ETH
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inf | Informatik
Computer Science

Introduction to Machine Learning

Discriminative vs. Generative Modeling

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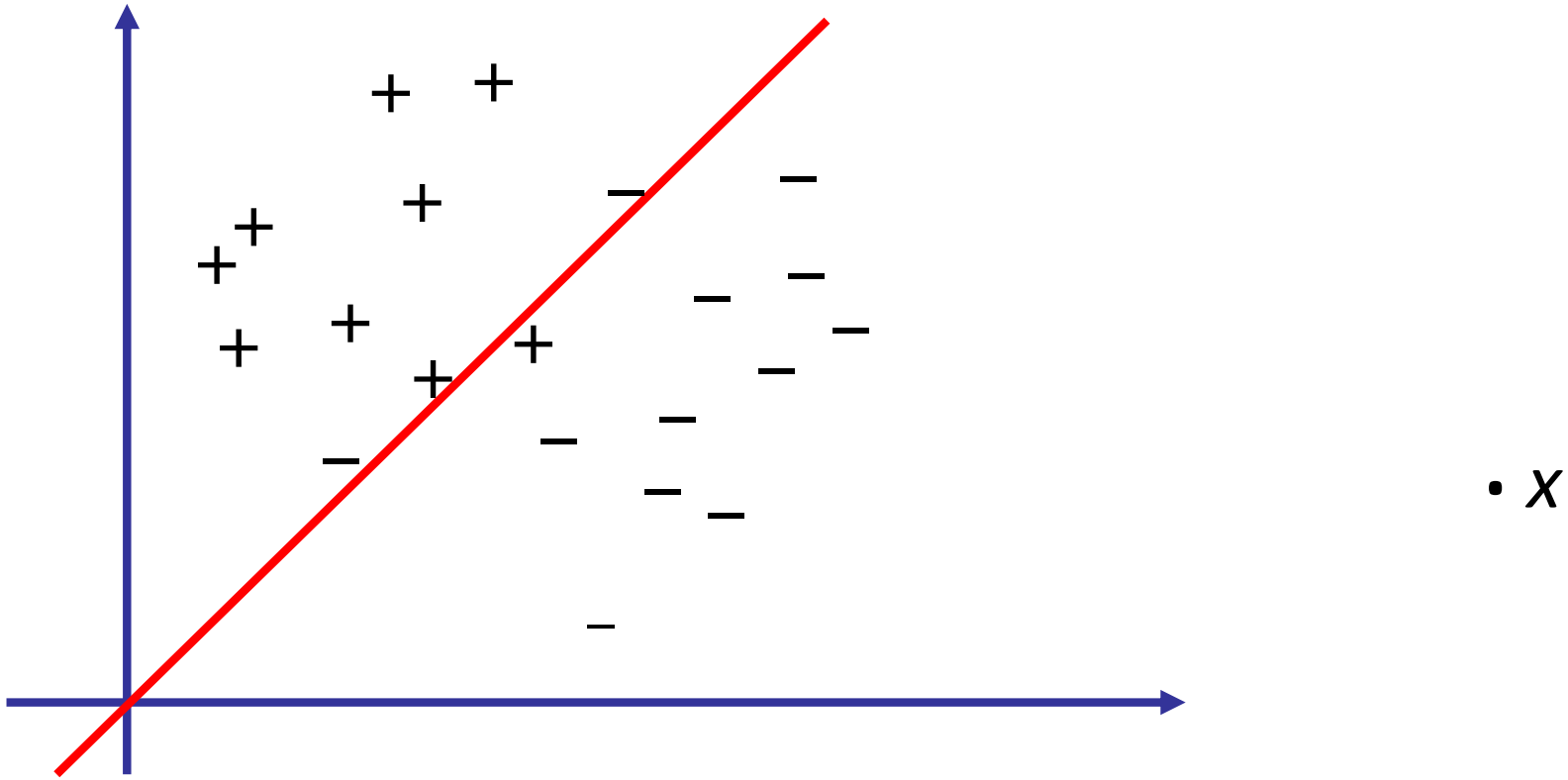
Motivating example: Logistic regression



- What will logistic regression predict for data point *x*?
- Logistic regression can be overconfident about labels for outliers

Discriminative vs. Generative models

- Discriminative models aim to estimate

$$P(y \mid \mathbf{x})$$

- Generative models aim to estimate joint distribution

$$P(y, \mathbf{x})$$

- Can derive conditional from joint distribution, but not vice versa!

Typical approach to generative modeling

1. Estimate prior on labels $P(y)$

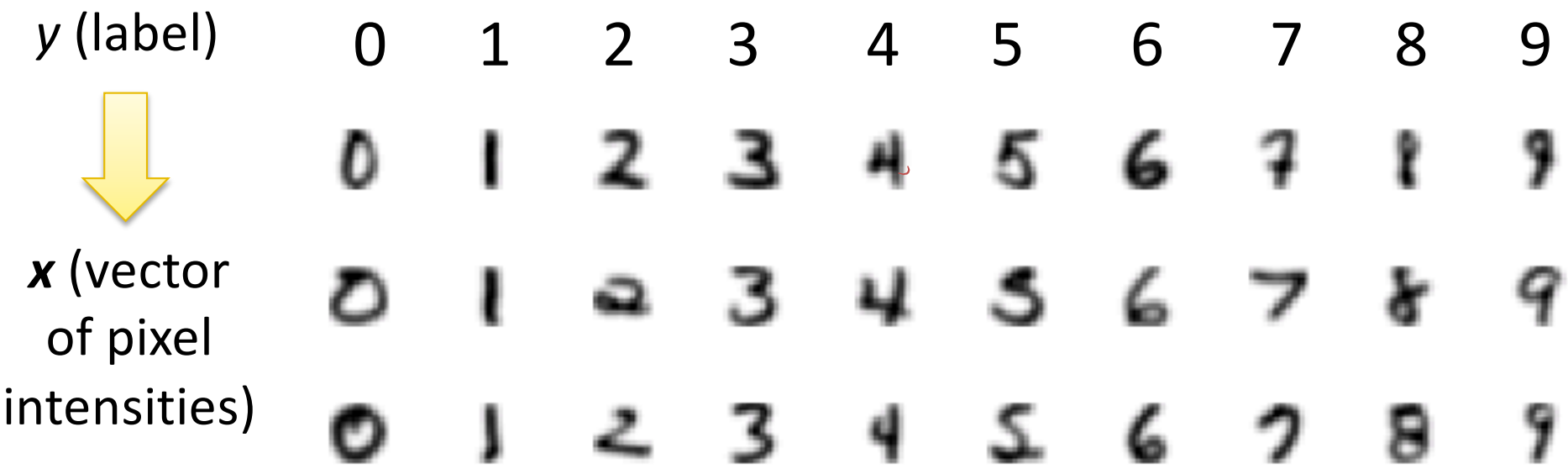
2. Estimate conditional distribution $P(\mathbf{x} \mid y)$ for each class *y*

3. Obtain predictive distribution using Bayes' rule:

$$P(y \mid \mathbf{x}) = \frac{1}{Z} P(y) P(\mathbf{x} \mid y)$$

A note on generative modeling

- Generative modeling attempts to infer the process, according to which examples are generated
- First generate class label $P(y)$
- Then, generate features given class $P(\mathbf{x} \mid y)$



Example: Naive Bayes Model

- Model class label as generated from categorical variable

$$P(Y = y) = p_y \qquad y \in \mathcal{Y} = \{1, \ldots, c\}$$

- Model features as conditionally independent given Y

$$P(X_1, \ldots, X_d \mid Y) = \prod_{i=1}^{d} P(X_i \mid Y)$$

- I.e., given class label, each feature is „generated“ independently of the other features.
- Need to still specify feature distributions $P(X_i \mid Y)$

Gaussian Naive Bayes Classifiers

- Learning given data $D = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)\}$
  - MLE for class prior: $\hat{P}(Y = y) = \hat{p}_y = \dfrac{\text{Count}(Y = y)}{n}$
  - MLE for feature distribution: $\hat{P}(x_i \mid y) = \mathcal{N}(x_i; \hat{\mu}_{y,i}, \sigma^2_{y,i})$

$$\hat{\mu}_{y,i} = \frac{1}{\text{Count(Y=y)}} \sum_{j:y_j=y} x_{j,i}$$

$$\sigma^2_{y,i} = \frac{1}{\text{Count(Y=y)}} \sum_{j:y_j=y} (x_{j,i} - \hat{\mu}_{y,i})^2$$

- Prediction given new point ***x:***

$$y = \arg\max_{y'} \hat{P}(y' \mid \mathbf{x}) = \arg\max_{y'} \hat{P}(y') \prod_{i=1}^{d} \hat{P}(x_i \mid y')$$

Gaussian NB vs. Logistic regression

- Gaussian NB with shared variance uses discriminant

$$f(\mathbf{x}) = \log \frac{P(Y=1 \mid \mathbf{x})}{P(Y=-1 \mid \mathbf{x})}$$

where $f(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + w_0$ and

$$w_0 = \log \frac{\hat{p}_+}{1-\hat{p}_+} + \sum_{i=1}^{d} \frac{\hat{\mu}^2_{-,i} - \hat{\mu}^2_{+,i}}{2\hat{\sigma}^2_i}$$

$$w_i = \frac{\mu_{+,i} - \mu_{-,1}}{\sigma^2_i}$$

- The corresponding class distribution

$$P(Y=1 \mid \mathbf{x}) = \frac{1}{1+\exp(-f(\mathbf{x}))} = \sigma(\mathbf{w}^T\mathbf{x} + w_0)$$

is of the same form as logistic regression!

- If model assumptions are met, GNB will make same predictions as Logistic Regression!

Issue with Naive Bayes models

- Conditional independence assumption means that features are generated independently given class label
- If there is (conditional) correlation between class labels, then this assumption is violated
- Due to conditional independence assumption, predictions can become overconfident (very close to 1 or 0)
- This might be fine if we care about most likely class only, but not if we want to use probilities for making decisions (e.g., asymmetric losses etc.)

More general: Gaussian Bayes classifiers

- Model class label as generated from categorical variable

$$P(Y = y) = p_y \qquad\qquad y \in \mathcal{Y} = \{1, \ldots, c\}$$

- Model features as generated by multivariate Gaussian

$$P(\mathbf{x} \mid y) = \mathcal{N}(\mathbf{x}; \mu_y, \Sigma_y)$$

- How do we estimate the parameters?

MLE for Gaussian Bayes Classifier

- Given data set $D = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)\}$
- MLE for class label distribution $\hat{P}(Y = y) = \hat{p}_y$

$$\hat{p}_y = \frac{\text{Count}(Y = y)}{n}$$

- MLE for feature distribution $\hat{P}(\mathbf{x} \mid y) = \mathcal{N}(\mathbf{x}; \hat{\mu}_y, \hat{\Sigma}_y)$

$$\hat{\mu}_y = \frac{1}{\text{Count(Y=y)}} \sum_{i:y_i=y} \mathbf{x}_i$$

$$\hat{\Sigma}_y = \frac{1}{\text{Count(Y=y)}} \sum_{i:y_i=y} (\mathbf{x}_i - \hat{\mu}_y)(\mathbf{x}_i - \hat{\mu}_y)^T$$

Discriminant functions for GBCs

- Given: $P(Y = 1) = p$ and $P(\mathbf{x} \mid y) = \mathcal{N}(\mathbf{x}; \mu_y, \Sigma_y)$
- Want:

$$f(\mathbf{x}) = \log \frac{P(Y = 1 \mid \mathbf{x})}{P(Y = -1 \mid \mathbf{x})}$$

- This discriminant function is given by

$$f(\mathbf{x}) = \log \frac{p}{1-p} + \frac{1}{2}\left[\log \frac{|\hat{\Sigma}_-|}{|\hat{\Sigma}_+|} + \left((\mathbf{x} - \hat{\mu}_-)^T \hat{\Sigma}_-^{-1} (\mathbf{x} - \hat{\mu}_-)\right) - \left((\mathbf{x} - \hat{\mu}_+)^T \hat{\Sigma}_+^{-1} (\mathbf{x} - \hat{\mu}_+)\right)\right]$$

Fisher's linear discriminant analysis LDA (c=2)

- Suppose we fix *p=.5*
- Further, assume covariances are equal: $\hat{\Sigma}_- = \hat{\Sigma}_+ = \hat{\Sigma}$
- Then the discriminant function

$$f(\mathbf{x}) = \log \frac{p}{1-p} + \frac{1}{2}\left[\log \frac{|\hat{\Sigma}_-|}{|\hat{\Sigma}_+|} + \left((\mathbf{x}-\hat{\mu}_-)^T\hat{\Sigma}_-^{-1}(\mathbf{x}-\hat{\mu}_-)\right) - \left((\mathbf{x}-\hat{\mu}_+)^T\hat{\Sigma}_+^{-1}(\mathbf{x}-\hat{\mu}_+)\right)\right]$$

simplifies: $f(\mathbf{x}) = \mathbf{x}^T\hat{\Sigma}^{-1}(\hat{\mu}_+ - \hat{\mu}_-) + \frac{1}{2}(\hat{\mu}_-^T\Sigma^{-1}\hat{\mu}_- - \hat{\mu}_+^T\Sigma^{-1}\hat{\mu}_+)$

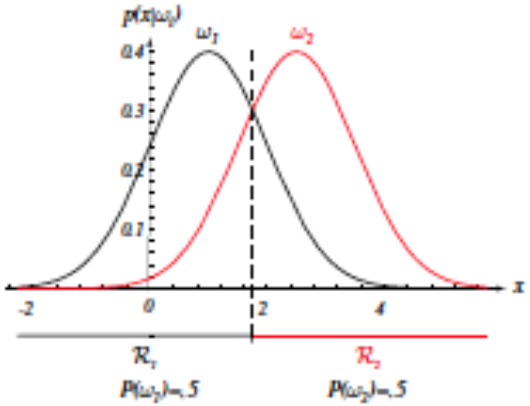
- Under these assumptions, we predict

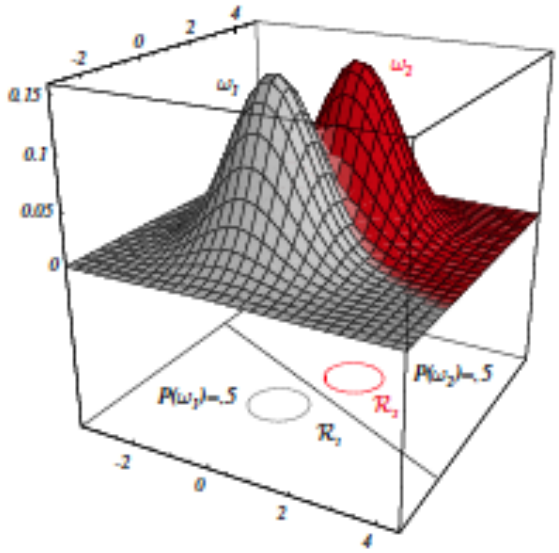
$$y = \text{sign}(f(\mathbf{x})) = \text{sign}(\mathbf{w}^T\mathbf{x} + w_0) \quad \mathbf{w} = \hat{\Sigma}^{-1}(\hat{\mu}_+ - \hat{\mu}_-)$$

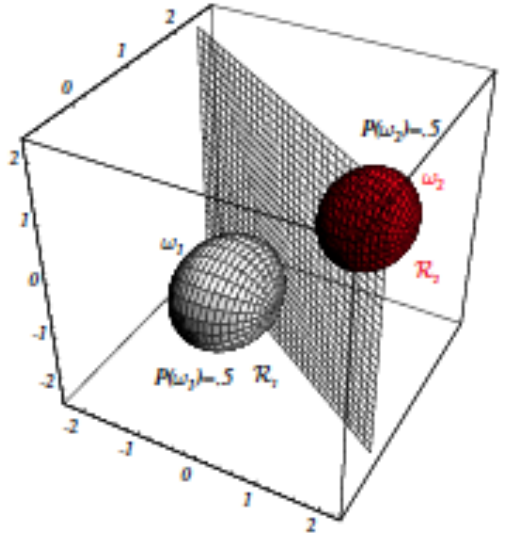
$$w_0 = \frac{1}{2}(\hat{\mu}_-^T\Sigma^{-1}\hat{\mu}_- - \hat{\mu}_+^T\Sigma^{-1}\hat{\mu}_+)$$

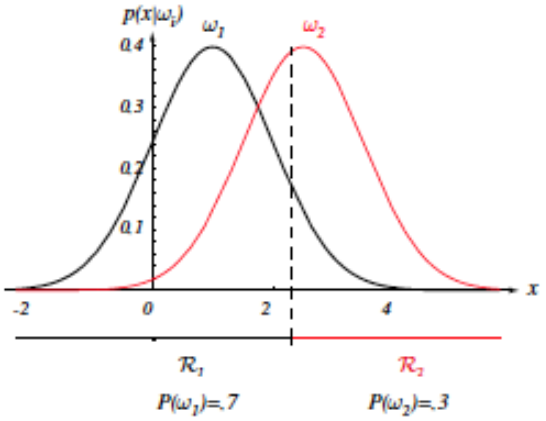
- This linear classifier is called Fisher's linear discriminant analysis

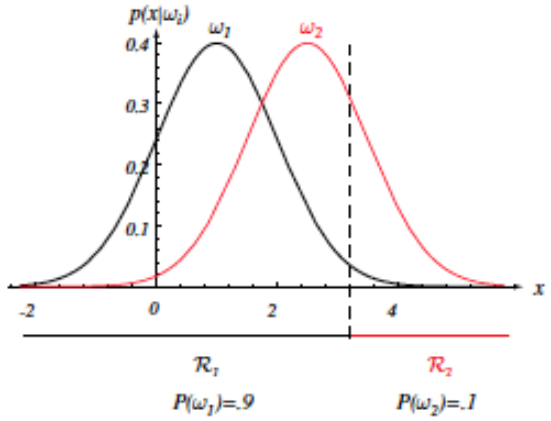
Illustration

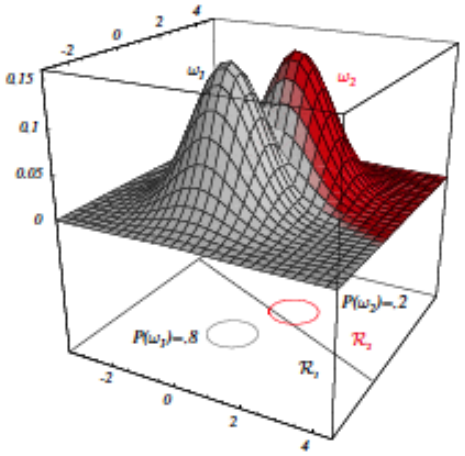


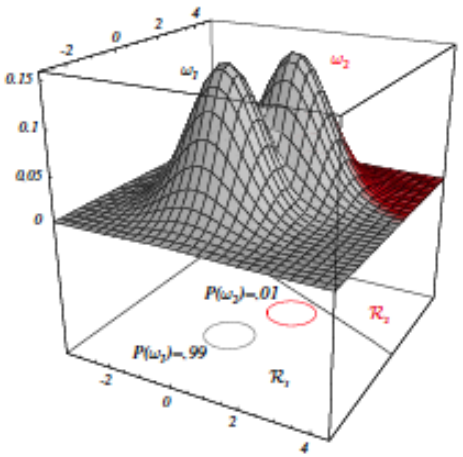


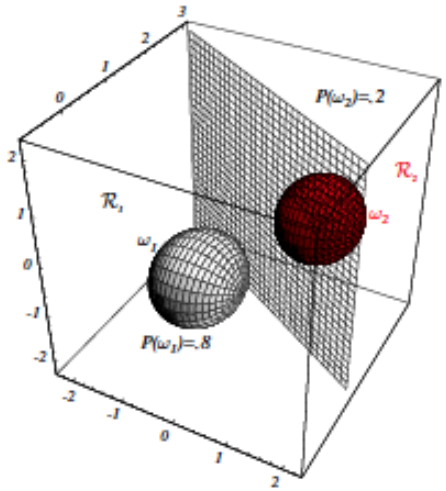


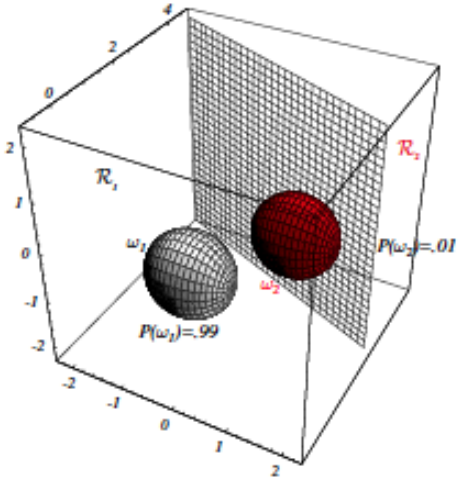

$p(x|\omega_i)$
ω_1
ω_2
0.4
0.3
0.2
0.1
x
-2
0
2
4
$\mathcal{R}_1$
$\mathcal{R}_2$
$P(\omega_1)=.7$
$P(\omega_2)=.3$


$p(x|\omega_i)$
ω_1
ω_2
0.4
0.3
0.2
0.1
x
-2
0
2
4
$\mathcal{R}_1$
$\mathcal{R}_2$
$P(\omega_1)=.9$
$P(\omega_2)=.1$


0.15
0.1
0.05
0
ω_1
ω_2
$P(\omega_2)=.2$
$P(\omega_1)=.8$
$\mathcal{R}_2$
$\mathcal{R}_1$


0.15
0.1
0.05
0
ω_1
ω_2
$P(\omega_2)=.01$
$P(\omega_1)=.99$
$\mathcal{R}_2$
$\mathcal{R}_1$


$P(\omega_2)=.2$
$\mathcal{R}_2$
$\mathcal{R}_1$
ω_2
ω_1
$P(\omega_1)=.8$


$\mathcal{R}_2$
$\mathcal{R}_1$
$P(\omega_2)=.01$
ω_2
ω_1
$P(\omega_1)=.99$

Fisher's LDA vs. Logistic regression

- Fisher's LDA uses the discriminant function:

$$f(\mathbf{x}) = \log \frac{P(Y=1 \mid \mathbf{x})}{P(Y=-1 \mid \mathbf{x})}$$

where $f(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + w_0$ and $\mathbf{w} = \hat{\Sigma}^{-1}(\hat{\mu}_+ - \hat{\mu}_-)$

$$w_0 = \frac{1}{2}(\hat{\mu}_-^T\Sigma^{-1}\hat{\mu}_- - \hat{\mu}_+^T\Sigma^{-1}\hat{\mu}_+)$$

- Can derive the class distribution

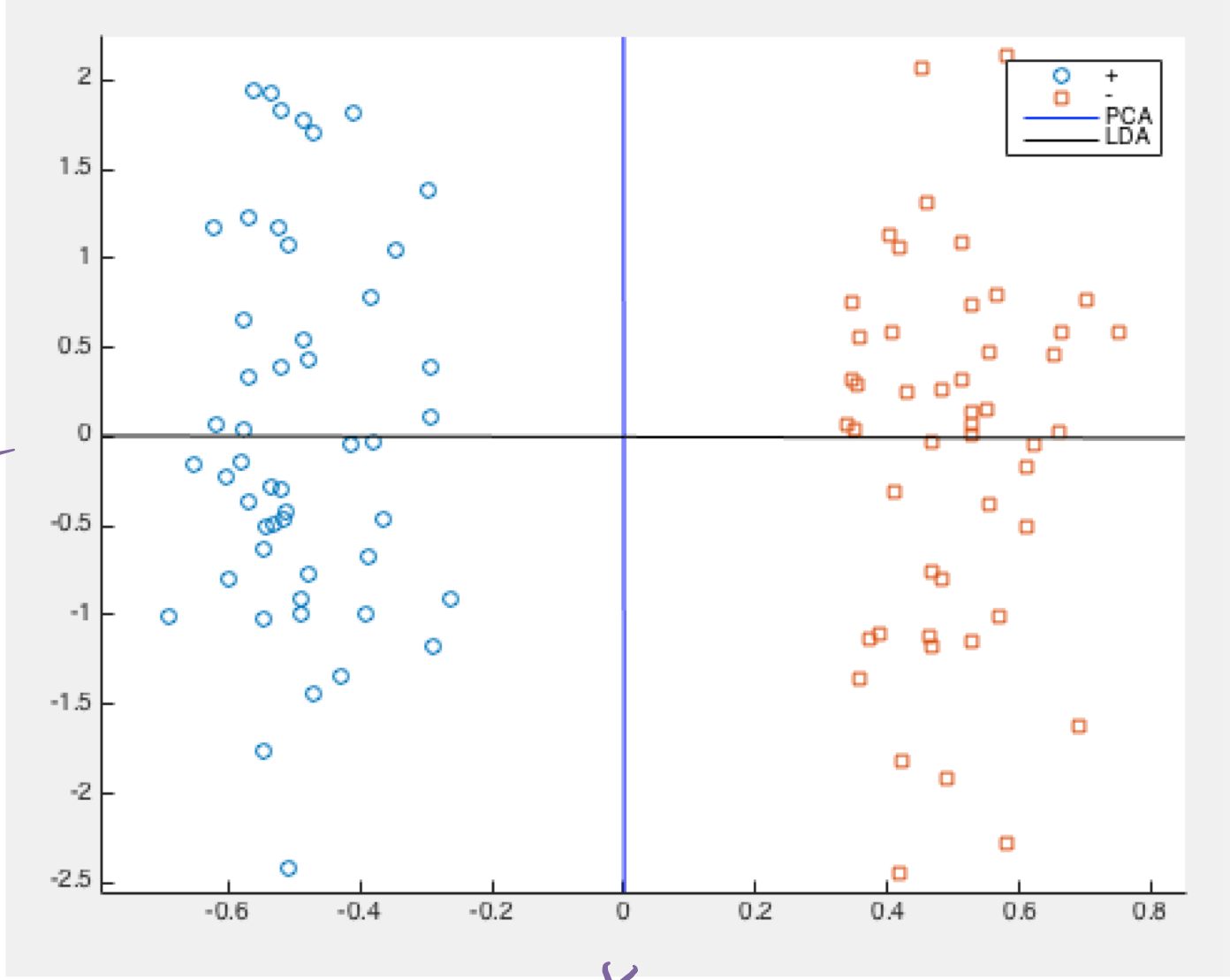
$$P(Y=1 \mid \mathbf{x}) = \frac{1}{1+\exp(-f(\mathbf{x}))} = \sigma(\mathbf{w}^T\mathbf{x} + w_0)$$

- This is the same form as logistic regression*!
- If model assumptions are met, LDA will make same predictions as Logistic Regression!

LDA vs. PCA

- LDA can be viewed as a projection to a 1-dim. subspace that maximizes ratio of between-class and within-class variances
- In constrast, PCA (k=1) maximizes the variance of the resulting 1-dim. projection

LDA vs. PCA



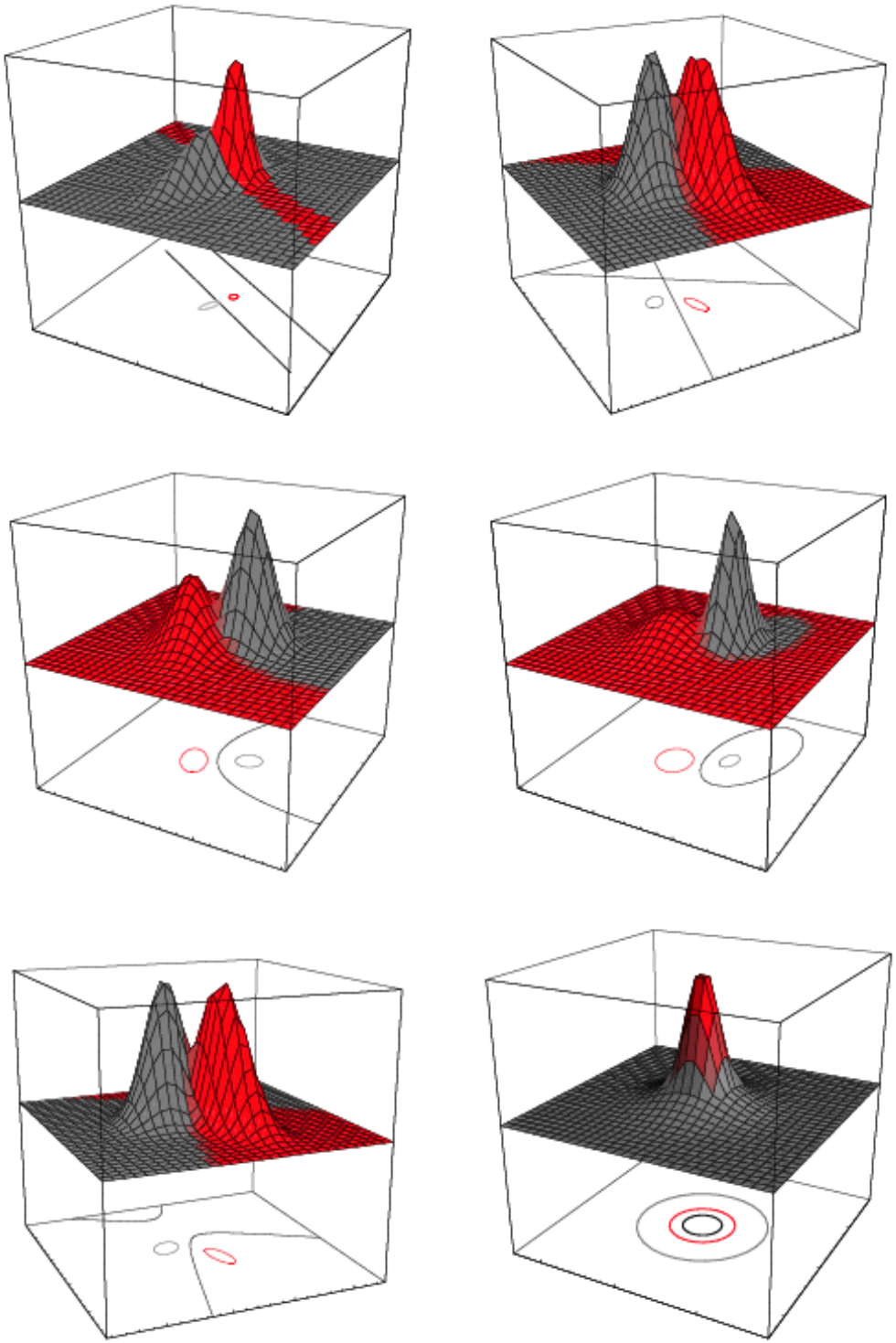
Quadratic discriminant analysis

- In the general case,

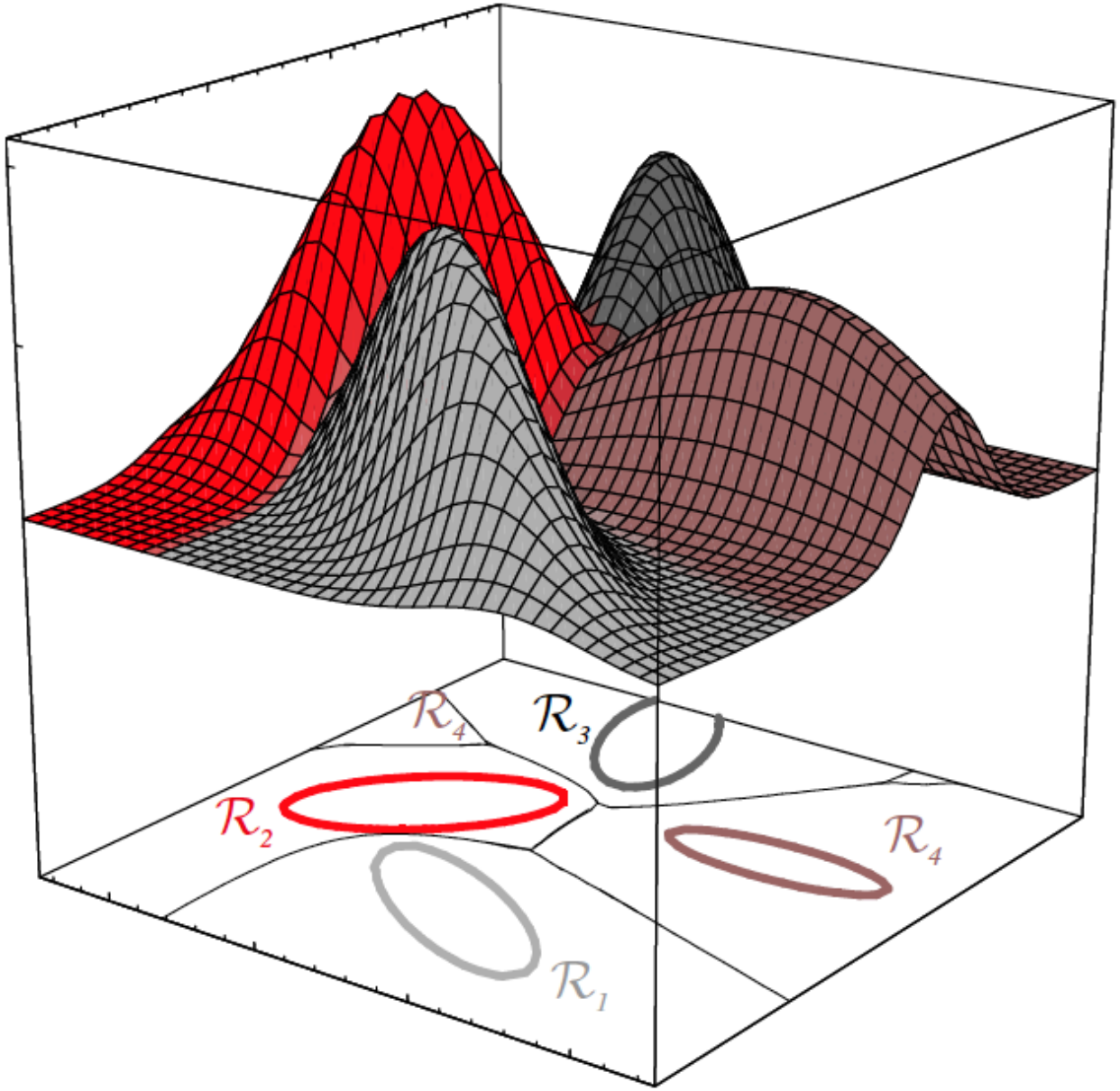
$$f(\mathbf{x}) = \log \frac{p}{1-p} + \frac{1}{2}\left[\log \frac{|\hat{\Sigma}_-|}{|\hat{\Sigma}_+|} + \left((\mathbf{x}-\hat{\mu}_-)^T \hat{\Sigma}_-^{-1}(\mathbf{x}-\hat{\mu}_-)\right) - \left((\mathbf{x}-\hat{\mu}_+)^T \hat{\Sigma}_+^{-1}(\mathbf{x}-\hat{\mu}_+)\right)\right]$$

- and we predict $y = \text{sign}(f(\mathbf{x}))$

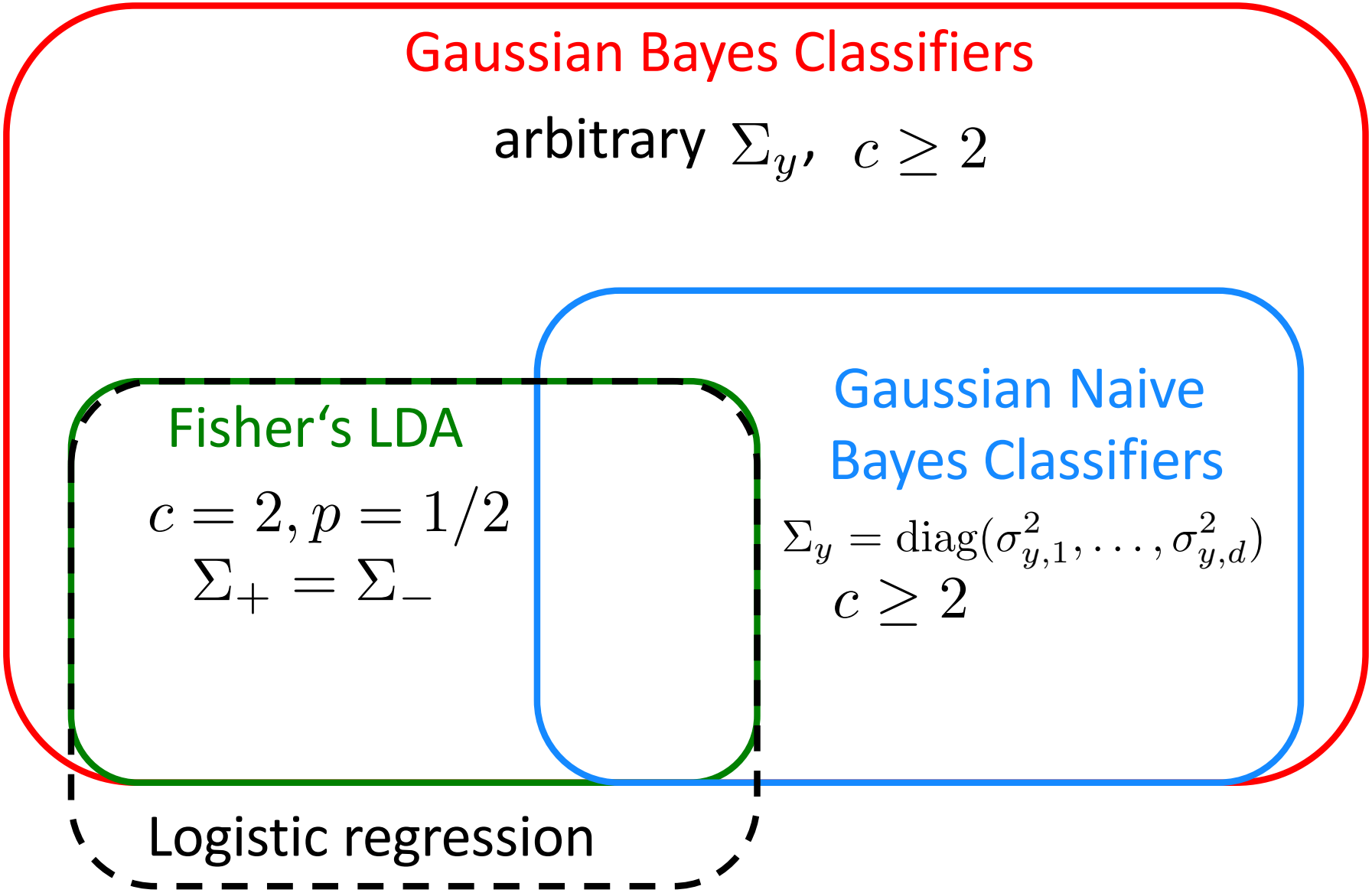
- This is called quadratic discriminant analysis



Multiple classes



Gaussian Bayes Classifiers Big Picture



Fisher‘s LDA vs. Logistic regression

- Fisher‘s LDA
  - Generative model, i.e., models $P(\boldsymbol{X}, Y)$
  - Can be used to detect outliers: $P(\boldsymbol{X}) < t$
  - Assumes normality of $\boldsymbol{X}$
  - not very robust against violation of this assumption
- Logistic regression
  - Discriminative model, i.e., models $P(Y|\boldsymbol{X})$ only
  - Cannot detect outliers
  - Makes no assumptions on $\boldsymbol{X}$
  - More robust

Gaussian Naive Bayes vs. General GBCs

- Gaussian Naive Bayes models
  - Conditional independence assumption may lead to overconfidence
  - Predictions might still be useful
  - #parameters = O(c d)
  - Complexity (memory + inference) linear in d
- General Gaussian Bayes models
  - Captures correlations among features
  - Avoids overconfidence
  - #parameters = O(c d^2)
  - Complexity quadratic in d

What if we have discrete features?

- So far we assumed that $\mathbf{x} \in \mathbb{R}^d$
- Suppose some X_i take discrete values
  - Gender
  - Nationality
  - …
- Might not make sense to model X_i as a Gaussian
- Generative models allow to easily swap different distributions. E.g., model $P(X_i|Y)$ as
  - Bernoulli
  - Categorial
  - Multinomial
  - …

Example: Categorical *Naive* Bayes classifiers

- Model class label as generated from categorical variable

$$P(Y = y) = p_y \qquad\qquad y \in \mathcal{Y} = \{1, \ldots, c\}$$

- Model features by (conditionally) independent categorical random variables

$$P(X_i = c \mid Y = y) = \theta^{(i)}_{c|y}$$

- How do we estimate the parameters?

MLE for Categorial Naive Bayes Classifier

- Given data set $D = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)\}$
- MLE for class label distribution $\hat{P}(Y = y) = \hat{p}_y$

$$\hat{p}_y = \frac{\text{Count}(Y = y)}{n}$$

- MLE for distribution of feature i $\hat{P}(X_i = c \mid y) = \theta^{(i)}_{c|y}$

$$\theta^{(i)}_{c|y} = \frac{\text{Count}(X_i = c, Y = y)}{\text{Count}(Y = y)}$$

Categorical Naive Bayes Classifiers

- Learning given data $D = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)\}$
  - MLE for class prior: $\hat{P}(Y = y) = \hat{p}_y = \dfrac{\text{Count}(Y = y)}{n}$
  - MLE for distribution of feature i: $\hat{P}(X_i = c \mid y) = \theta^{(i)}_{c|y}$

$$\theta^{(i)}_{c|y} = \frac{\text{Count}(X_i = c, Y = y)}{\text{Count}(Y = y)}$$

- Prediction given new point ***x:***

$$y = \arg\max_{y'} \hat{P}(y' \mid \mathbf{x}) = \arg\max_{y'} \hat{P}(y') \prod_{i=1}^{d} \hat{P}(x_i \mid y')$$

Beyond categorical Naive Bayes

- Could in principle lift the Naive Bayes assumption by modeling joint (conditional) distribution of the features: $P(X_1,\ldots,X_d|Y)$
- What's the issue?

- Requires exponentially (in d) many parameters
  - Computationally intractable
  - Fantastic way to overfit!
- Remedy: Graphical models / Bayesian networks (see Probabilistic AI course)

What if I have both discrete and continuous features?

- The (Naive) Bayes classifier does not require each feature to follow the same type of conditional distribution
- For example, can model some features as Gaussian, and some others as categorical
- Training (MLE) and prediction remains the same!

Avoiding overfitting

- So far we always used Maximum Likelihood Estimation -- didn‘t we say that‘s prone to overfitting?
- Can avoid overfitting by
  - Restricting model class (e.g., assumptions on covariance structure, e.g., Gaussian Naive Bayes) ➔ fewer parameters
  - Using priors ➔ „smaller“ parameters

Prior over parameters (case c=2)

- As prior for our class probabilities, have assumed

$$P(Y = 1) = \theta$$

- Maximum likelihood estimate: $\hat{\theta} = \frac{\text{Count}(Y = 1)}{n}$

- What happens in the extreme case *n=1*?

Prior over parameters (case c=2)

- As prior for our class probabilities, have assumed

$$P(Y = 1) = \theta$$

- Maximum likelihood estimate: $\hat{\theta} = \frac{\text{Count}(Y = 1)}{n}$

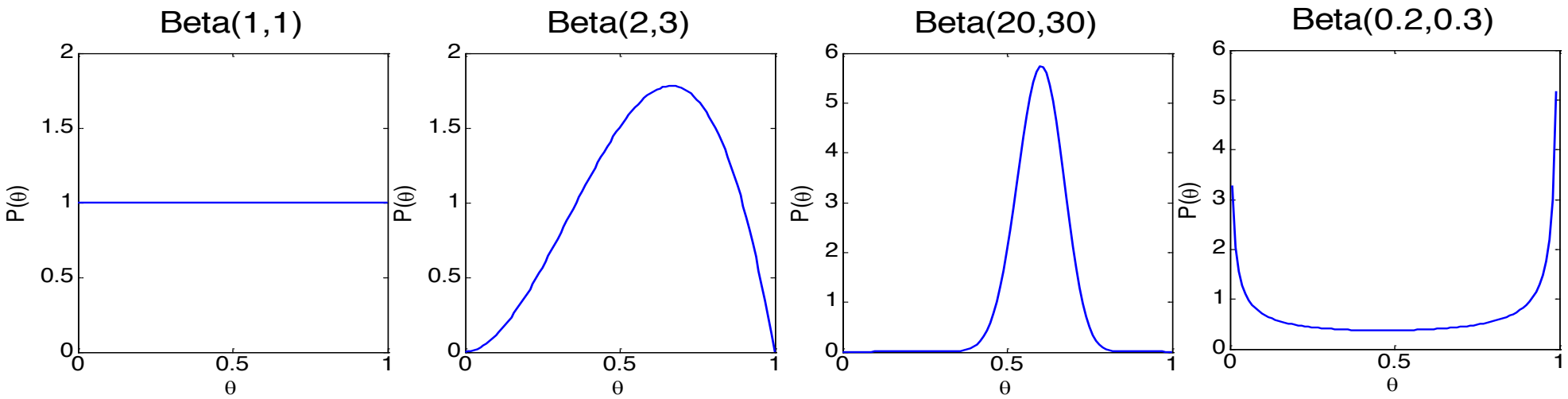
- May want to put prior distribution $P(\theta)$ and compute posterior distribution

$$P(\theta \mid y_1, \ldots, y_n)$$

- In which cases can we do this efficiently?

Beta prior over parameters

$$\text{Beta}(\theta; \alpha_+, \alpha_-) = \frac{1}{B(\alpha_+, \alpha_-)} \theta^{\alpha_+ - 1} (1-\theta)^{\alpha_- - 1}$$



Conjugate distributions

- A pair of prior distributions and likelihood functions is called conjugate if the posterior distribution remains in the same family as the prior
- **Example**: Beta priors and Binomial likelihood
  - **Prior**: $\mathrm{Beta}(\theta; \alpha_+, \alpha_-)$
  - **Observations**: Suppose we observe n_+ positive and n_- negative labels
  - **Posterior**: $\mathrm{Beta}(\theta; \alpha_+ + n_+, \alpha_- + n_-)$
- Thus α_+, α_- act as „pseudo-counts“
- **MAP estimate**:

$$\hat{\theta} = \arg\max_{\theta} P(\theta \mid y_1, \ldots, y_n; \alpha_+, \alpha_-) = \frac{\alpha_+ + n_+ - 1}{\alpha_+ + n_+ + \alpha_- + n_- - 2}$$

Conjugate priors

Prior / Posterior	**Likelihood function**
Beta	Bernoulli/Binomial
Dirichlet	Categorical/Multinomial
Gaussian (fixed covariance)	Gaussian
Gaussian-inverse Wishart	Gaussian
Gaussian process	Gaussian

- Can use conjugate priors as regularizers
- (Almost) no computational cost
- How to choose hyperparameters??
  - crossvalidation ☺

Summary: Generative vs Discriminative

- **Discriminative models**
  - Model $P(y|\boldsymbol{x})$. Do not attempt to model $P(\boldsymbol{x})$
  - Cannot detect outliers (property of P(x))
  - Are typically more robust, since accurately modeling $\boldsymbol{x}$ may be difficult
- **Generative models**
  - Model joint distribution $P(\boldsymbol{x},y)$
  - This is a strictly more ambitious goal!
  - Can be more powerful (e.g., detect outliers) if model assumptions are met
  - Are typically less robust against outliers

What you need to be able to do

- Apply (Gaussian / Categorical) Naive Bayes classifiers
- Relate different Gaussian Bayes classifiers
  - Naive Bayes
  - Fisher's LDA
  - General GBCs
- Use pseudocounts / conjugate priors as regularizers
- Compute distributions over features, and use them for outlier / anomaly detection

Representation/ features	Linear hypotheses; nonlinear hypotheses with nonlinear feature transforms, kernels, learn nonlinear features via neural nets		
Paradigm:	Discriminative vs. generative		
Probabilistic / Optimization	Likelihood	*	Prior
	Loss-function	+	Regularization
Model:	Squared loss = Gaussian lik., 0/1, Perceptron, Hinge, cost sensitive, multi-class hinge, reconstruction error, logistic loss=Bernoulli lik., cross-entropy loss=Categorical lik.		L^2 norm (=Gaussian prior), L^1 norm (=Laplace prior), early stopping, dropout Categorical;. Beta/Dirichlet priors
Method:	Exact solution, Gradient Descent, (mini-batch) SGD, Reductions, Bayesian model averaging		
Evaluation metric:	Mean squared error, Accuracy, F1 score, AUC, Confusion matrices, compression performance, log-likelihood on validation set		
Model selection:	K-fold Cross-Validation, Monte Carlo CV, Bayesian model selection		