ then Light Post

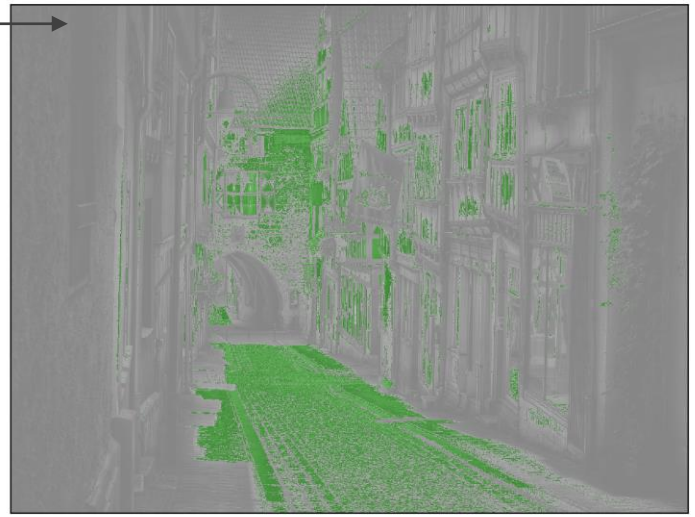
else Dark Alley



Class 1: Light Post y_1

Class 0: Dark Alley y_0

Green = classified as from Light Post
Grey = classified as from Dark Alley

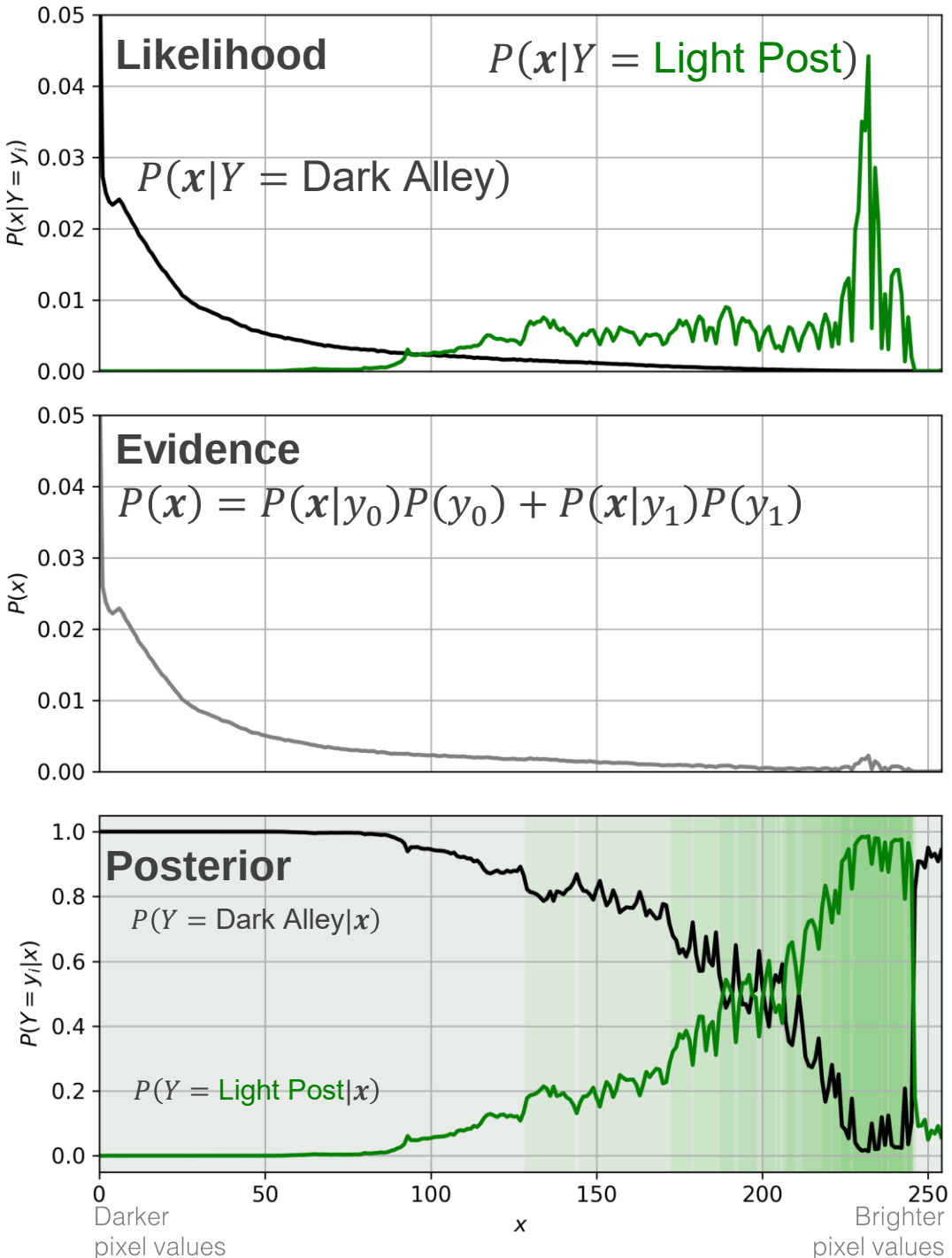


Classifying each of the individual pixels as being either from **Light Post** or **Dark Alley** results in classification above

Decision rule:

If $P(Y = \text{Light Post}|x) > P(Y = \text{Dark Alley}|x)$ then Light Post

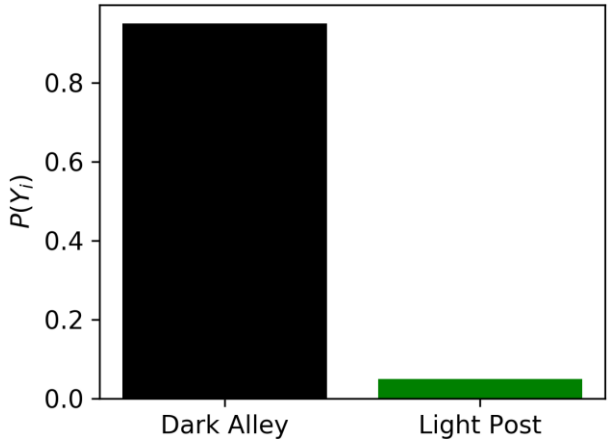
else Dark Alley



Class 1: Light Post y_1

Class 0: Dark Alley y_0

Prior: $P(Y = y_i)$

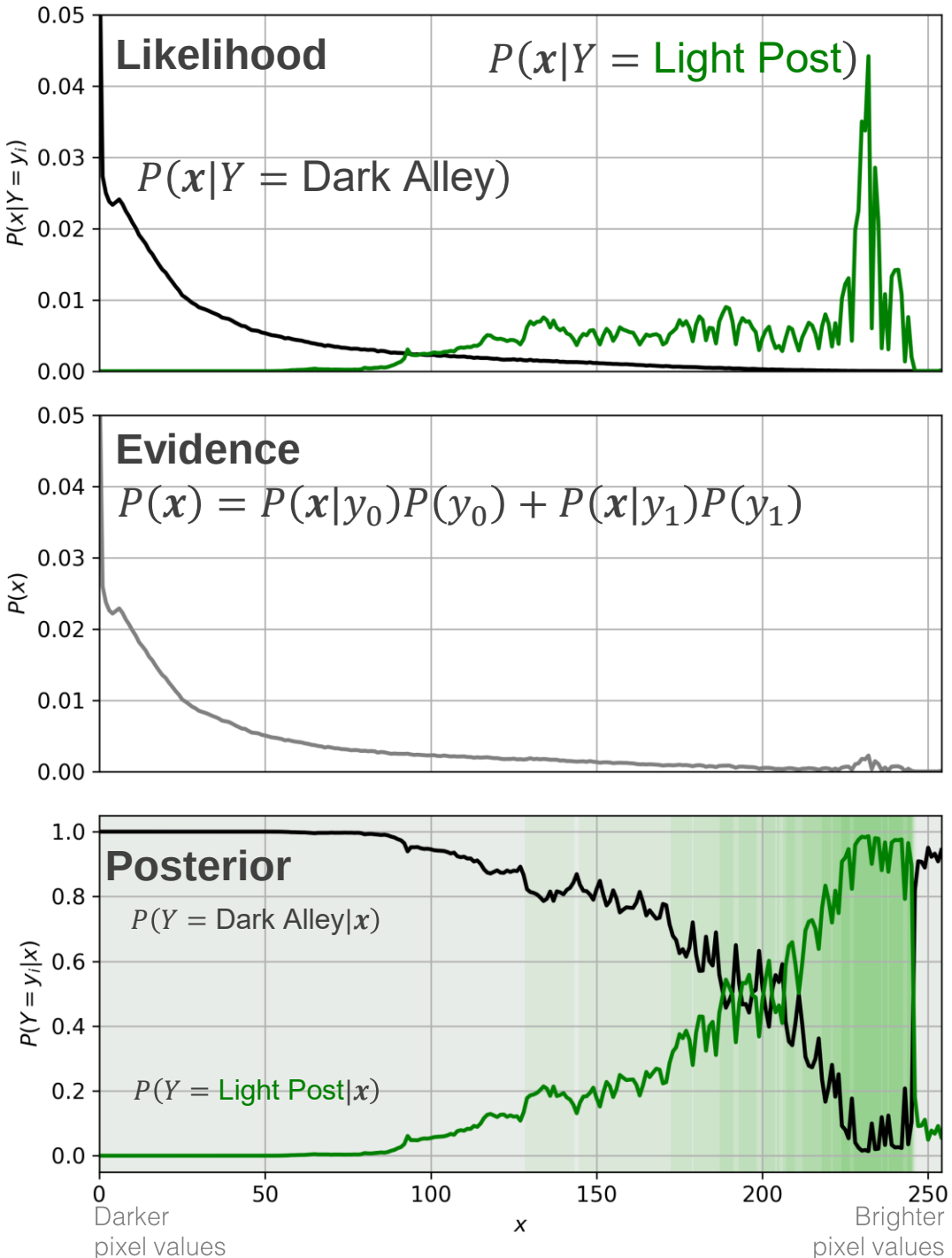


Let's assume the sampling of pixels occurred more from the **Dark Alley**

Bayes' Rule

$$P(Y = y_i|\boldsymbol{x}) = \frac{\overbrace{P(\boldsymbol{x}|Y = y_i)}^{\text{Likelihood}}\overbrace{P(Y = y_i)}^{\text{Prior}}}{\underbrace{P(\boldsymbol{x})}_{\text{Evidence}}}$$

Posterior

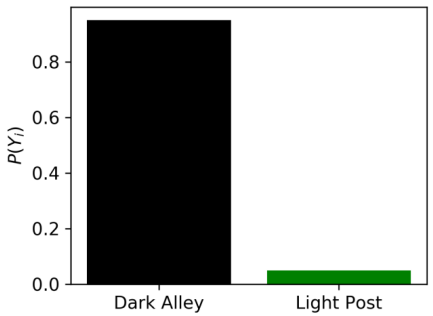


Class 1: Light Post y_1

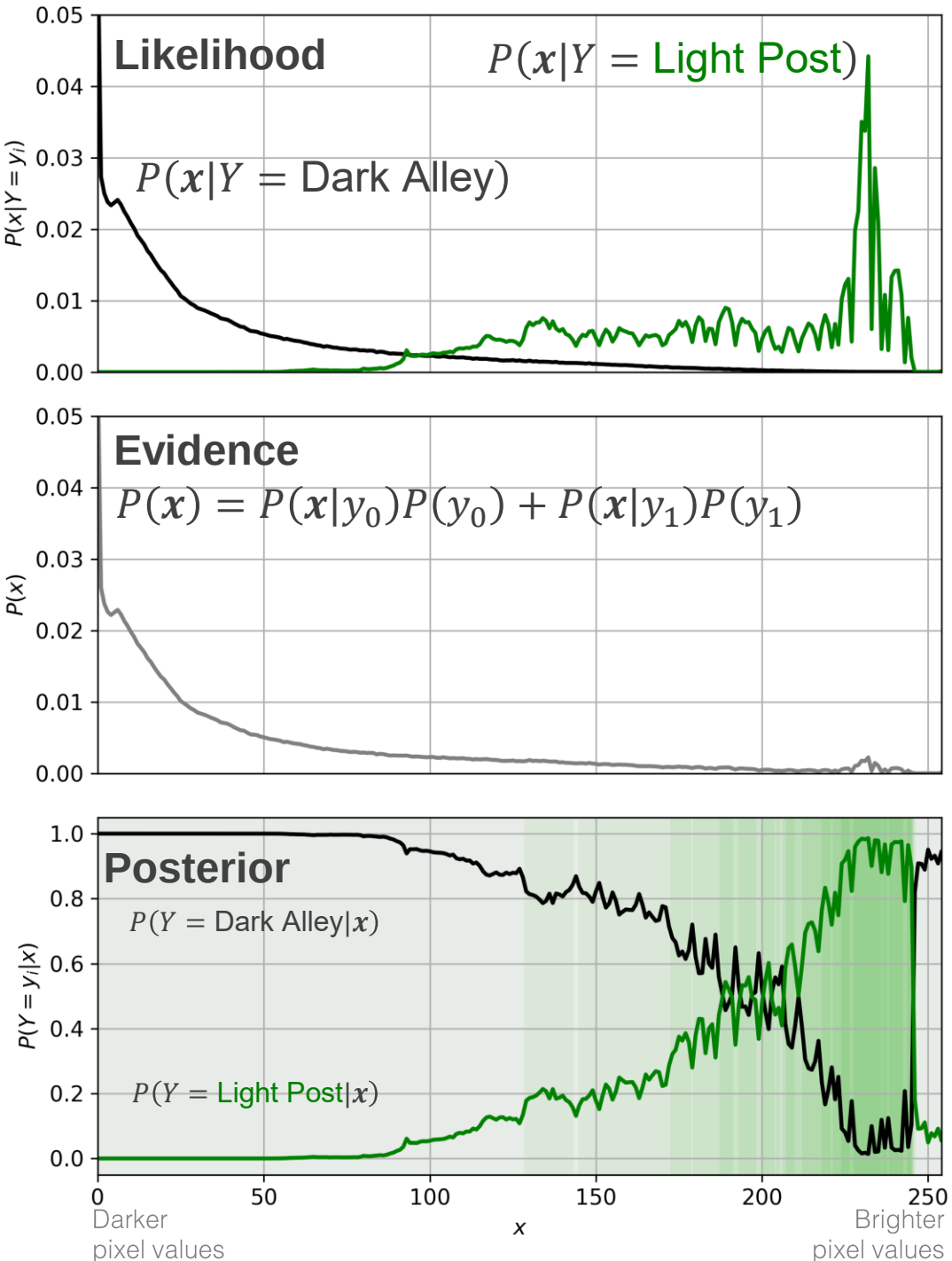
Class 0: Dark Alley y_0

Green = classified as from Light Post
Grey = classified as from Dark Alley

Prior: $P(Y = y_i)$



Assuming we the sampling of pixels occurred more from the **Dark Alley**



Generative models model the **likelihood**

These can also be used to generate synthetic data

$$\text{Posterior}\quad P(Y = y_i|x) = \frac{\overbrace{P(x|Y = y_i)}^{\text{Likelihood}}\overbrace{P(Y = y_i)}^{\text{Prior}}}{\underbrace{P(x)}_{\text{Evidence}}}$$

Discriminative models model the **posterior**

Or they just directly estimate labels without a probabilistic interpretation, $f(x) \rightarrow y$

Discriminant Functions

Assume we have c **different classes**

Define the **posterior probability** as a discriminant function: $d_i(x) = P(y = i|\boldsymbol{x})$

For a new sample, classify it as the class with the **largest** $d_i(x)$

Discriminant Functions

If we have c different classes, we define a discriminant function, $d_i(\boldsymbol{x})$ for $i = 1, \ldots, c$

If $d_i(\boldsymbol{x}) > d_j(\boldsymbol{x})$ for $i \neq j$, then we assign feature $\boldsymbol{x}$ to class i

$$d_i(x) = P(y = i|\boldsymbol{x}) = \frac{P(\boldsymbol{x}|y = i)P(y = i)}{P(\boldsymbol{x})}$$

Bayes' Rule: $P(Y|\boldsymbol{X}) = \frac{P(\boldsymbol{X}|Y)P(Y)}{P(\boldsymbol{X})}$

Likelihood, Prior, Posterior, Evidence

$$= \frac{P(\boldsymbol{x}|y = i)P(y = i)}{\sum_{i=1}^{c} P(\boldsymbol{x}|y = i)P(y = i)}$$

Denominator is the same for all classes i, so it won't help us tell which class's posterior is higher relative to other classes, so we ignore it going forward

We can simply write $d_i(x) = P(\boldsymbol{x}|y = i)P(y = i)$

Or in log form: $\ln d_i(x) = \ln P(\boldsymbol{x}|y = i) + \ln P(y = i)$

If we know the **true likelihood and prior** for our data, this process yields our **Bayes' classifier** (minimum misclassification error classifier)

Discriminant Functions

$$d_i(x) = P(y = i|\boldsymbol{x}) = P(\boldsymbol{x}|y = i)P(y = i)$$

Or in log form:

$$d_i(x) = \ln P(\boldsymbol{x}|y = i) + \ln P(y = i)$$

Equally valid discriminant functions since log is monotonic

1. Assume a form for $P(\boldsymbol{x}|y = i)$

   Gaussian for Linear and Quadratic Discriminant Analysis
   Gaussian mixture models
   Nonparametric density estimates
   Naïve Bayes models

2. Assign the class, i, for which $d_i(x)$ is largest

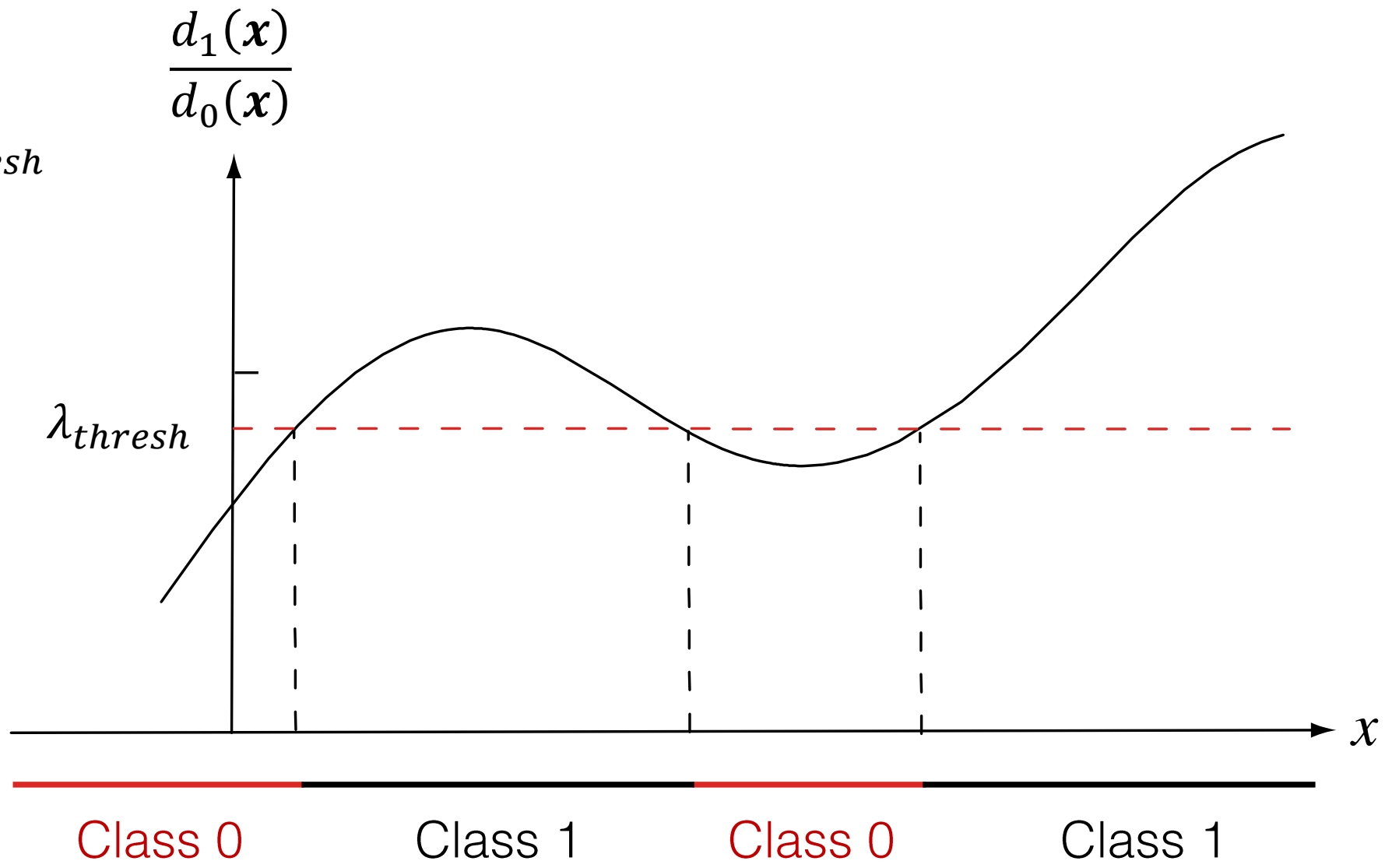
   Applies to both binary and multiclass problems

Discriminant Functions: 2 classes

Decision rule:

Class 1 if: $\frac{d_1(\boldsymbol{x})}{d_0(\boldsymbol{x})} > \lambda_{thresh}$

Otherwise, class 0



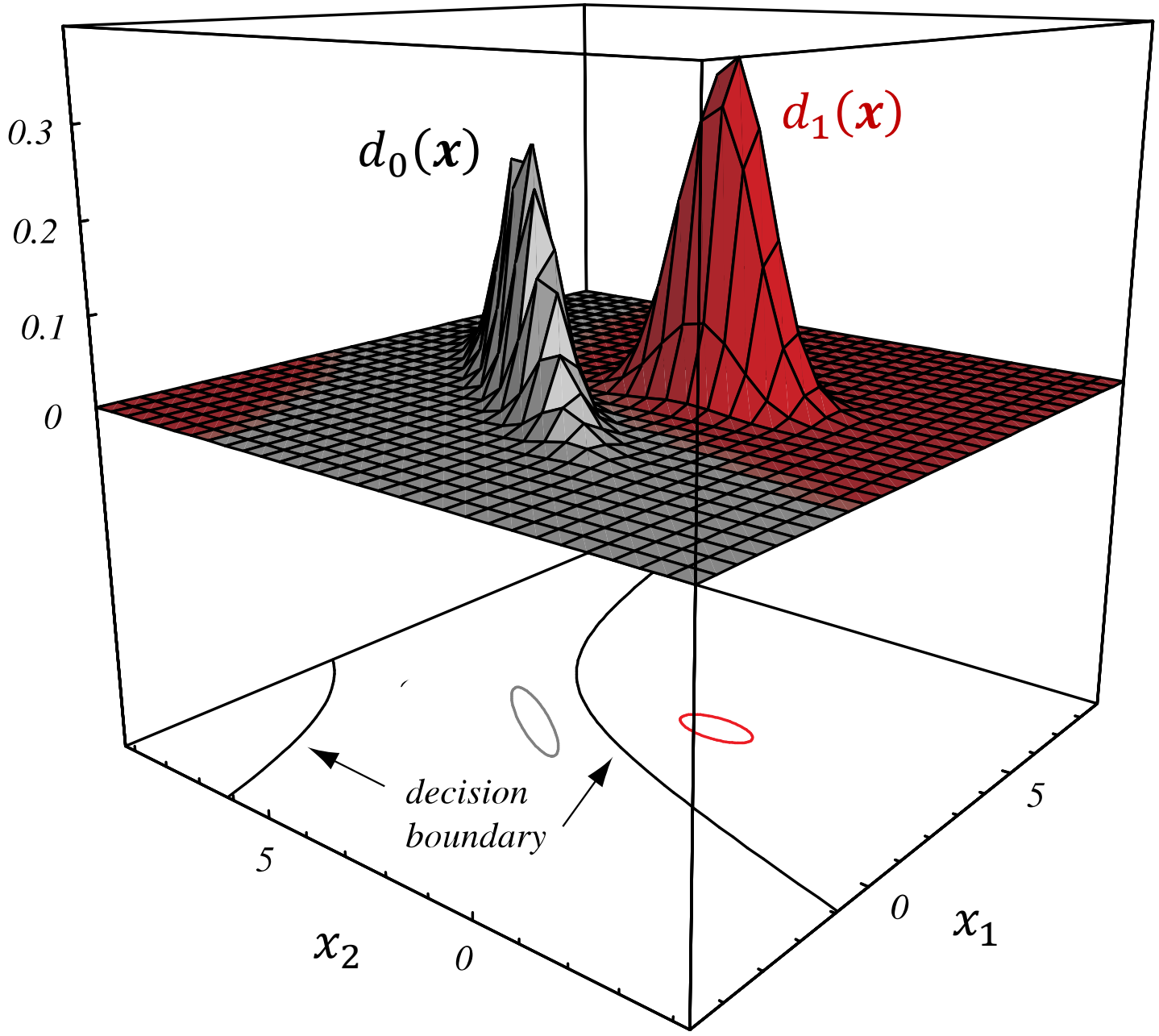
Duda, Hart, and Stork, Pattern Classification, 2006

Discriminant Functions: 2 classes, 2 dimensions

Decision rule:

Class 1 if: $\frac{d_1(\boldsymbol{x})}{d_0(\boldsymbol{x})} > \lambda_{thresh}$

Otherwise, class 0



Duda, Hart, and Stork, Pattern Classification, 2006

Discriminant Function: 2 classes

We build a classifier that assigns the class with the higher posterior probability:

If $$\frac{P(y=1|\boldsymbol{x})}{P(y=0|\boldsymbol{x})} = \frac{P(\boldsymbol{x}|y=1)P(y=1)}{P(\boldsymbol{x}|y=0)P(y=0)} > 1$$ Assign class 1, else class 0

Assumes these likelihoods are normal

$$\frac{P(\boldsymbol{x}|y=1)}{P(\boldsymbol{x}|y=0)} > \frac{P(y=0)}{P(y=1)}$$

$N(\mu_1, \Sigma_1)$

$N(\mu_0, \Sigma_0)$

Estimate the class-conditional mean and covariance matrix from the data

Discriminant Function: 2 classes

We build a classifier that assigns the class with the higher posterior probability:

Likelihood ratio:

$$\frac{P(\boldsymbol{x}|y=1)}{P(\boldsymbol{x}|y=0)} > \frac{P(y=0)}{P(y=1)}$$

$P(\boldsymbol{x}|y=1) \sim N(\mu_1, \Sigma_1)$

$P(\boldsymbol{x}|y=0) \sim N(\mu_0, \Sigma_0)$

If we assume the class conditional distributions are Gaussian, this represents

Quadratic Discriminant Analysis

If we further assume the covariance matrices are the same, $\Sigma_0 = \Sigma_1$, this represents

Linear Discriminant Analysis

Multivariate Gaussian

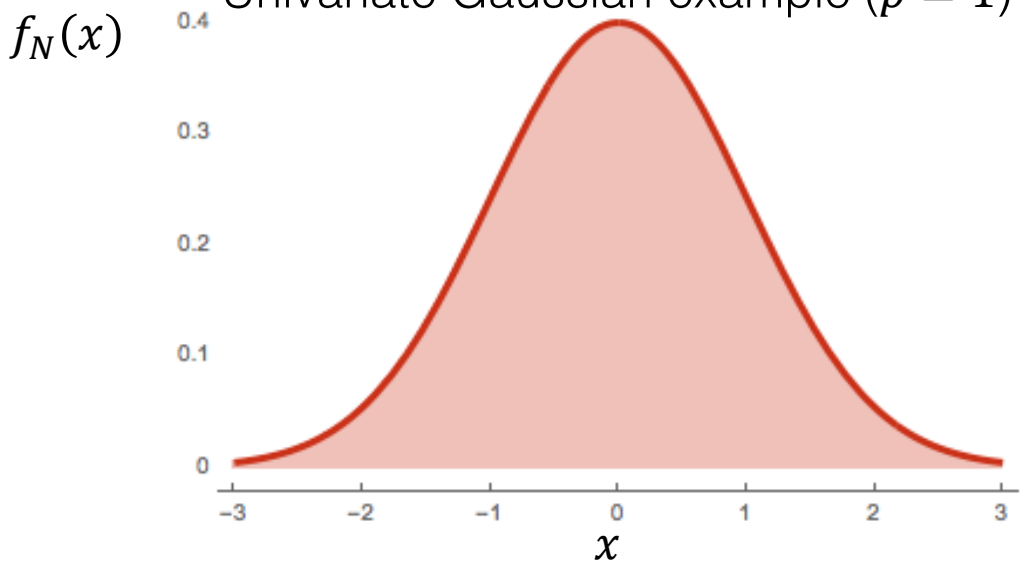
Univariate Gaussian (1 predictor)

$$f_N(x) = \frac{1}{(2\pi)^{1/2}\sigma}\exp\left[-\frac{1}{2\sigma^2}(x-\mu)^2\right]$$

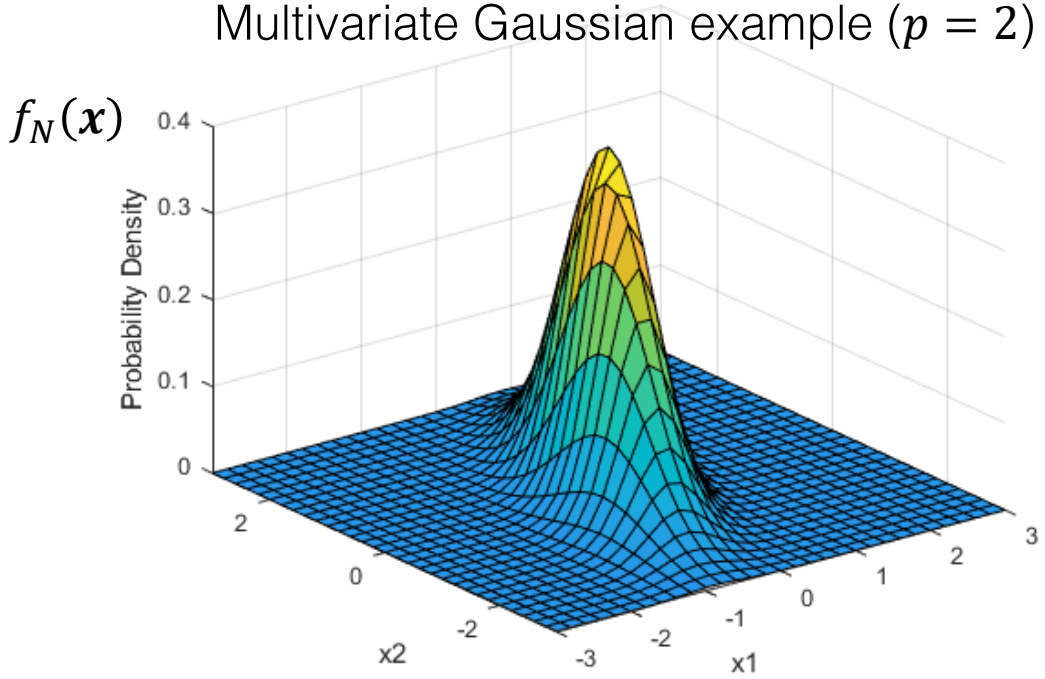
Multivariate Gaussian (p predictors)

$$f_N(\boldsymbol{x}) = \frac{1}{(2\pi)^{p/2}|\boldsymbol{\Sigma}|^{1/2}}\exp\left[-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^T\boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu})\right]$$

Univariate Gaussian example ($p = 1$)



Multivariate Gaussian example ($p = 2$)



Images from Brilliant.org (top) and the Mathworks (bottom)

Linear Discriminant Analysis: 2 Class

Σ is the same for both classes

$$\ln\left|\frac{P(\boldsymbol{x}|y=1)}{P(\boldsymbol{x}|y=0)}\right| = \boldsymbol{x}^T\boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_1-\boldsymbol{\mu}_0) - \frac{1}{2}(\boldsymbol{\mu}_1+\boldsymbol{\mu}_0)\boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_1-\boldsymbol{\mu}_0)$$

Since our decision rule is to classify as class 1 if the following is true:

$$\ln\left|\frac{P(\boldsymbol{x}|y=1)}{P(\boldsymbol{x}|y=0)}\right| > \ln\left|\frac{P(y=0)}{P(y=1)}\right|$$

We can rewrite our decision rule as:

(see appendix slides for full derivation)

$$\boldsymbol{x}^T\boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_1-\boldsymbol{\mu}_0) > \frac{1}{2}(\boldsymbol{\mu}_1+\boldsymbol{\mu}_0)\boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_1-\boldsymbol{\mu}_0) + \ln\left|\frac{P(y=0)}{P(y=1)}\right|$$

Or simply as:

$$\boldsymbol{x}^T\boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_1-\boldsymbol{\mu}_0) > \lambda_{thresh}$$

If we define $\boldsymbol{w} = \boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_1-\boldsymbol{\mu}_0)$, then this becomes $\boldsymbol{x}^T\boldsymbol{w} = \boldsymbol{w}^T\boldsymbol{x} > \lambda_{thresh}$

This approach is a supervised dimensionality reduction technique that we use for classification

Linear Discriminant Analysis: Multiclass

Σ is the same for all classes

We build a classifier that assigns the class with the higher posterior probability:

$$\delta_k(\boldsymbol{x}) = P(\boldsymbol{x}|y=k)P(y=k) = \frac{1}{(2\pi)^{d/2}|\boldsymbol{\Sigma}|^{1/2}} \exp\left[-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu}_k)^T\boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu}_k)\right]\pi_k \qquad P(y=k) \triangleq \pi_k$$

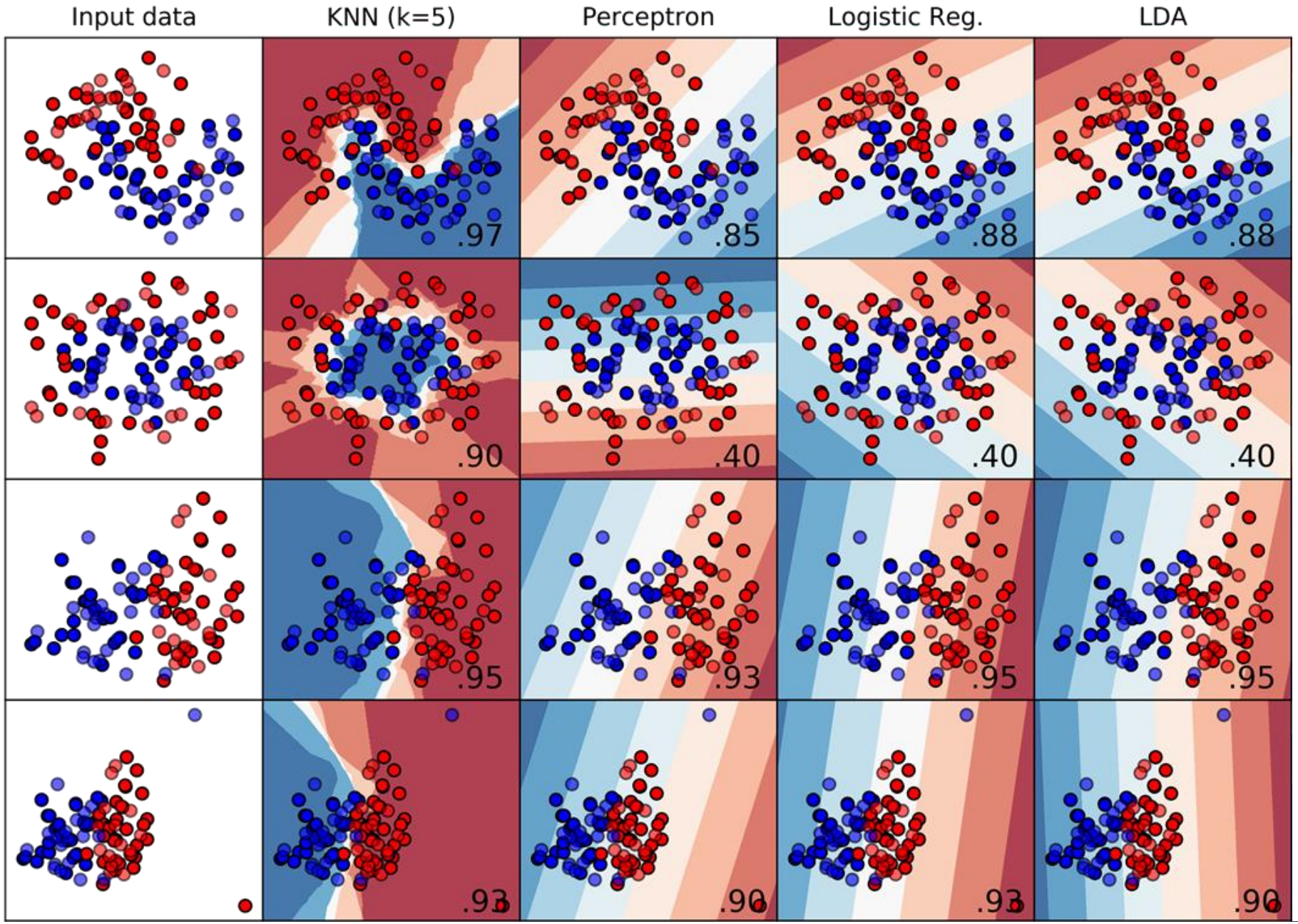
$$\ln|\delta_k(\boldsymbol{x})| = -\frac{p}{2}\ln|2\pi| - \frac{p}{2}\ln|\boldsymbol{\Sigma}| - \underbrace{\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu}_k)^T\boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu}_k)}_{-\frac{1}{2}[\boldsymbol{x}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{x} - 2\boldsymbol{x}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_k + \boldsymbol{\mu}_k{}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_k]} + \ln|\pi_k|$$

$$\ln|\delta_k(\boldsymbol{x})| = -\cancel{\frac{p}{2}\ln|2\pi|} - \cancel{\frac{p}{2}\ln|\boldsymbol{\Sigma}|} - \cancel{\frac{1}{2}\boldsymbol{x}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{x}} - \boldsymbol{x}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_k + \frac{1}{2}\boldsymbol{\mu}_k{}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_k + \ln|\pi_k|$$

$$\ln|\delta_k(\boldsymbol{x})| = -\boldsymbol{x}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_k + \frac{1}{2}\boldsymbol{\mu}_k{}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_k + \ln|\pi_k|$$

Since we'll be looking for the choice of class k that maximizes the value of $\delta_k(\boldsymbol{x})$, we can ignore terms that are independent of class

We compute this for each k and assign the class with the largest discriminant $\delta_k(\boldsymbol{x})$


Input data
KNN (k=5)
Perceptron
Logistic Reg.
LDA
.97
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.90
.93
.90

Quadratic Discriminant Analysis

We build a classifier that assigns the class with the higher posterior probability:

$$d_k(\boldsymbol{x}) = \frac{1}{(2\pi)^{d/2}|\boldsymbol{\Sigma}_k|^{1/2}} \exp\left[-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu}_k)^T \boldsymbol{\Sigma}_k^{-1}(\boldsymbol{x}-\boldsymbol{\mu}_k)\right]\pi_k$$

We assume a normal distribution, but **different covariance matrices**

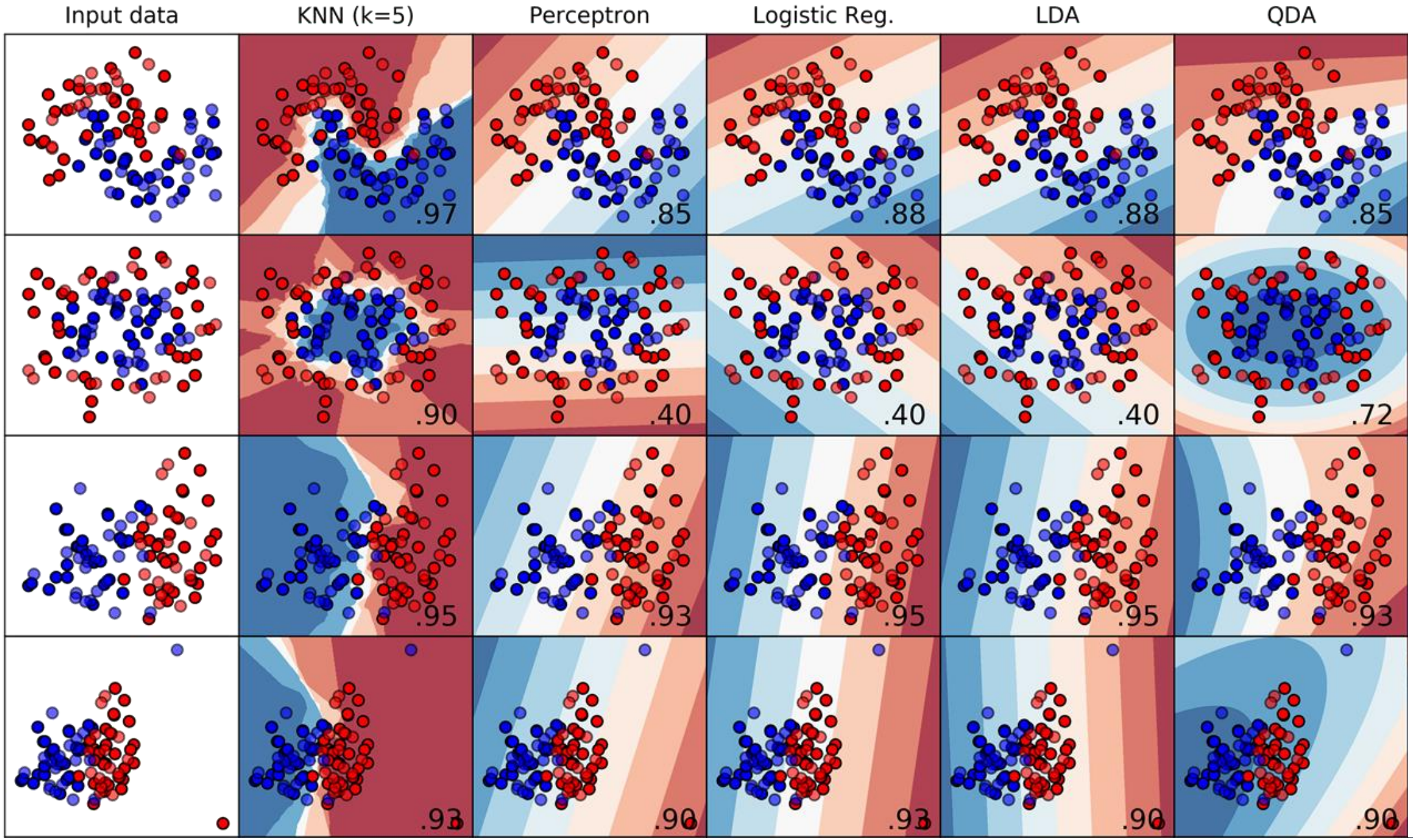
Produces a quadric decision boundary

Summary Comparison

	Fisher's Linear Discriminant (FLD)	Linear Discriminant Analysis (LDA)	Quadratic Discriminant Analysis (QDA)
Assumes Gaussian Likelihood $P(\boldsymbol{x}\|y)$ (class conditional density)	No	Yes	Yes
Assumes equivalent covariance matrices $\boldsymbol{\Sigma}_i = \boldsymbol{\Sigma}_j$	No	Yes	No

LDA & FLD reduce the dimensionality of the data to make them more separable

LDA and QDA easily extend to multiclass problems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Joint vs Marginal Densities

The marginal densities don't factor in relationships between features

What if the joint density is too hard to estimate?

Note: The plot in the middle is actually a scatterplot, but could be used to estimate $P(x_1, x_2|Y)$

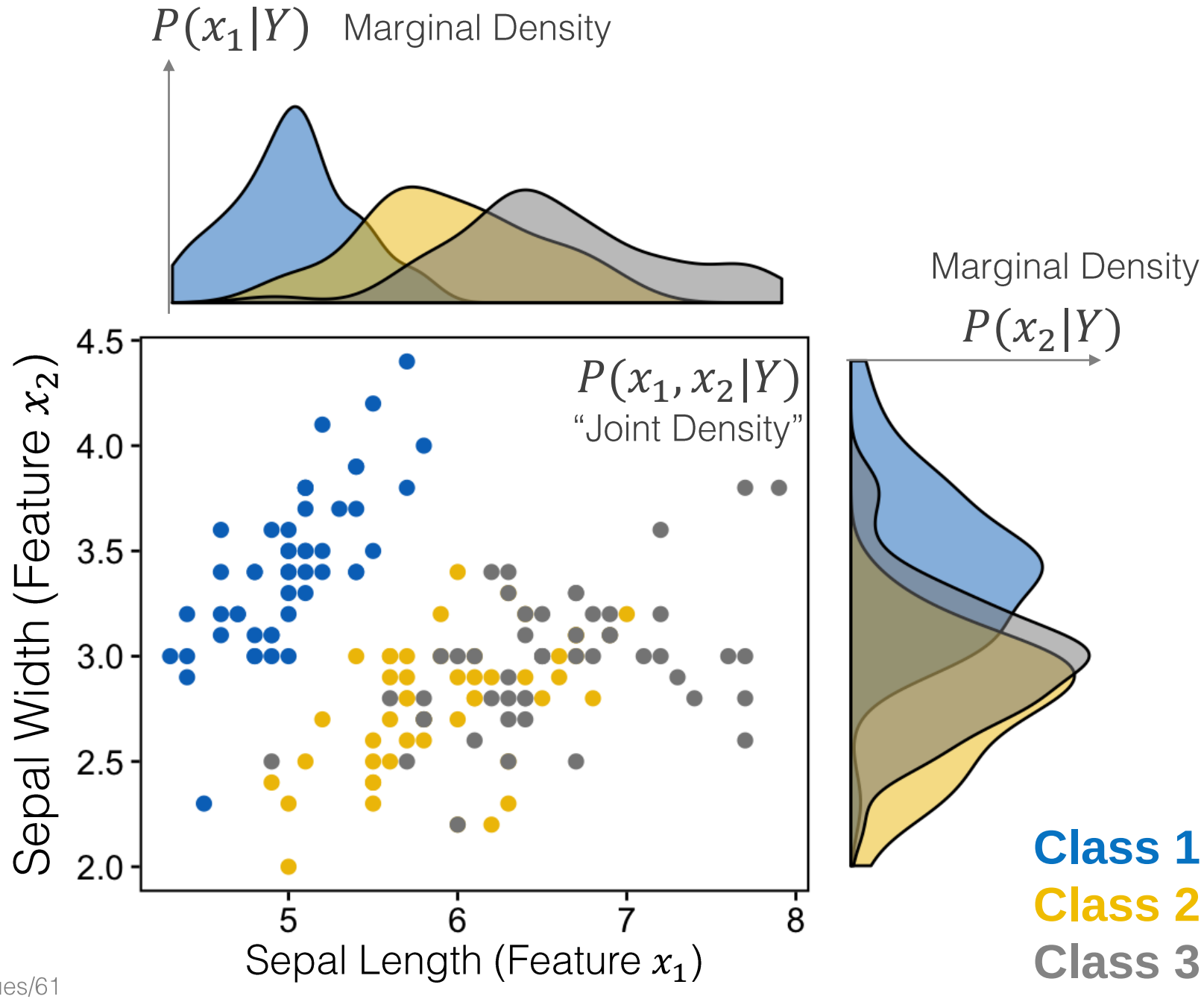


Image adapted from: https://github.com/daattali/ggExtra/issues/61

Naïve Bayes

Sometimes called "Idiot's Bayes"

For independent events: A, B, and C

$$P(A \text{ and } B \text{ and } C) = P(A)P(B)P(C)$$

Start with our original expression for our posterior distribution

$$P(y = i|\boldsymbol{x}) = \frac{P(\boldsymbol{x}|y = i)P(y = i)}{P(\boldsymbol{x})}$$

Write out the full expression with all the terms in $\boldsymbol{x}$

(assume p predictors/features)

$$P(y = i|x_1, x_2, \dots, x_p) = \frac{P(x_1, x_2, \dots, x_p|y = i)P(y = i)}{P(x_1, x_2, \dots, x_p)}$$

Assumption: Given the class, the features are independent

Note: The denominator (evidence) is a constant if we know the values of the predictor variables

$$P(y = i|x_1, x_2, \dots, x_p) = \frac{P(y = i)\prod_{j=1}^{p} P(x_j|y = i)}{P(x_1, x_2, \dots, x_p)}$$

Predict the class with the highest posterior probability

$$P(y = i|x_1, x_2, \dots, x_p) \propto P(y = i)\prod_{j=1}^{p} P(x_j|y = i)$$

Naïve Bayes

We assign the class that has the largest posterior, $P(y = i|x_1, x_2, \dots, x_p)$

$$P(y = i|x_1, x_2, \dots, x_p) \propto P(y = i) \prod_{j=1}^{p} P(x_j|y = i)$$

This implies we estimate the density of each feature **separately**

This independence assumption is a strong assumption that is rarely valid

Considerably simplifies computation and data needs

Is flexible to allow for different distributional forms (i.e. Gaussian) or nonparametric techniques

Naïve Bayes: Gaussian example

We assign the class that has the largest posterior, $P(y = i|x_1, x_2, \dots, x_p)$

$$P(y = i|x_1, x_2, \dots, x_p) \propto P(y = i) \prod_{j=1}^{p} P(x_j|y = i)$$

This implies we estimate the density of each feature **separately**

If $P(x_j|y = i)$ is $N(\mu_{ji}, \sigma_{ji}^2)$, so for each class we estimate one mean and variance for each of the p features and for each class. We multiply **univariate** distributions together

$$P(y = i|x_1, x_2, \dots, x_p) \propto P(y = i) \prod_{j=1}^{p} N(\mu_{ji}, \sigma_{ji}^2)$$

Naïve Bayes: Parameters

p predictors, c classes

For each predictor, x_i, and class, y_j:

$$(\mu_{ij}, \sigma_{ij}^2)$$

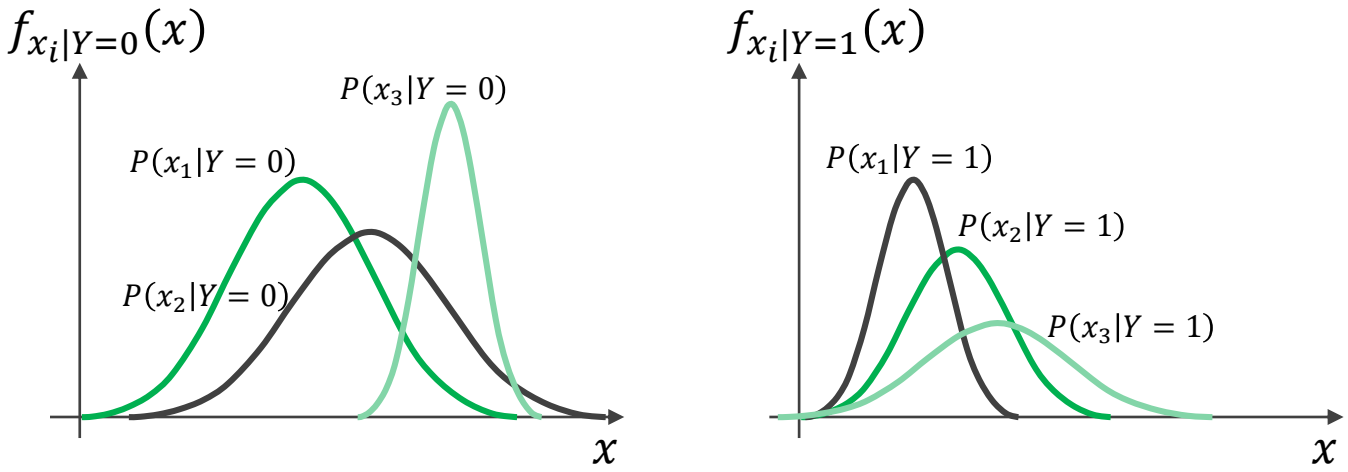
Total parameters = $2cp$

Without the Naïve Bayes assumption, each class would be a multivariate Gaussian with $(\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)$

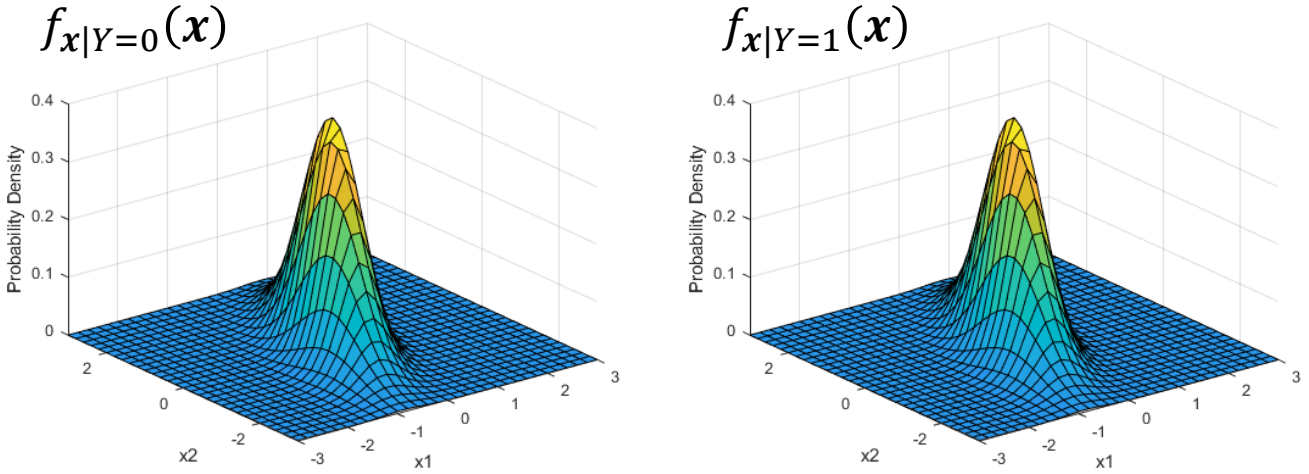
$$\boldsymbol{\mu}_j = \begin{bmatrix} \mu_1 \\ \mu_2 \\ \vdots \\ \mu_p \end{bmatrix}, \boldsymbol{\Sigma}_j = \begin{bmatrix} \sigma_{11}^2 & \sigma_{12}^2 & \cdots & \sigma_{1p}^2 \\ \sigma_{21}^2 & \sigma_{22}^2 & \cdots & \sigma_{2p}^2 \\ \vdots & \vdots & & \vdots \\ \sigma_{p1}^2 & \sigma_{p2}^2 & \cdots & \sigma_{pp}^2 \end{bmatrix}$$

Total parameters = $c(p + p^2)$

Naïve Bayes ($p = 3$)



Multivariate Gaussian (example shown for $p = 2$)



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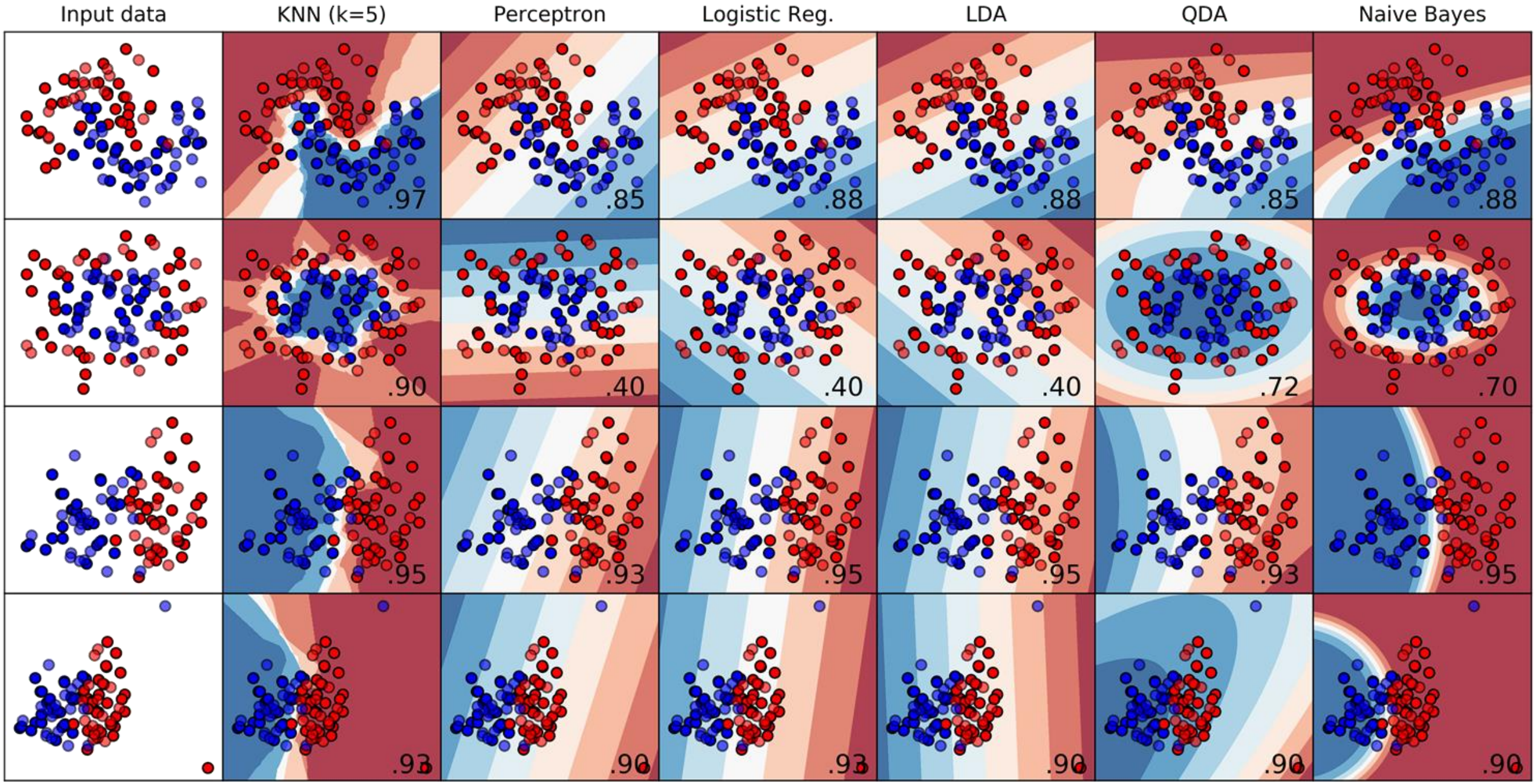
Input data
KNN (k=5)
Perceptron
Logistic Reg.
LDA
QDA
Naive Bayes
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Classifiers

Covered so far

- K-Nearest Neighbors
- Perceptron
- Logistic Regression
- Fisher's Linear Discriminant
- Linear Discriminant Analysis
- Quadratic Discriminant Analysis
- Naïve Bayes

Have closed-form solutions
Apply to multiclass problems
Have no hyperparameters
Fast to train

Requires small amounts of training data
Only model choice is the form of P(X|Y)
Fast to train

Appendix (Derivations)

FLD: Fisher Criterion Maximization

$$J(\boldsymbol{w}) = \frac{(m_2 - m_1)^2}{s_1^2 + s_2^2}$$

$$= \frac{\boldsymbol{w}^T(\boldsymbol{m}_2 - \boldsymbol{m}_1)(\boldsymbol{m}_2 - \boldsymbol{m}_1)^T\boldsymbol{w}}{\sum_{i \in \boldsymbol{C_1}}(y_n - m_k)^2 + \sum_{i \in \boldsymbol{C_2}}(y_n - m_k)^2}$$

$$m_2 - m_1 = \boldsymbol{w}^T(\boldsymbol{m}_2 - \boldsymbol{m}_1)$$

$$s_k^2 = \sum_{i \in \boldsymbol{C_k}}(y_n - m_k)^2$$

$$= \frac{\boldsymbol{w}^T(\boldsymbol{m}_2 - \boldsymbol{m}_1)(\boldsymbol{m}_2 - \boldsymbol{m}_1)^T\boldsymbol{w}}{\sum_{i \in \boldsymbol{C_1}}(\boldsymbol{w}^T\boldsymbol{x}_i - \boldsymbol{w}^T\boldsymbol{m}_1)^2 + \sum_{i \in \boldsymbol{C_2}}(\boldsymbol{w}^T\boldsymbol{x}_i - \boldsymbol{w}^T\boldsymbol{m}_2)^2}$$

$$m_k = \boldsymbol{w}^T\boldsymbol{m}_k$$

$$y_k = \boldsymbol{w}^T\boldsymbol{x}_k$$

$$= \frac{\boldsymbol{w}^T(\boldsymbol{m}_2 - \boldsymbol{m}_1)(\boldsymbol{m}_2 - \boldsymbol{m}_1)^T\boldsymbol{w}}{\boldsymbol{w}^T\left[\sum_{i \in \boldsymbol{C_1}}(\boldsymbol{x}_i - \boldsymbol{m}_1)(\boldsymbol{x}_i - \boldsymbol{m}_1)^T + \sum_{i \in \boldsymbol{C_2}}(\boldsymbol{x}_i - \boldsymbol{m}_2)(\boldsymbol{x}_i - \boldsymbol{m}_2)^T\right]\boldsymbol{w}}$$

Factoring out the $\boldsymbol{w}$ in denominator

FLD: Fisher Criterion Maximization

$$\boldsymbol{S}_B = (\boldsymbol{m}_2 - \boldsymbol{m}_1)(\boldsymbol{m}_2 - \boldsymbol{m}_1)^T$$

$$J(\boldsymbol{w}) = \frac{\boldsymbol{w}^T(\boldsymbol{m}_2 - \boldsymbol{m}_1)(\boldsymbol{m}_2 - \boldsymbol{m}_1)^T\boldsymbol{w}}{\boldsymbol{w}^T\left[\sum_{i\in C_1}(\boldsymbol{x}_i - \boldsymbol{m}_1)(\boldsymbol{x}_i - \boldsymbol{m}_1)^T + \sum_{i\in C_2}(\boldsymbol{x}_i - \boldsymbol{m}_2)(\boldsymbol{x}_i - \boldsymbol{m}_2)^T\right]\boldsymbol{w}}$$

$$\boldsymbol{S}_W = \sum_{i\in C_1}(\boldsymbol{x}_i - \boldsymbol{m}_1)(\boldsymbol{x}_i - \boldsymbol{m}_1)^T + \sum_{i\in C_2}(\boldsymbol{x}_i - \boldsymbol{m}_2)(\boldsymbol{x}_i - \boldsymbol{m}_2)^T$$

$$= \boldsymbol{\Sigma}_1 + \boldsymbol{\Sigma}_2$$

$\boldsymbol{\Sigma}_i$ = covariance matrix for class i

$$J(\boldsymbol{w}) = \frac{\boldsymbol{w}^T\boldsymbol{S}_B\boldsymbol{w}}{\boldsymbol{w}^T\boldsymbol{S}_W\boldsymbol{w}}$$

Generalized Raleigh Quotient

We want to maximize this and solve for $\boldsymbol{w}$

FLD: Fisher Criterion Maximization

$$J(\boldsymbol{w}) = \frac{\boldsymbol{w}^T \boldsymbol{S}_B \boldsymbol{w}}{\boldsymbol{w}^T \boldsymbol{S}_W \boldsymbol{w}}$$

Take the derivative (gradient), set it equal to zero, solve for $\boldsymbol{w}$

Recall the quotient rule for differentiation:

$$f(x) = \frac{u(x)}{v(x)} \qquad \frac{df}{dx} = \frac{u'v - uv'}{v^2}$$

Matrix derivatives of the form $\boldsymbol{x}^T \boldsymbol{A} \boldsymbol{x}$ with respect to $\boldsymbol{x}$ are:

$$\frac{d\boldsymbol{x}^T \boldsymbol{A} \boldsymbol{x}}{d\boldsymbol{x}} = \boldsymbol{x}^T (\boldsymbol{A} + \boldsymbol{A}^T)$$

If A is symmetric (as it is for our scatter matrices), then $\boldsymbol{A} = \boldsymbol{A}^T$, therefore:

$$\boldsymbol{x}^T (\boldsymbol{A} + \boldsymbol{A}^T) = 2\boldsymbol{x}^T \boldsymbol{A}$$

Therefore, we can write:

$$\frac{dJ(\boldsymbol{w})}{d\boldsymbol{w}} = \frac{(2\boldsymbol{w}^T \boldsymbol{S}_B)(\boldsymbol{w}^T \boldsymbol{S}_W \boldsymbol{w}) - (\boldsymbol{w}^T \boldsymbol{S}_B \boldsymbol{w})(2\boldsymbol{w}^T \boldsymbol{S}_W)}{(\boldsymbol{w}^T \boldsymbol{S}_W \boldsymbol{w})^2} = 0$$

We want to solve this for $\boldsymbol{w}$

FLD: Fisher Criterion Maximization

$$\frac{dJ(\boldsymbol{w})}{d\boldsymbol{w}} = \frac{(2\boldsymbol{w}^T\boldsymbol{S}_B)(\boldsymbol{w}^T\boldsymbol{S}_W\boldsymbol{w}) - (\boldsymbol{w}^T\boldsymbol{S}_B\boldsymbol{w})(2\boldsymbol{w}^T\boldsymbol{S}_W)}{(\boldsymbol{w}^T\boldsymbol{S}_W\boldsymbol{w})^2} = 0$$

We want to solve this for $\boldsymbol{w}$

Since the denominator will not approach infinity, only the numerator matters

$$(2\boldsymbol{w}^T\boldsymbol{S}_B)(\boldsymbol{w}^T\boldsymbol{S}_W\boldsymbol{w}) - (\boldsymbol{w}^T\boldsymbol{S}_B\boldsymbol{w})(2\boldsymbol{w}^T\boldsymbol{S}_W) = 0$$

$$(\underbrace{\boldsymbol{w}^T\boldsymbol{S}_W\boldsymbol{w}}_{\alpha})(\boldsymbol{w}^T\boldsymbol{S}_B) = (\underbrace{\boldsymbol{w}^T\boldsymbol{S}_B\boldsymbol{w}}_{\beta})(\boldsymbol{w}^T\boldsymbol{S}_W)$$

$$[1 \times D][D \times D][D \times 1] \rightarrow \text{scalar}$$

These will only affect magnitude. We assume that $\boldsymbol{w}$ is of unit length, so we replace these with variables α and β.

$$\alpha\boldsymbol{w}^T\boldsymbol{S}_B = \beta\boldsymbol{w}^T\boldsymbol{S}_W$$

FLD: Fisher Criterion Maximization

$$\alpha \boldsymbol{w}^T \boldsymbol{S}_B = \beta \boldsymbol{w}^T \boldsymbol{S}_W$$

$$\alpha \boldsymbol{S}_B^T \boldsymbol{w} = \beta \boldsymbol{S}_W^T \boldsymbol{w}$$

$$\alpha \boldsymbol{S}_B \boldsymbol{w} = \beta \boldsymbol{S}_W \boldsymbol{w}$$

$$\alpha (\boldsymbol{m}_2 - \boldsymbol{m}_1)(\boldsymbol{m}_2 - \boldsymbol{m}_1)^T \boldsymbol{w} = \beta \boldsymbol{S}_W \boldsymbol{w}$$

scalar $\boldsymbol{m}_2 - \boldsymbol{m}_1$, call this γ

$$\alpha \gamma (\boldsymbol{m}_2 - \boldsymbol{m}_1) = \beta \boldsymbol{S}_W \boldsymbol{w}$$

Property of matrix transposition:

$$(\boldsymbol{AB})^T = \boldsymbol{B}^T \boldsymbol{A}^T$$

The scatter matrices are symmetric:

$$\boldsymbol{S}_B = \boldsymbol{S}_B^T \qquad \boldsymbol{S}_W = \boldsymbol{S}_W^T$$

Between-class scatter matrix:

$$\boldsymbol{S}_B = (\boldsymbol{m}_2 - \boldsymbol{m}_1)(\boldsymbol{m}_2 - \boldsymbol{m}_1)^T$$

Aside: dimensionality reduction

Rearranging, this is an eigenvalue problem

$$\boldsymbol{S}_W^{-1} \boldsymbol{S}_B \boldsymbol{w} = \lambda \boldsymbol{w}$$

For multiclass problems, we can use the eigenvalue of $\boldsymbol{S}_W^{-1} \boldsymbol{S}_B$, much like PCA to get projections into lower dimensional subspaces where the classes are well-separated

FLD: Fisher Criterion Maximization

$$\alpha\gamma(\boldsymbol{m}_2 - \boldsymbol{m}_1) = \beta \boldsymbol{S}_W \boldsymbol{w}$$

Solving for $\boldsymbol{w}$:

$$\boldsymbol{w} = \frac{\alpha\gamma}{\beta} \boldsymbol{S}_W^{-1}(\boldsymbol{m}_2 - \boldsymbol{m}_1)$$

We only care about the direction of $\boldsymbol{w}$

$$\boldsymbol{w} \propto \boldsymbol{S}_W^{-1}(\boldsymbol{m}_2 - \boldsymbol{m}_1)$$

Note: if $\boldsymbol{S}_w$ is isotropic (proportional to the identity matrix, i.e. if $\boldsymbol{S}_w = a\boldsymbol{I}$), then this is just the difference between the means

$$\boldsymbol{w} \propto (\Sigma_1 + \Sigma_2)^{-1} (\boldsymbol{m}_2 - \boldsymbol{m}_1)$$

Linear Discriminant Analysis ($\Sigma_0 = \Sigma_1$)

We build a classifier that assigns the class with the higher posterior probability:

$$\frac{P(\boldsymbol{x}|y=1)}{P(\boldsymbol{x}|y=0)} = \frac{\frac{1}{(2\pi)^{d/2}|\boldsymbol{\Sigma}|^{1/2}} \exp\left[-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu}_1)^T\boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu}_1)\right]}{\frac{1}{(2\pi)^{d/2}|\boldsymbol{\Sigma}|^{1/2}} \exp\left[-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu}_0)^T\boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu}_0)\right]}$$

$$= \frac{\exp\left[-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu}_1)^T\boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu}_1)\right]}{\exp\left[-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu}_0)^T\boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu}_0)\right]}$$

$$\ln\left|\frac{P(\boldsymbol{x}|y=1)}{P(\boldsymbol{x}|y=0)}\right| = -\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu}_1)^T\boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu}_1) + \frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu}_0)^T\boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu}_0)$$

Linear Discriminant Analysis ($\Sigma_0 = \Sigma_1$)

$$\ln\left|\frac{P(\boldsymbol{x}|y=1)}{P(\boldsymbol{x}|y=0)}\right| = -\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu}_1)^T\boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu}_1) + \frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu}_0)^T\boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu}_0)$$

Expanding this expression yields:

These combine since $\boldsymbol{x}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_i = \boldsymbol{\mu}_i^T\boldsymbol{\Sigma}^{-1}\boldsymbol{x}$ for symmetric matrices

$$= -\frac{1}{2}[\boldsymbol{x}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{x} - \boldsymbol{x}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_1 - \boldsymbol{\mu}_1^T\boldsymbol{\Sigma}^{-1}\boldsymbol{x} + \boldsymbol{\mu}_1^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_1$$

$$-\boldsymbol{x}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{x} + \boldsymbol{x}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_0 + \boldsymbol{\mu}_0^T\boldsymbol{\Sigma}^{-1}\boldsymbol{x} - \boldsymbol{\mu}_0^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_0$$

$$= \frac{1}{2}[2\boldsymbol{x}^T\boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_1-\boldsymbol{\mu}_0) - (\boldsymbol{\mu}_1+\boldsymbol{\mu}_0)\boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_1-\boldsymbol{\mu}_0)]$$

$$= \boldsymbol{x}^T\boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_1-\boldsymbol{\mu}_0) - \frac{1}{2}(\boldsymbol{\mu}_1+\boldsymbol{\mu}_0)\boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_1-\boldsymbol{\mu}_0)$$

Linear Discriminant Analysis ($\Sigma_0 = \Sigma_1$)

$$\ln \left| \frac{P(\boldsymbol{x}|y=1)}{P(\boldsymbol{x}|y=0)} \right| = \boldsymbol{x}^T \boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0) - \frac{1}{2}(\boldsymbol{\mu}_1 + \boldsymbol{\mu}_0)\boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0)$$

Since our decision rule is to classify as class 1 if the following is true:

$$\ln \left| \frac{P(\boldsymbol{x}|y=1)}{P(\boldsymbol{x}|y=0)} \right| > \ln \left| \frac{P(y=0)}{P(y=1)} \right|$$

We can rewrite our decision rule as:

$$\boldsymbol{x}^T \boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0) > \frac{1}{2}(\boldsymbol{\mu}_1 + \boldsymbol{\mu}_0)\boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0) + \ln \left| \frac{P(y=0)}{P(y=1)} \right|$$

Or simply as:

$$\boldsymbol{x}^T \boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0) > C$$

If we define $\boldsymbol{w} = \boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0)$, then this becomes $\boldsymbol{x}^T \boldsymbol{w} > C$