# Generative Models for Classification

# Supervised learning in practice

# Preprocessing Explore & prepare data

Data Visualization and Exploration

Identify patterns that can be leveraged for learning

Data Cleaning

- Missing dataNoisy data
- Erroneous data

Scaling (Standardization)

Prepare data for use in scale-dependent algorithms.

Feature Extraction

Dimensionality reduction eliminates redundant information

**Model training** Supervised Learning Models: Linear models fine tune and KNN the model (enough to get started using supervised learning) Select model options Other algorithms and concepts: **Generative vs** discriminative models Parametric vs nonparametric models Model ensembles Feature/representation learning (neural networks, deep learning) How to control model overfit: regularization strategies for model refinement

**Performance** evaluation Make a prediction on validation data Evaluating model performance and comparing models Classification Precision Recall F How to make decisions using models Regression MSE, explained variance, R<sup>2</sup>

### Classifiers

Covered so far

K-Nearest Neighbors

Perceptron

Logistic Regression

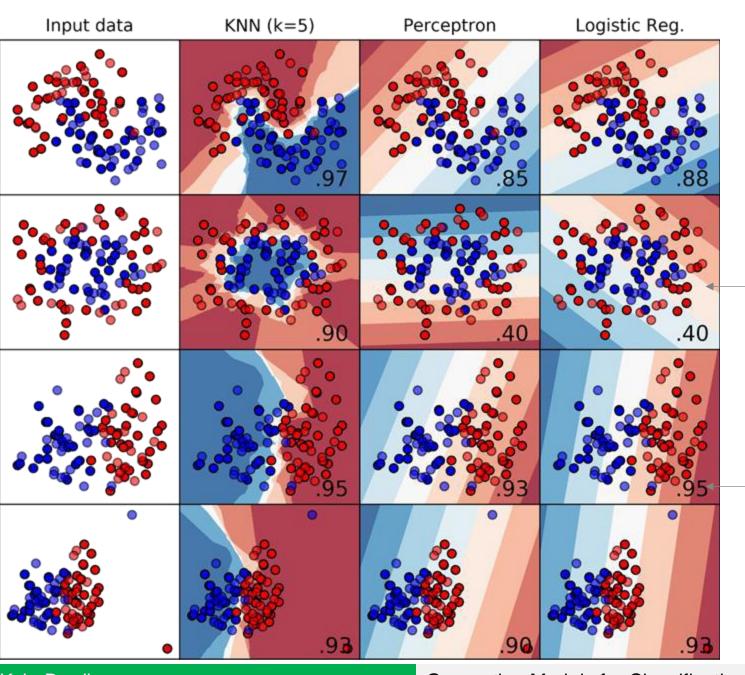
Linear Discriminant Analysis

Quadratic Discriminant Analysis

Naïve Bayes

#### Along the way...

Revisiting Bayes' Rule
Projections from higher dimensions
Multivariate normal distributions



# Comparison of classifiers we have seen so far

The color gradient shows the confidence scores

Test data accuracy

### Bayes' rule in the context of classification

### Bayes' Rule

$$P(C|X) = \frac{P(X|C)P(C)}{P(X)}$$
Posterior
$$P(X|C) = \frac{P(X|C)P(C)}{P(X)}$$
Evidence

#### **X** Features

C Class label i.e.  $C \in \{c_0, c_1\}$  for the binary case

### **Bayes' Decision Rule:**

choose the most probable class given the data

If 
$$P(C_i=c_1|X_i)>P(C_i=c_0|X_i)$$
 then  $\hat{y}=c_1$  otherwise  $\hat{y}=c_0$ 

- If the distributions are correct, this decision rule is optimal
- Rarely do we have enough information to use this in practice





**Class 1: Light Image** 

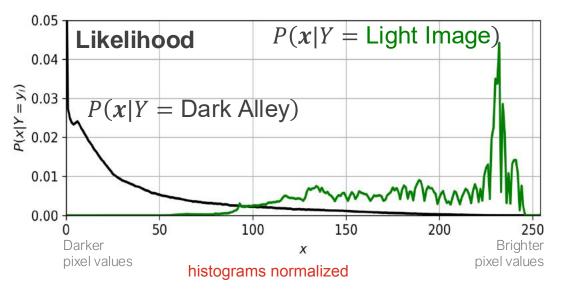
Randomly draw a pixel from either of the images:

**Class 0: Dark Image** 

$$x_i = 149$$
 Darker pixel valu (closer to 0), bright numbers (closer

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

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

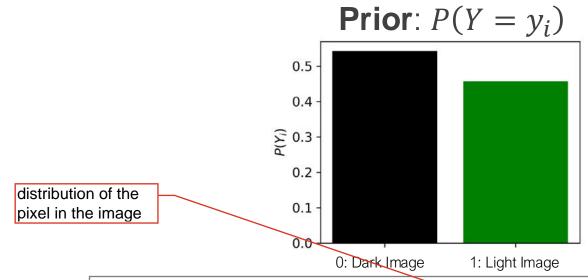




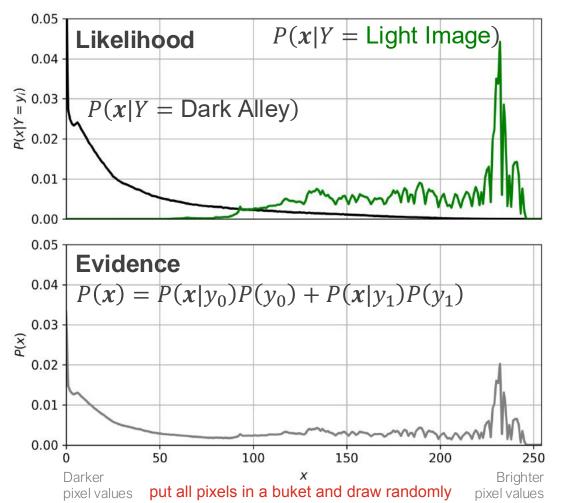


Class 1: Light Image  $y_1$ 

Class 0: Dark Image  $y_0$ 



Bayes' Rule 
$$P(Y = y_i | x) = \frac{P(x | Y = y_i)P(Y = y_i)}{P(x)}$$
 Evidence

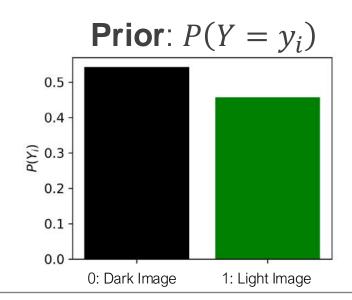




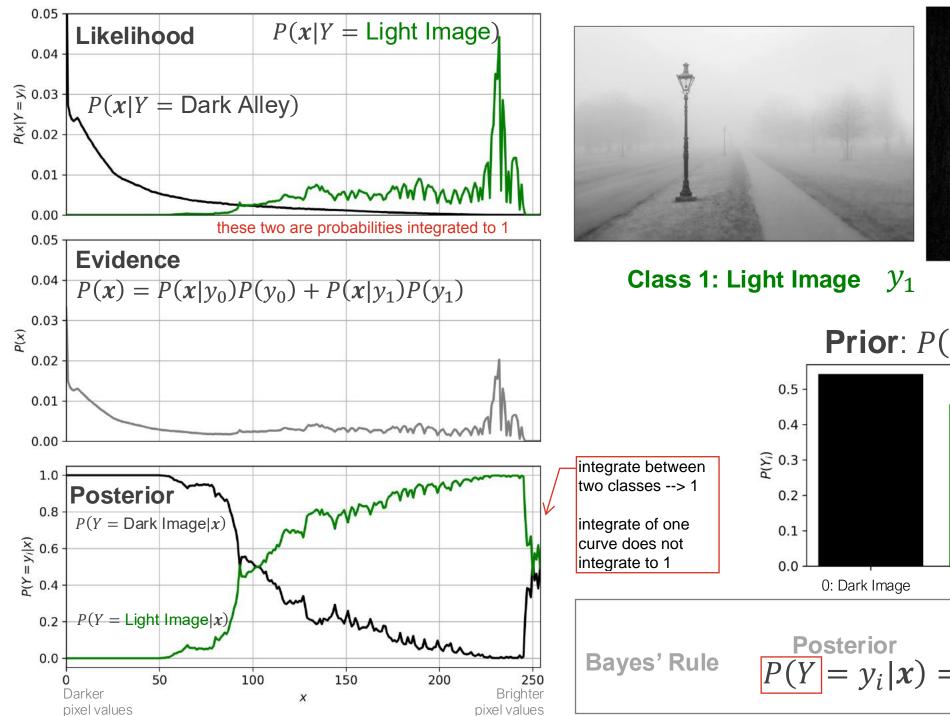


Class 1: Light Image  $y_1$ 

Class 0: Dark Image  $y_0$ 

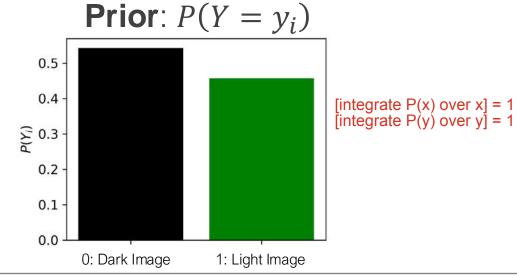


Bayes' Rule 
$$P(Y = y_i | x) = \frac{P(x | Y = y_i)P(Y = y_i)}{P(x)}$$
 Evidence

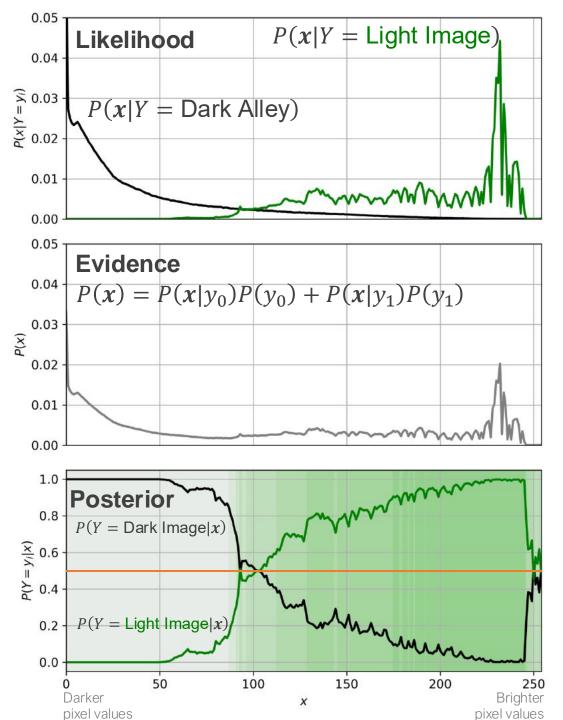




Class 0: Dark Image  $y_0$ 



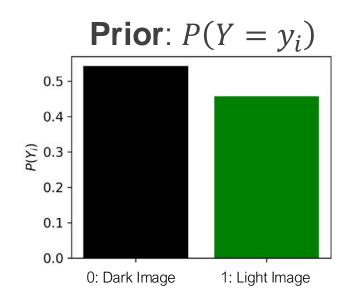
Posterior
$$P(Y = y_i | \mathbf{x}) = \frac{P(\mathbf{x} | Y = y_i)P(Y = y_i)}{P(\mathbf{x}) \text{ Evidence}}$$





Class 1: Light Image  $y_1$ 

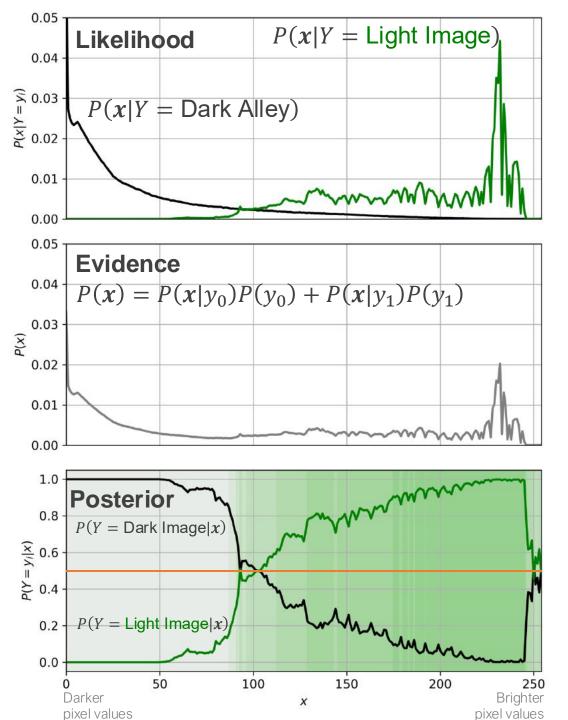
Class 0: Dark Image  $y_0$ 



pick the bigger one

#### **Decision rule:**

If P(Y = Light Image|x) > P(Y = Dark Image|x) then else Dark Image

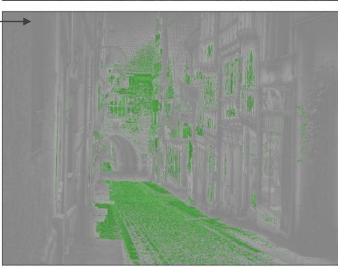


Class 1: Light Image  $y_1$ 





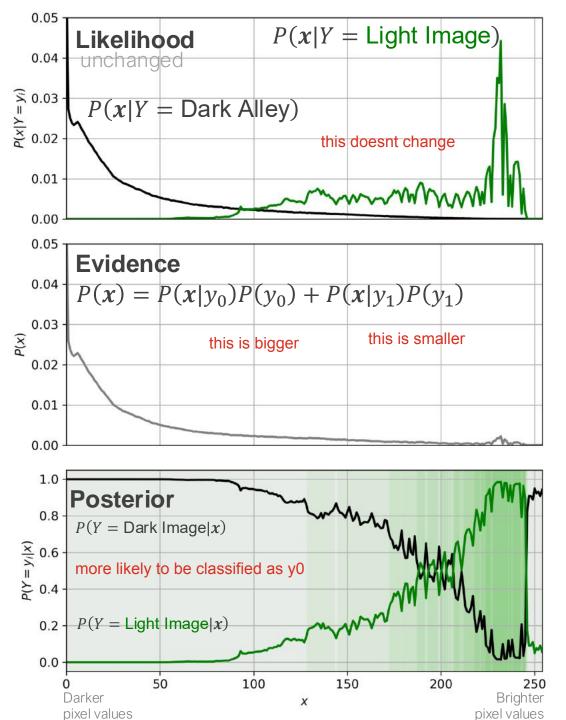
Green = classified as from Light Image Grey = classified as from Dark Image



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

#### **Decision rule:**

If P(Y = Light Image|x) > P(Y = Dark Image|x) then Light Image else Dark Image

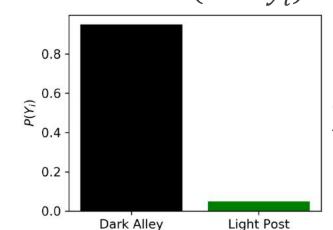




Class 1: Light Image  $y_1$ 

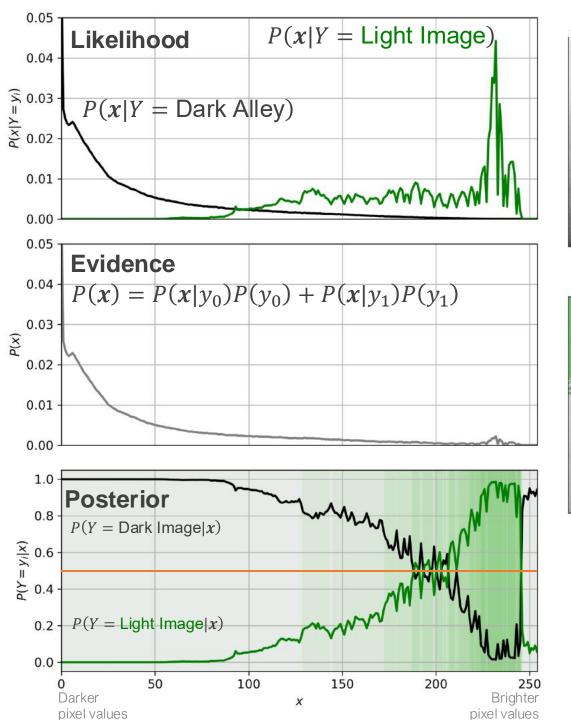
Class 0: Dark Image  $y_0$ 

Prior:  $P(Y = y_i)$ 

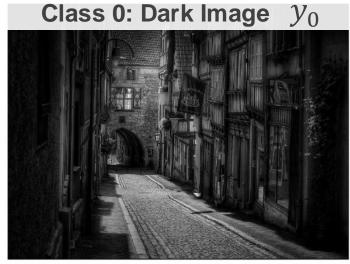


Let's assume the sampling of pixels occurred more from the **Dark Image** 

Posterior
$$P(Y = y_i | \mathbf{x}) = \frac{P(\mathbf{x} | Y = y_i)P(Y = y_i)}{P(\mathbf{x}) \text{ Fyidence}}$$











Prior: 
$$P(Y = y_i)$$
  $\hat{z}_{0.4}$ 

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

#### 0.05 P(x|Y = Light Image).ikelihood 0.04 (x = 0.03)P(x|Y = Dark Alley)0.01 0.00 0.05 **Evidence** 0.04 $P(x) = P(x|y_0)P(y_0) + P(x|y_1)P(y_1)$ 0.03 0.02 0.01 0.00 Posterior 4 6 1 0.8 P(Y = Dark Image|x) $0.0 = \frac{(x | x)}{10.0}$ P(Y = Light Image|x)0.0 50 100 150 200 pixel values

#### Generative models model the likelihood

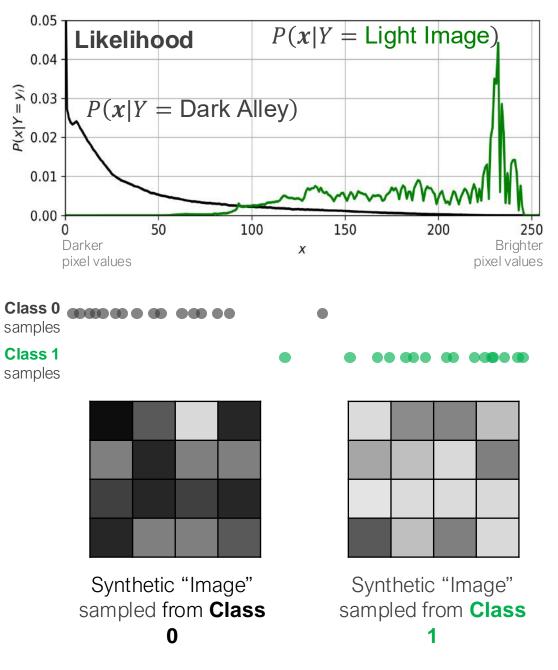
- These can also be used to generate synthetic data
- Often good performance when sample size is small Examples: linear discriminant analysis, naïve Bayes, hidden Markov models, Guassian mixture models, Generative Adversarial Networks

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

#### Discriminative models model the posterior

- Or they just directly estimate labels without a probabilistic interpretation,  $f(x) \rightarrow y$
- Often better performance for large sample sizes

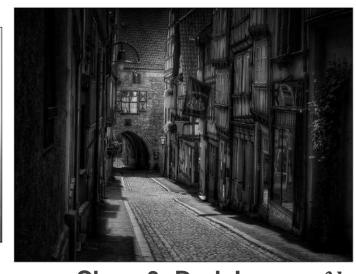
  Examples: logistic regression, support vector machines, neural networks, k nearest neighbors



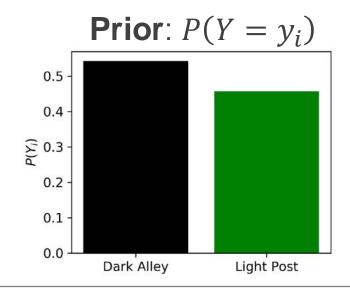
**How to "Generate" Data?** 



Class 1: Light Image  $y_1$ 



Class 0: Dark Image  $y_0$ 



Bayes' Rule 
$$P(Y = y_i | x) = \frac{P(x | Y = y_i)P(Y = y_i)}{P(x)}$$
 Evidence

# Generative modeling for classification

Assume we have *c* different classes

For a new sample, classify it as the class with the **largest posterior** P(y = i | x)

i = 1, ..., c

# Generative modeling for classification

If we have c different classes, we define a discriminant function,  $d_i(x)$  for i = 1, ..., c

If P(y = i | x) > P(y = j | x) for  $i \neq j$ , then we classify feature x to class i

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

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

 $= \frac{P(x|y=i)P(y=i)}{\sum_{i=1}^{c} P(x|y=i)P(y=i)} \longrightarrow \begin{array}{l} \text{Denominator is the same for all classes } i, \text{ so it} \\ \text{won't help us tell which class's posterior is higher} \\ \text{relative to other classes, so we ignore it going} \\ \text{forward} \end{array}$ 

We can define the discriminant function as:

$$d_i(x) = P(x|y=i)P(y=i)$$

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

Likelihood

# Generative modeling for classification

$$d_i(x) = P(x|y=i)P(y=i)$$

We **rarely** know our **true likelihood** for our data so we need to assume a form for the distributions and approximate

1 Assume a form for P(x|y=i)

Gaussian → Linear and Quadratic Discriminant Analysis
Gaussian mixture models
Nonparametric density estimates

If we assume independent features → Naïve Bayes

2 Assign the class, i, for which  $d_i(x)$  is largest Applies to both binary and multiclass problems

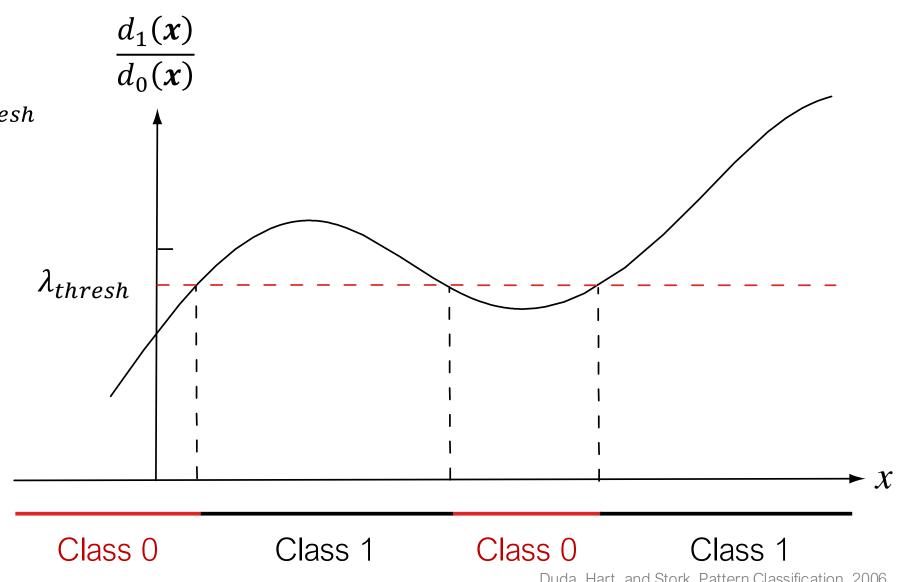
(remember  $d_i(x)$  proportional to the posterior)

### Discriminant Function: 2 classes

Decision rule:

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

Otherwise, class 0



Duda, Hart, and Stork, Pattern Classification, 2006

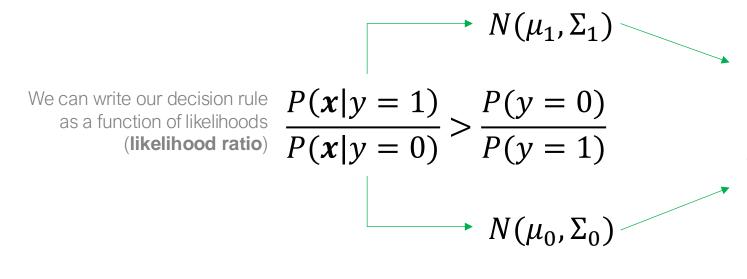
### **Discriminant Function: 2 classes**

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

If 
$$\frac{d_1(x)}{d_0(x)} = \frac{P(x|y=1)P(y=1)}{P(x|y=0)P(y=0)} > 1$$

Assign class 1, else class 0

Assumes these likelihoods are normal



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: 
$$\frac{P(x|y=1)}{P(x|y=0)} > \frac{P(y=0)}{P(y=1)}$$
 
$$N(\mu_0, \Sigma_0)$$

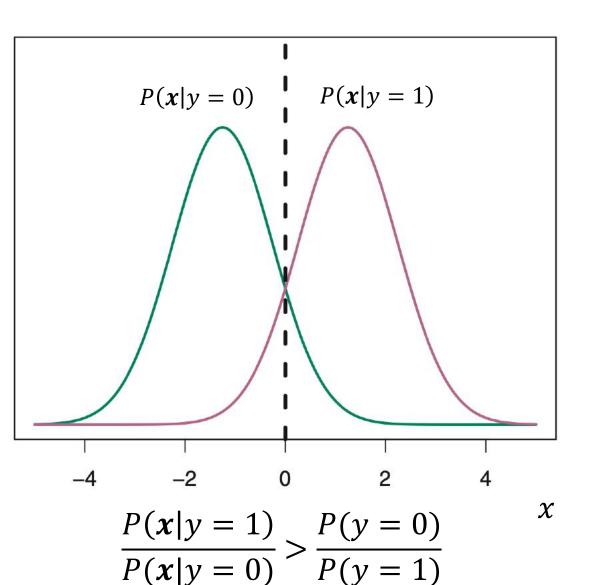
If we assume the class conditional distributions are Gaussian, this represents

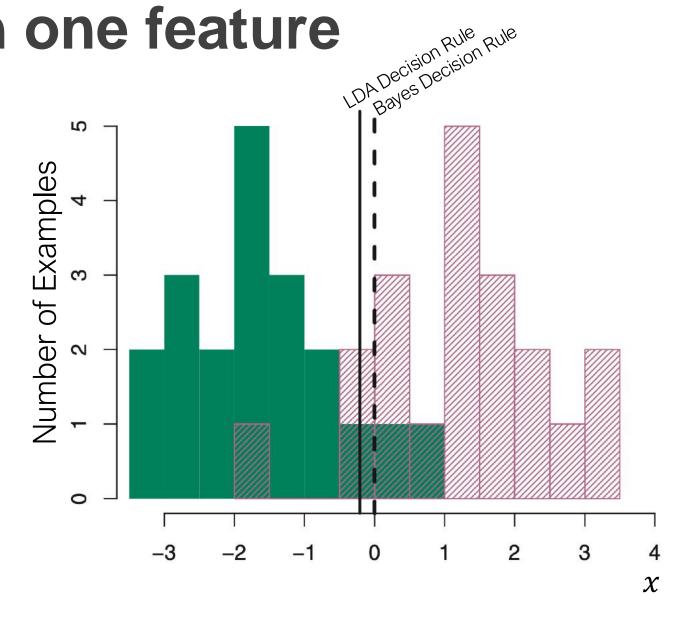
#### **Quadratic Discriminant Analysis**

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

#### **Linear Discriminant Analysis**

### Simple example with one feature





Figures from James et al. - Introduction to Statistical Learning

### **Covariance matrix**

$$\mathbf{X}_{\boldsymbol{i}} = \begin{bmatrix} x_{i1} \\ x_{i2} \\ \vdots \\ x_{iD} \end{bmatrix}$$
Vector of observation  $i$ 

$$\mathbf{X}_{i} = \begin{bmatrix} x_{i1} \\ x_{i2} \\ \vdots \\ x_{iD} \end{bmatrix}$$

$$\mathbf{X}_{i}$$

$$\mathbf{X}_{i$$

$$\Sigma = \frac{1}{N} \sum_{i=1}^{N} (\mathbf{x}_{i} - \overline{\mathbf{x}}) (\mathbf{x}_{i} - \overline{\mathbf{x}})^{T} \rightarrow [D \times D]$$

$$[D \times 1][1 \times D]$$

$$\boldsymbol{\Sigma} = \begin{bmatrix} \boldsymbol{\Sigma}_{11} & \boldsymbol{\Sigma}_{12} & \cdots & \boldsymbol{\Sigma}_{1D} \\ \boldsymbol{\Sigma}_{21} & \boldsymbol{\Sigma}_{22} & \cdots & \boldsymbol{\Sigma}_{2D} \\ \vdots & \vdots & \ddots & \vdots \\ \boldsymbol{\Sigma}_{D1} & \boldsymbol{\Sigma}_{D2} & \cdots & \boldsymbol{\Sigma}_{DD} \end{bmatrix}$$

$$\Sigma = \begin{bmatrix} \sigma_1^2 & \Sigma_{12} & \cdots & \Sigma_{1D} \\ \Sigma_{21} & \sigma_2^2 & \cdots & \Sigma_{2D} \\ \vdots & \vdots & \ddots & \vdots \\ \Sigma_{D1} & \Sigma_{D2} & \cdots & \sigma_D^2 \end{bmatrix} \qquad \sigma_j^2 = \frac{1}{N} \sum_{i=1}^N (x_{ij} - \bar{x}_j)^2 \\ = E[(X_j - \mu_j)^2]$$

$$\Sigma = \begin{bmatrix} \Sigma_{11} & \Sigma_{12} & \cdots & \Sigma_{1D} \\ \Sigma_{21} & \Sigma_{22} & \cdots & \Sigma_{2D} \\ \vdots & \vdots & \ddots & \vdots \\ \Sigma_{D1} & \Sigma_{D2} & \cdots & \Sigma_{DD} \end{bmatrix} \qquad \Sigma_{jk} = \frac{1}{N} \sum_{i=1}^{N} (x_{ij} - \bar{x}_j)(x_{ik} - \bar{x}_k)$$

$$= \operatorname{cov}(X_j, X_k)$$

$$= E[(X_j - \mu_j)(X_k - \mu_k)]$$

$$\sigma_j^2 = \frac{1}{N} \sum_{i=1}^N (x_{ij} - \bar{x}_j)^2$$
$$= E[(X_i - \mu_i)^2]$$

Mean of each predictor

If 
$$\dot{\bar{x}}_j = 0$$
 for all  $j$ 

This will be the case IF the data are standardized

$$\Sigma_{jk} = \frac{1}{N} \sum_{i=1}^{N} x_{ij} x_{ik}$$
$$= \frac{1}{N} \mathbf{x}_{j}^{T} \mathbf{x}_{k}$$
$$= E[X_{j} X_{k}]$$

$$\mathbf{\Sigma} = \frac{1}{N} \mathbf{X}^{\mathrm{T}} \mathbf{X}$$

### **Covariance and Correlation**

differences please!

Relationship between covariance and correlation

$$corr(X,Y) = \frac{cov(X,Y)}{\sqrt{var(X)var(Y)}}$$

When var(X) = var(Y) = 1, then:

$$corr(X, Y) = cov(X, Y)$$

If each of the features have been standardized, this means this matrix is:

$$\mathbf{\Sigma} = \begin{bmatrix} 1 & \rho_{12} & \cdots & \rho_{1D} \\ \rho_{21} & 1 & \cdots & \rho_{2D} \\ \vdots & \vdots & \ddots & \vdots \\ \rho_{D1} & \rho_{D2} & \cdots & 1 \end{bmatrix}$$

### **Covariance Matrix Examples**

diagonal only --> no correlation

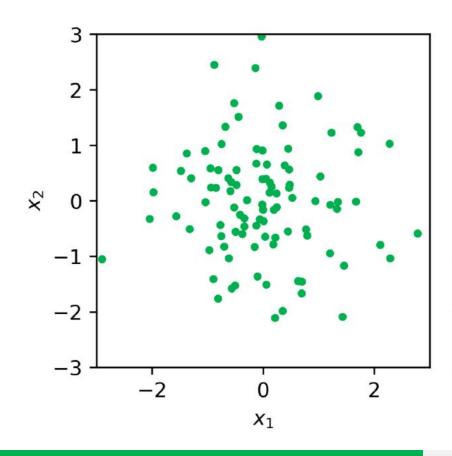
some correlation

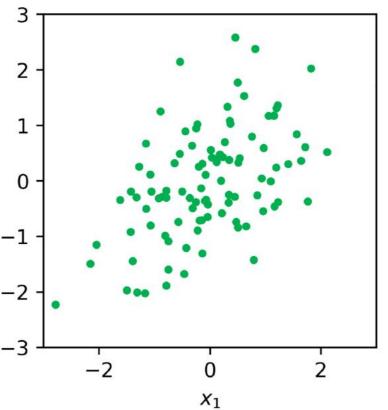
strong correlation

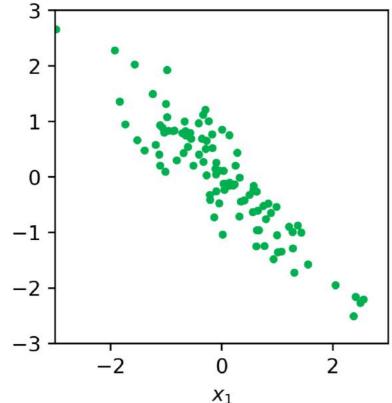
$$\Sigma = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$\Sigma = \begin{bmatrix} 1 & 0.5 \\ 0.5 & 1 \end{bmatrix}$$

$$\Sigma = \begin{bmatrix} 1 & -0.9 \\ -0.9 & 1 \end{bmatrix}$$







### Key model differences

Quadratic Discriminant Analysis (QDA)

$$\Sigma_0 \neq \Sigma_1$$

Each class (e.g., 0 or 1) may have a unique covariance matrix

Linear Discriminant Analysis (LDA)

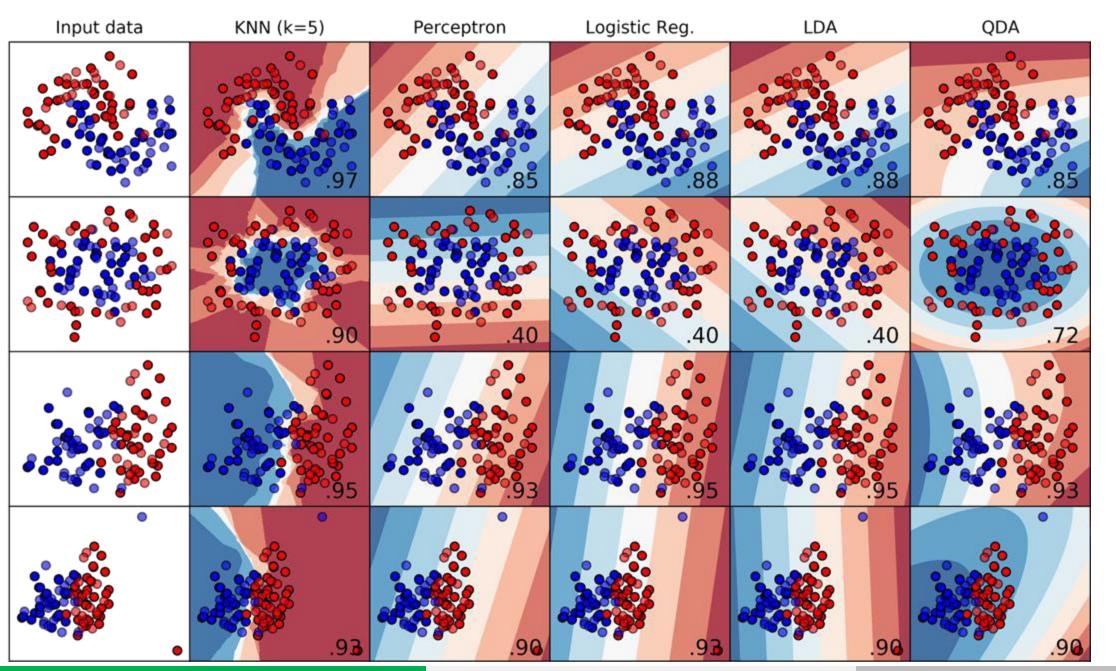
$$\Sigma_0 = \Sigma_1$$

Every class (e.g., 0 or 1) has an identical covariance matrix

Naïve Bayes with Gaussian Likelihoods

$$\Sigma_i = \begin{bmatrix} \sigma_1^2 & 0 & \cdots & 0 \\ 0 & \sigma_2^2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sigma_D^2 \end{bmatrix}$$
Every class (e.g.,  $i = 0$  or 1) has a **diagonal** covariance matrix

covariance matrix



# Joint vs Marginal Densities

The marginal densities don't factor in relationships between features

What if the joint density is too hard to estimate?

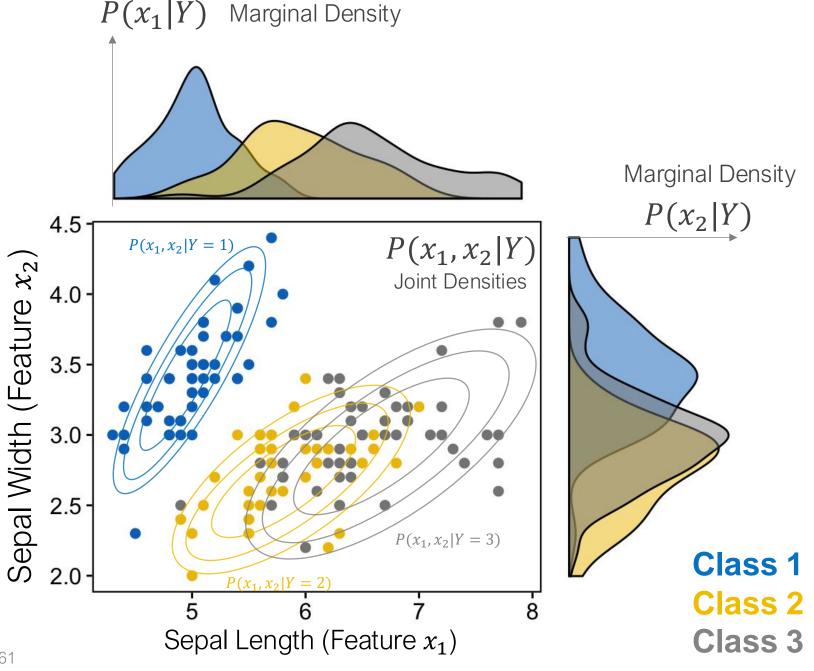


Image adapted from: https://github.com/daattali/ggExtra/issues/61

# Naïve Bayes

For independent events: A, B, and C P(A and B and C) = P(A)P(B)P(C)

Start with our original expression for our discriminant function

(proportional to posterior distribution)

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

Write out the full expression with all the 
$$d_i(x_1, x_2, ..., x_p) = P(x_1, x_2, ..., x_p | y = i)P(y = i)$$

(assume p predictors/features)

### Assumption: Given the class, the features are independent

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

Predict the class with the highest discriminant function (i.e. posterior probability)

terms in x

### Naïve Bayes

We assign the class that has the largest discriminant (i.e. posterior probability)

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

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 for the likelihood  $P(x_i|y=i)$ 

### Naïve Bayes: Gaussian example

We assign the class that has the largest discriminant (i.e. posterior probability)

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

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

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

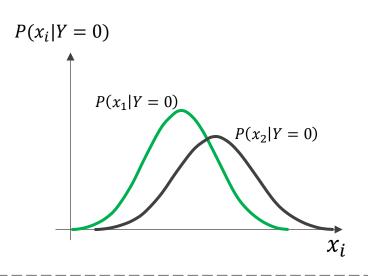
### Naïve Bayes: Parameters

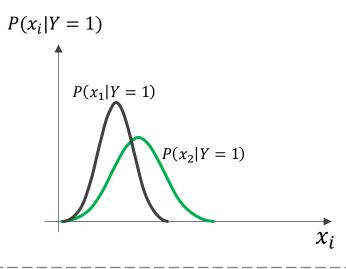
Gaussian Naïve Bayes (p = 2)

p predictors, c classes

For each predictor,  $x_i$ , and class,  $y_j$ :  $(\mu_{ij}, \sigma_{ij}^2)$ 

Total parameters = 2cp



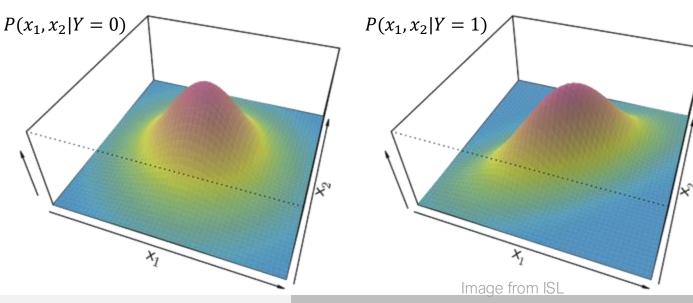


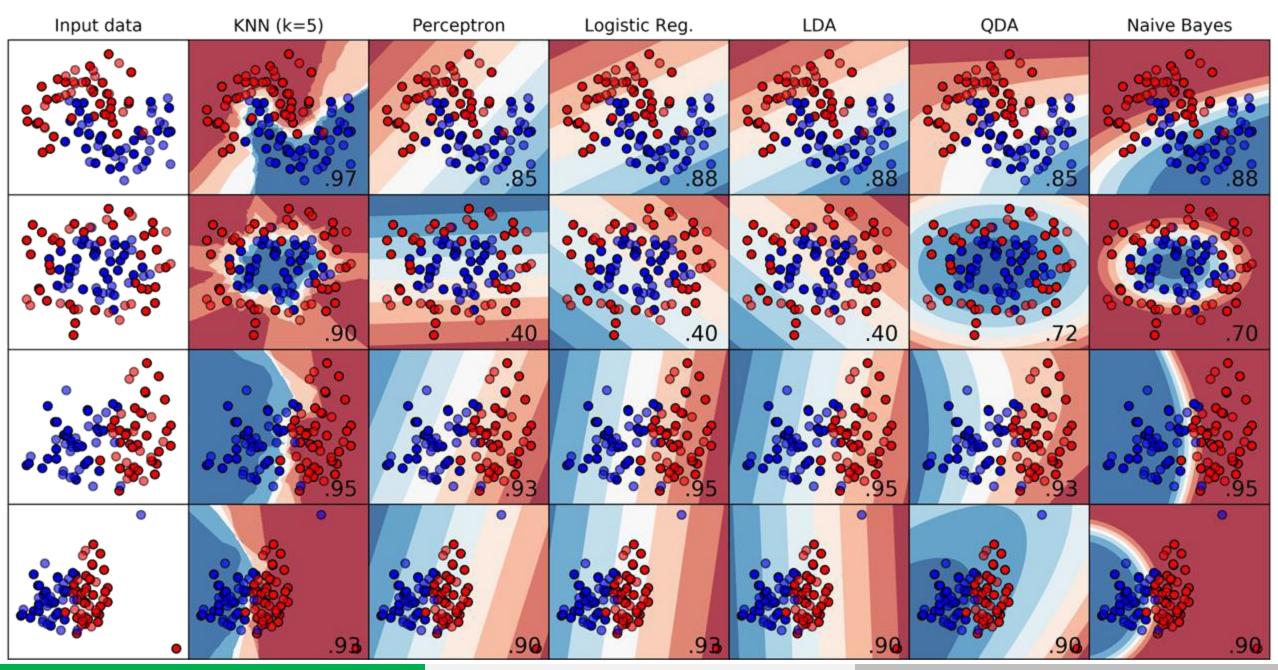
Without the Naïve Bayes independence assumption, each class would be a multivariate Gaussian with  $(\mu_j, \Sigma_j)$ 

$$\boldsymbol{\mu}_{j} = \begin{bmatrix} \mu_{1} \\ \mu_{2} \\ \vdots \\ \mu_{p} \end{bmatrix}, \, \boldsymbol{\Sigma}_{j} = \begin{bmatrix} \sigma_{11}^{2} & \sigma_{12}^{2} & \cdots & \sigma_{1p}^{2} \\ \sigma_{21}^{2} & \sigma_{22}^{2} & \cdots & \sigma_{2p}^{2} \\ \vdots & \vdots & & \vdots \\ \sigma_{p1}^{2} & \sigma_{p2}^{2} & \cdots & \sigma_{pp}^{2} \end{bmatrix}$$

Total parameters =  $c\left(p + \frac{p^2 - p}{2} + p\right)$ 

Multivariate Gaussian (p = 2)





### Classifiers

Covered so far

K-Nearest Neighbors

Perceptron

Logistic Regression

Linear Discriminant Analysis

Quadratic Discriminant Analysis

Naïve Bayes

Have closed-form solutions

Apply to multiclass problems

No hyperparameters

Fast to train

Requires small amounts of training data

Only choice is the form of P(X|Y) (otherwise no parameter choices)

Fast to train

### Examples of deep generative models...

Variational Auto Encoders

Normalizing Flows

Generative Adversarial Networks (GANs)

**Diffusion Models** 

### **Face Synthesis**

#### Image Synthesis (<u>link</u>)

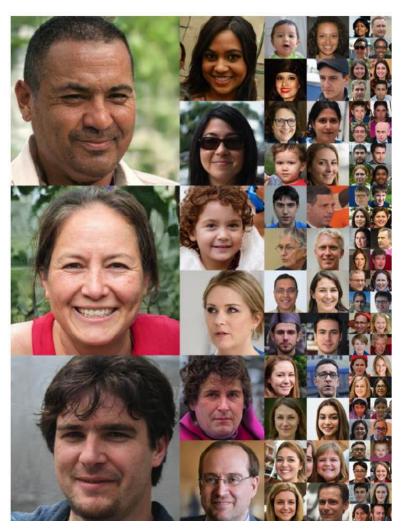
Karras et al. 2018, NVIDIA: Progressive growing of GANS for improved quality, stability, and variation

These images are all synthetic



# **Synthetic Generation**

Karras, T., Laine, S. and Aila, T., 2019. A style-based generator architecture for generative adversarial networks. In Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition (pp. 4401-4410).

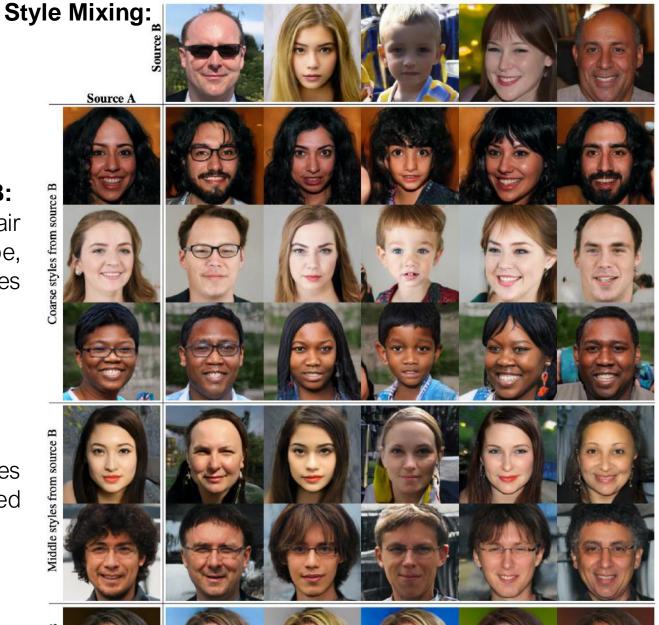


From source B:

Pose, general hair style, face shape, eyeglasses

Hair style, eyes open/closed

Color scheme and microstructure





# Supervised learning in practice

# Preprocessing Explore & prepare data

Data Visualization and Exploration

Identify patterns that can be leveraged for learning

Data Cleaning

- Missing data
- Noisy data
- Erroneous data

Scaling (Standardization)

Prepare data for use in scale-dependent algorithms.

Feature Extraction

Dimensionality reduction eliminates redundant information

**Model training** Supervised Learning Models: Linear models fine tune and KNN the model (enough to get started using supervised learning) Select model options Other algorithms and concepts: **Generative vs** discriminative models Parametric vs nonparametric models Model ensembles Feature/representation learning (neural networks, deep learning) How to control model overfit: regularization strategies for model refinement

**Performance** evaluation Make a prediction on validation data Evaluating model performance and comparing models Classification Precision Recall F How to make decisions using models Regression MSE, explained variance, R<sup>2</sup>