Classification: Three Different Methods

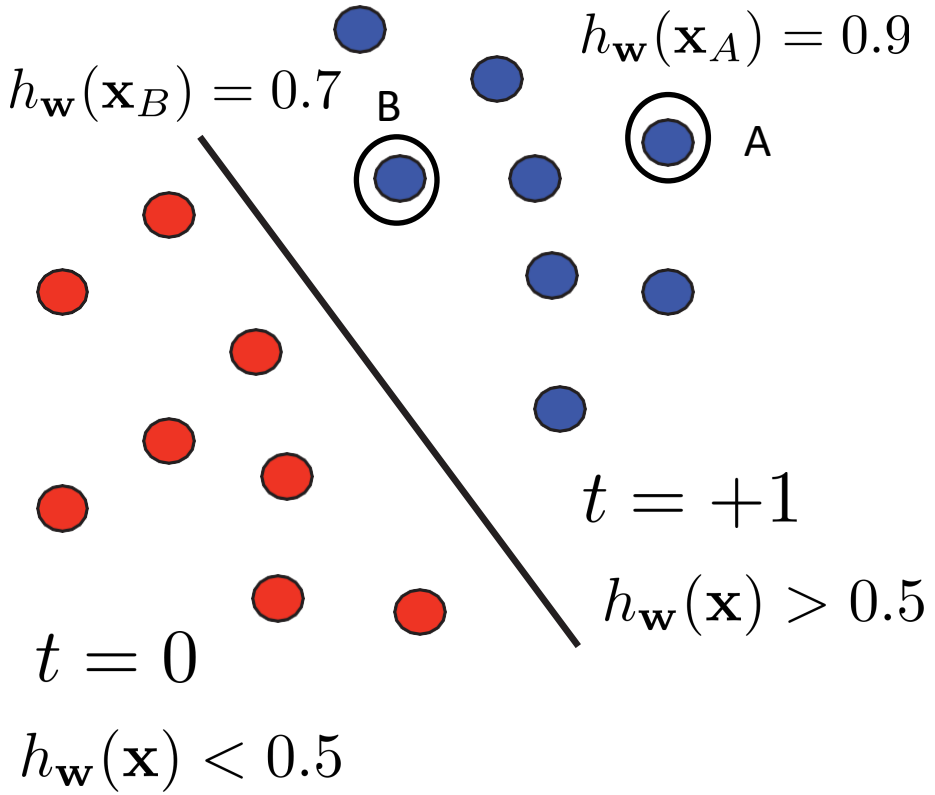
- **Discriminant models**
  - Given training data, assign each data x to one class C_k via a discriminant function
  - *Do not consider distribution* of the training data

- **Probabilistic discriminant models**
  - Given training data, model the posterior class distribution $p(C_k|x)$
  - Use the distribution $p(C_k|x)$ to perform classification for testing data

- **Probabilistic generative models**
  - Given training data, model the joint (data, class) distribution $p(x,C_k)$
  - Find class-conditional distribution $p(x|C_k)$ and class prior distribution $p(C_k)$
  - Then use Bayes rule to compute $p(C_k|x) \sim p(x|C_k)\,p(C_k)$

Probabilistic Generative Models: Gaussian Discriminant Analysis & Naïve Bayes Classifier

Recap: Logistic Regression

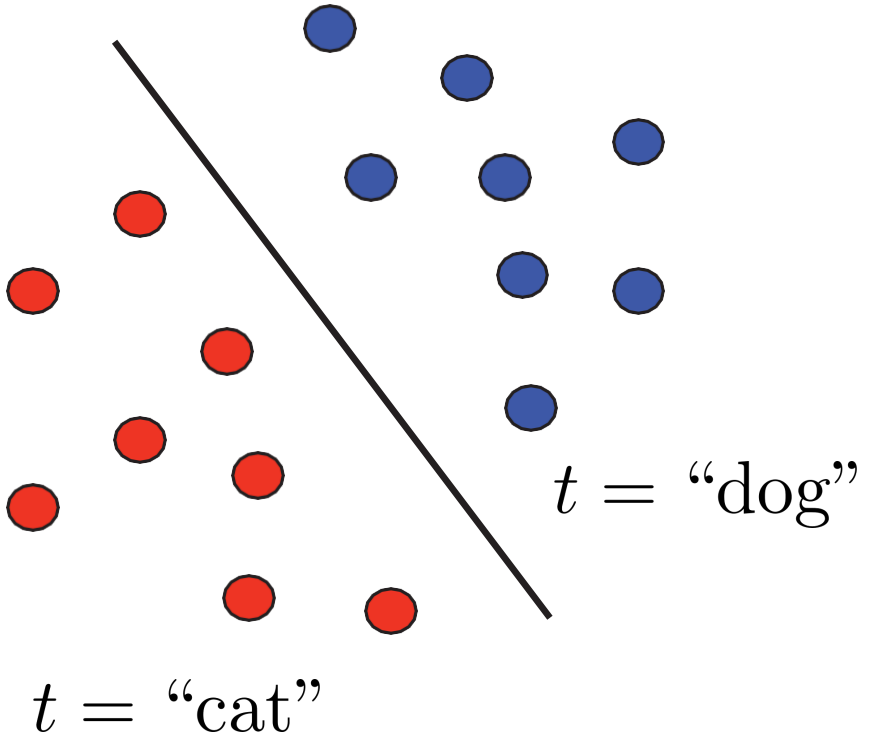


Model conditional/posterior distribution of t given x

$$p(t|\mathbf{x};\mathbf{w}) = ?$$

$$p(t=1|\mathbf{x};\mathbf{w})$$
$$= \frac{1}{1+\exp(-\mathbf{w}^T\mathbf{x})}$$
$$= h_{\mathbf{w}}(\mathbf{x})$$

Classification: Different Perspectives



Consider a classification problem: distinguish **dogs** (t = 1) vs **cats** (t = 0) based on features of an animal

Logistic regression: find a decision boundary to separate **cats** and **dogs**, via modeling **cat/dog label posterior distribution** given animal features

$$p(t = \text{“dog”}|\mathbf{x}) \textbf{ vs } p(t = \text{“cat”}|\mathbf{x})$$

A different perspective

- Look at dogs to build a model of what dogs look like
- Look at cats to build another model of what cats look like
- To classify a new animal, we match it to the dog/cat model, and see whether it looks more like the dog or cat

$$p(\mathbf{x}|t = \text{“dog”}) \textbf{ vs } p(\mathbf{x}|t = \text{“cat”})$$

Probabilistic Generative vs. Discriminative Models

Discriminative models: $p(t|\mathbf{x})$ Label posterior probability

Learn mappings directly from the space of inputs to the space of labels

Generative models: $p(\mathbf{x}|t)$ Likelihood $p(t)$ Label prior

Data generation process: model distribution of likelihood & label prior

Bayes rule to derive label t's posterior distribution given x

$$p(t|\mathbf{x}) = \frac{p(\mathbf{x}|t) \cdot p(t)}{p(\mathbf{x})}$$

$p(\mathbf{x})$ Normalization constant

Prediction $\arg\max_t p(t|\mathbf{x}) = \arg\max_t p(\mathbf{x}|t)p(t)$

Preliminaries

Bayes Rule

Joint probability distribution

$$P(A, B) = P(A|B)P(B) = P(B|A)P(A)$$

P(A|B) (P(B|A)): **Conditional probability** of event A (B) given event B (A) happens

P(A) (P(B)): **Prior probability** of observing event A (B)

Bayes Rule $$P(A|B) = \frac{P(B|A)P(A)}{P(B)}$$

Law of total probability $$P(B) = \sum_a P(A = a, B) = \sum_a P(B|A = a)P(A = a)$$

Multivariate Gaussian/Normal Distribution

$$p(\mathbf{x} \in \mathbb{R}^d; \mu, \Sigma) = \frac{1}{(2\pi)^{d/2}|\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(\mathbf{x}-\mu)^T \Sigma^{-1}(\mathbf{x}-\mu)\right)$$

$$\mathbf{x} \sim \mathcal{N}(\mu, \Sigma)$$

Mean vector: $\mu \in \mathbb{R}^d$ $\quad \mathbb{E}(\mathbf{x}) = \int_{\mathbf{x}} \mathbf{x} p(\mathbf{x}; \mu, \Sigma) d\mathbf{x} = \mu$

Covariance matrix: $\Sigma \in \mathbb{R}^{d \times d}$ $\quad \mathrm{Cov}(\mathbf{x}) = \mathbb{E}[(\mathbf{x} - \mathbb{E}[\mathbf{x}])(\mathbf{x} - \mathbb{E}[\mathbf{x}])^T] = \Sigma$

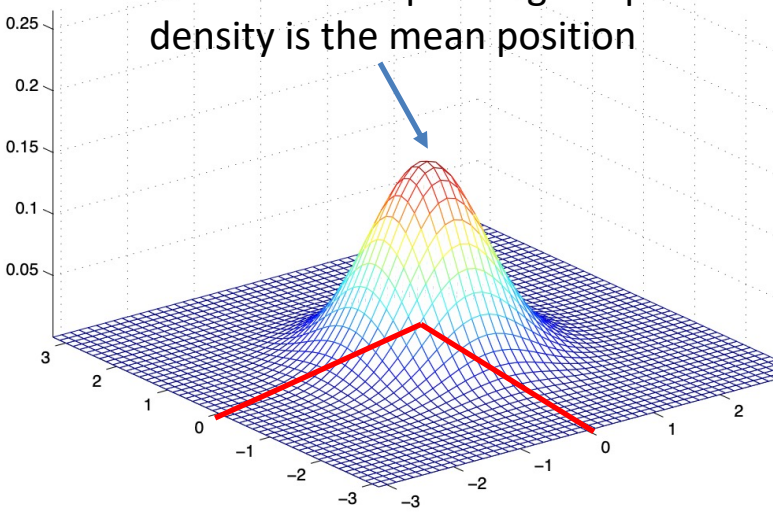
Determinant: $|\Sigma|$

Symmetric: $\Sigma^T = \Sigma$

Positive semi-definite: $\mathbf{v}^T \Sigma \mathbf{v} \geq 0, \forall \mathbf{v} \in \mathbb{R}^d$

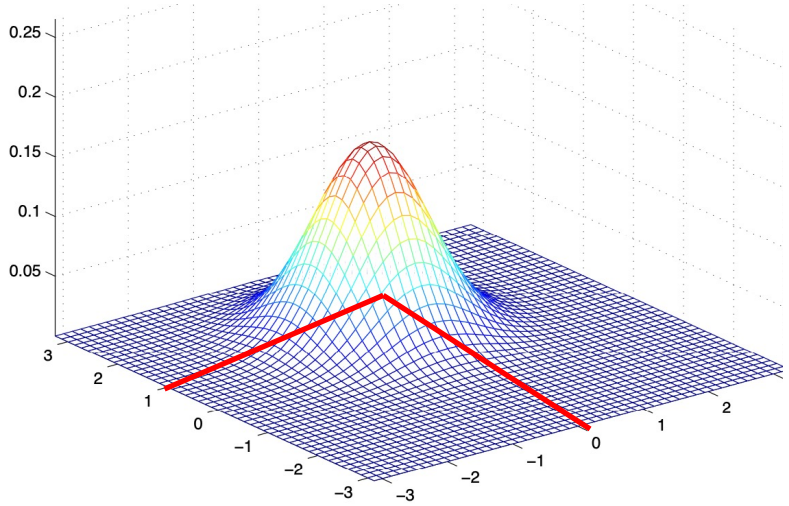
Density of Gaussian Distributions

Position corresponding the peak density is the mean position

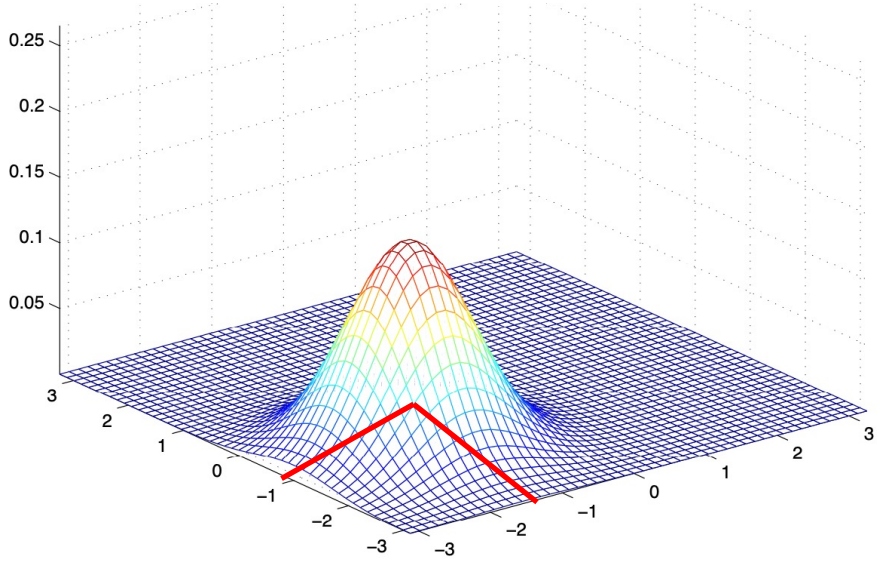


$$\mathcal{N}([0;0], \Sigma = \mathbf{I})$$

Standard Gaussian distribution



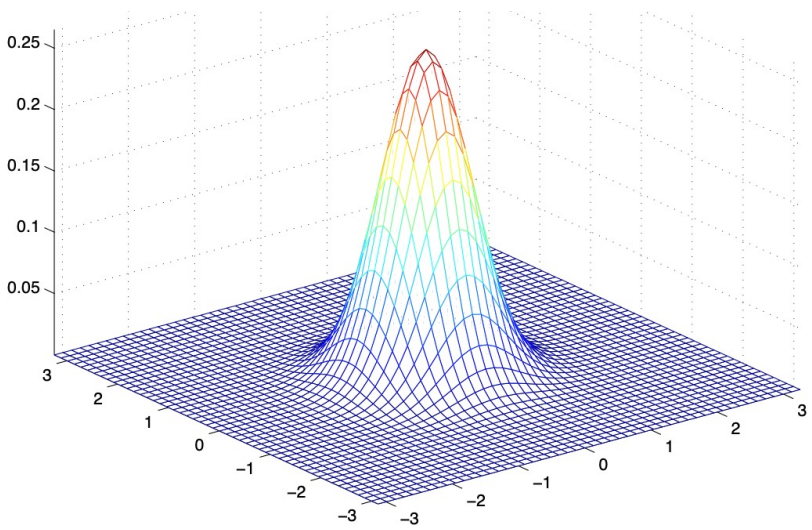
$$\mathcal{N}([1;0]; \Sigma = \mathbf{I})$$



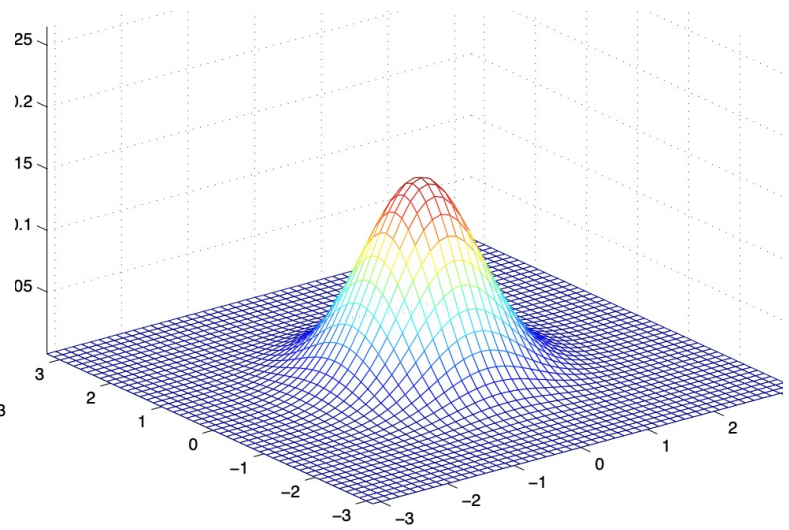
$$\mathcal{N}([-1;-1.5]; \Sigma = \mathbf{I})$$

Varying mean μ, move the peak positions of the density, but the density shapes are the same

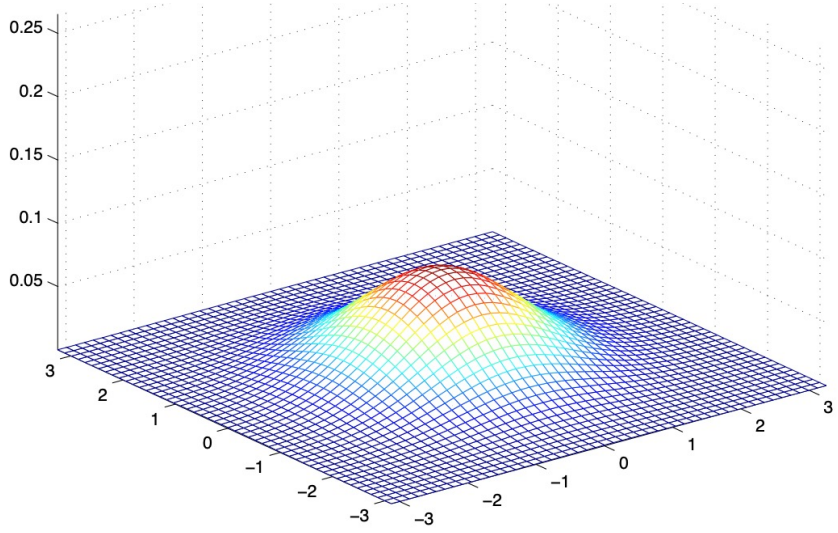
Density of Gaussian Distributions



$$\mathcal{N}([0;0], \Sigma = 0.6\mathbf{I})$$



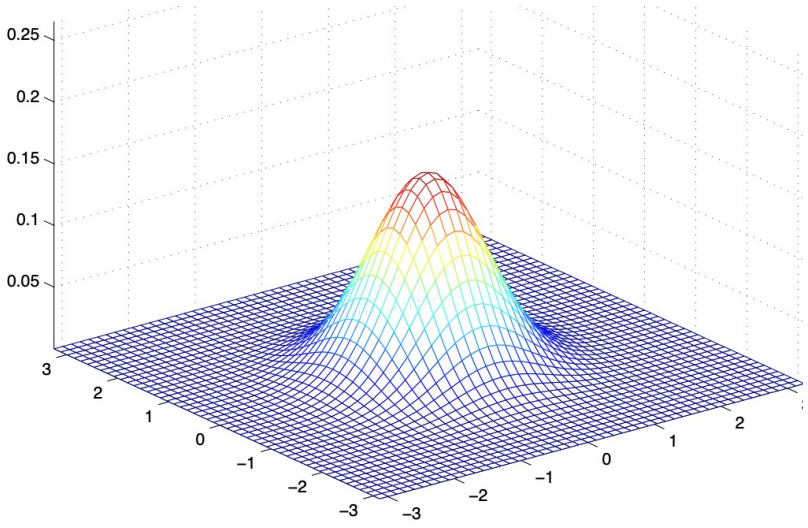
$$\mathcal{N}([0;0], \Sigma = \mathbf{I})$$



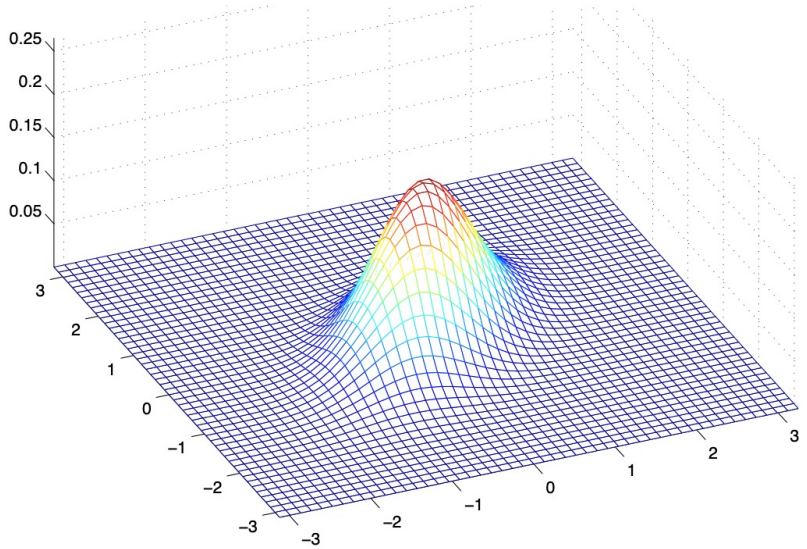
$$\mathcal{N}([0;0]\Sigma = 2\mathbf{I})$$

Σ ***larger*** (*smaller*), Gaussian becomes more spread-out (compressed)

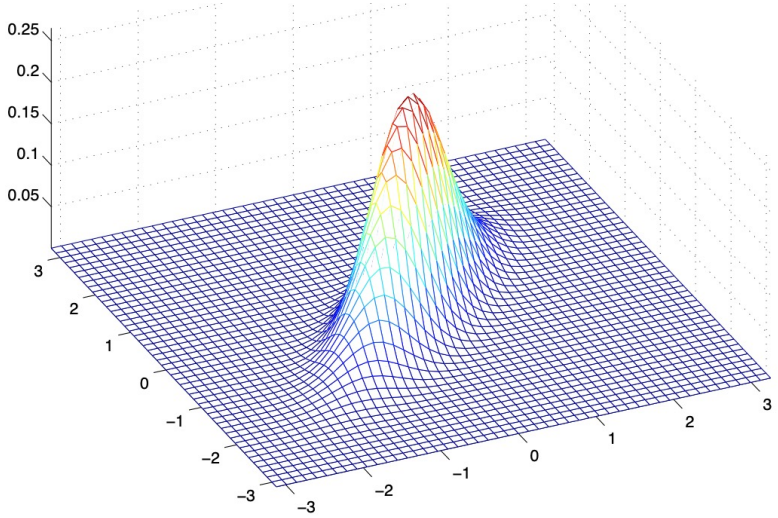
Density of Gaussian Distributions



$$\mathcal{N}([0;0], \Sigma = \mathbf{I})$$



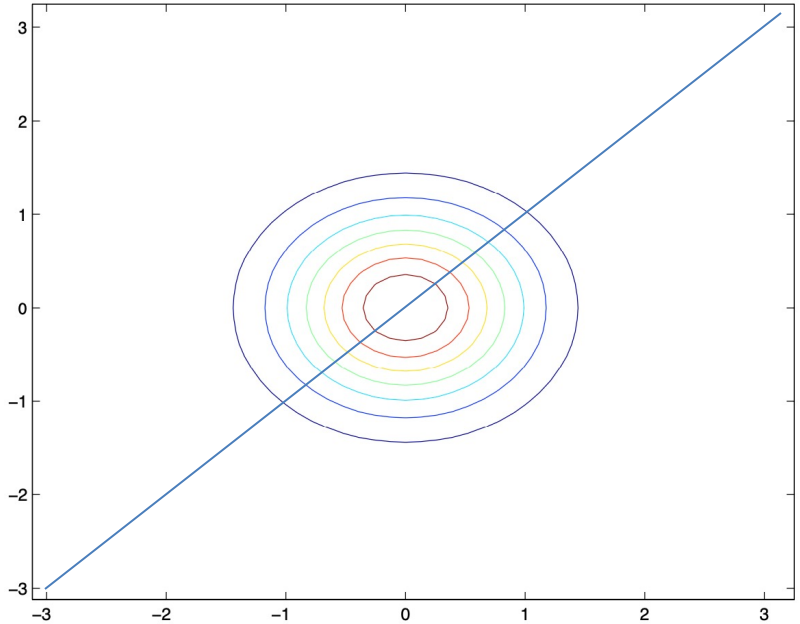
$$\mathcal{N}([0;0], \Sigma = \begin{bmatrix} 1 & 0.5 \\ 0.5 & 1 \end{bmatrix})$$



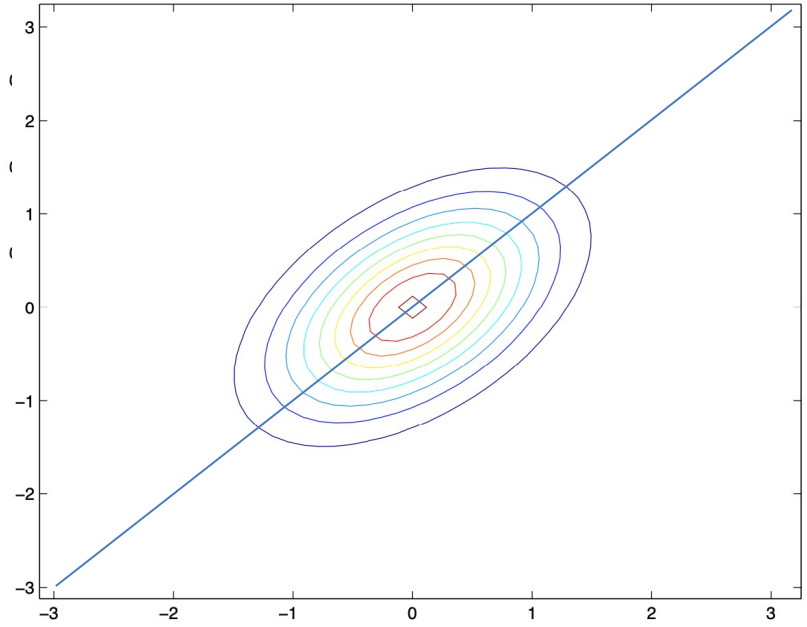
$$\mathcal{N}([0;0], \Sigma = \begin{bmatrix} 1 & 0.8 \\ 0.8 & 1 \end{bmatrix})$$

Increasing the off-diagonal entry in Σ, the density becomes more "compressed" towards the $x_2 = x_1$ line

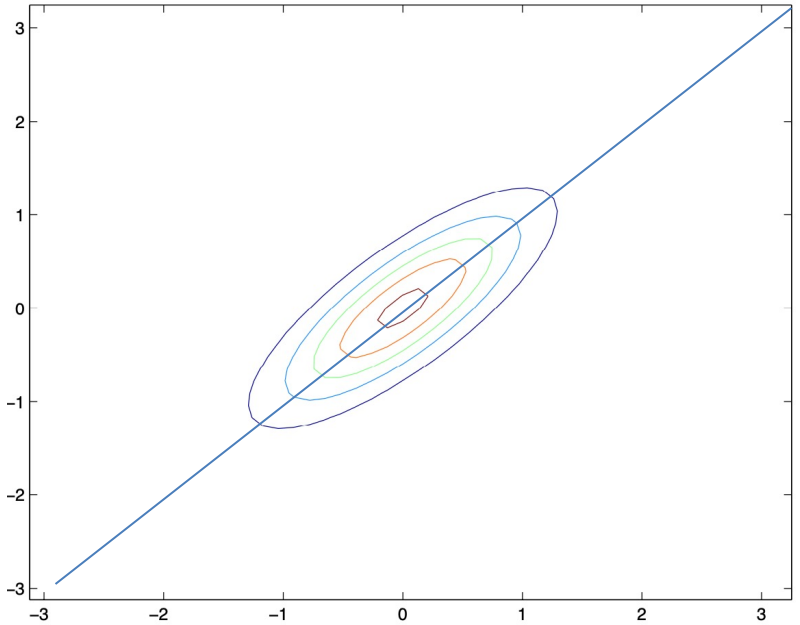
Contour of Density



$\mathcal{N}([0;0], \Sigma = \mathbf{I})$



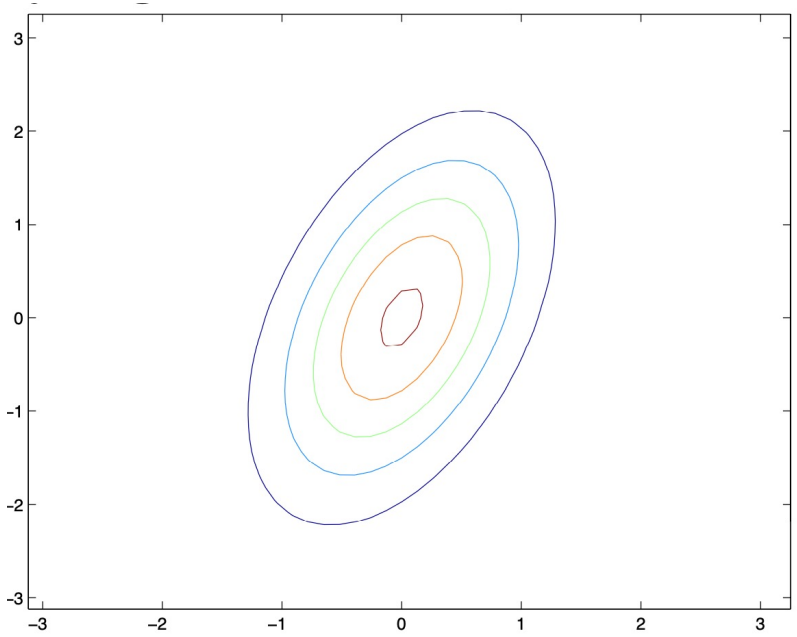
$\mathcal{N}([0;0], \Sigma = \begin{bmatrix} 1 & 0.5 \\ 0.5 & 1 \end{bmatrix})$

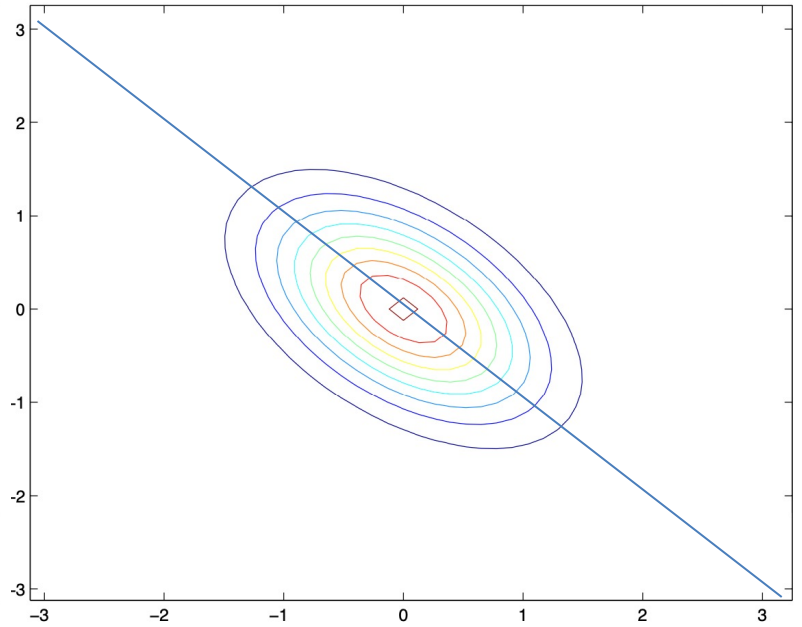


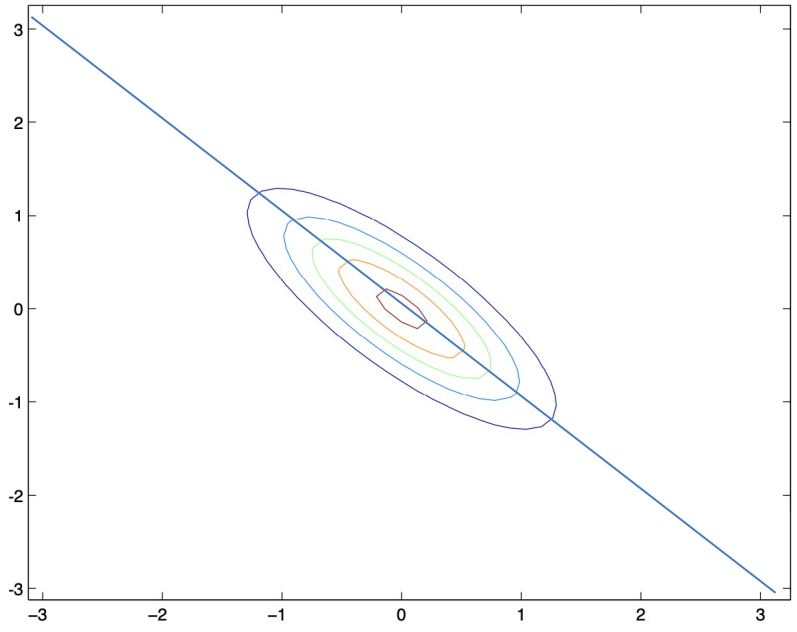
$\mathcal{N}([0;0], \Sigma = \begin{bmatrix} 1 & 0.8 \\ 0.8 & 1 \end{bmatrix})$

Increasing the off-diagonal entry in Σ, the density becomes more "compressed" towards the $x_2 = x_1$ line

Contour of Density







$$\mathcal{N}([0;0], \Sigma = \begin{bmatrix} 3 & 0.8 \\ 0.8 & 1 \end{bmatrix})$$

$$\mathcal{N}([0;0], \Sigma = \begin{bmatrix} 1 & -0.5 \\ -0.5 & 1 \end{bmatrix})$$

$$\mathcal{N}([0;0], \Sigma = \begin{bmatrix} 1 & -0.8 \\ -0.8 & 1 \end{bmatrix})$$

Decreasing the off-diagonal entry in Σ, the density becomes more “compressed” towards the $x_2 = -x_1$ line

Generally, the contours form ellipses by varying Σ parameters

Gaussian Discriminant Analysis (GDA)

Probabilistic Generative Models

Generative models: $p(\mathbf{x}|t)$ Likelihood $p(t)$ Label prior

Data generation process: model distribution of likelihood & label prior

Bayes rule to derive label t's posterior distribution given x

$$p(t|\mathbf{x}) = \frac{p(\mathbf{x}|t) \cdot p(t)}{p(\mathbf{x})}$$

Prediction $\arg\max_t p(t|\mathbf{x}) = \arg\max_t p(\mathbf{x}|t)p(t)$

Gaussian Discriminant Analysis: Continuous Random Variables

Binary classification t ∈ {0,1}

Likelihood

$$\mathbf{x}|t=0 \sim \mathcal{N}(\mu_0, \Sigma) \qquad p(\mathbf{x}|t=0) = \frac{1}{(2\pi)^{d/2}|\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(\mathbf{x}-\mu_0)^T\Sigma^{-1}(\mathbf{x}-\mu_0)\right)$$

$$\mathbf{x}|t=1 \sim \mathcal{N}(\mu_1, \Sigma) \qquad p(\mathbf{x}|t=1) = \frac{1}{(2\pi)^{d/2}|\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(\mathbf{x}-\mu_1)^T\Sigma^{-1}(\mathbf{x}-\mu_1)\right)$$

Note that there are two different mean vectors but just one covariance matrix

Label Prior

$$t \sim \text{Ber}(\phi) \qquad p(t) = \phi^t(1-\phi)^{1-t}$$

Parameters: $\phi, \mu_0, \mu_1, \Sigma$

(Log-) Likelihood of Data

Given N independent data samples $\{(x_n, t_n)\}_{n=1}^N$, the likelihood is defined as

$$\ell(\phi, \mu_0, \mu_1, \Sigma) = \log \prod_{n=1}^{N} p(\mathbf{x}_n, t_n) = \log \prod_{n=1}^{N} p(\mathbf{x}_n|t_n) \cdot p(t_n)$$

$$= \sum_{n=1}^{N} \log p(\mathbf{x}_n|t_n) + \sum_{n=1}^{N} \log p(t_n)$$

$$= \sum_{n:t_n=0} \log \Big[\frac{1}{(2\pi)^{d/2}|\Sigma|^{1/2}} \exp\Big(-\frac{1}{2}(\mathbf{x}-\mu_0)^T\Sigma^{-1}(\mathbf{x}-\mu_0)\Big)\Big]$$

$$+ \sum_{n:t_n=1} \log \Big[\frac{1}{(2\pi)^{d/2}|\Sigma|^{1/2}} \exp\Big(-\frac{1}{2}(\mathbf{x}-\mu_1)^T\Sigma^{-1}(\mathbf{x}-\mu_1)\Big)\Big]$$

$$+ \sum_{n=1}^{N} \phi^{t_n}(1-\phi)^{1-t_n}$$

Maximum Likelihood Estimation

$$\frac{\partial \ell}{\partial \phi} = 0 \qquad \phi = \frac{1}{N}\sum_{n=1}^{N} 1_{[t_n=1]}$$

Fraction of data points belonging to class *1*

$$\frac{\partial \ell}{\partial \mu_i} = 0 \qquad \mu_i = \frac{\sum_{n=1}^{N} 1_{[t_n=i]} \cdot \mathbf{x}_n}{\sum_{n=1}^{N} 1_{[t_n=i]}}$$

Average features of data points belonging to class *i*

$$\frac{\partial \ell}{\partial \Sigma} = 0 \qquad \Sigma = \frac{1}{N}\sum_{n=1}^{N} \left(\mathbf{x}_n - \mu_{t_n}\right)\left(\mathbf{x}_n - \mu_{t_n}\right)^T$$

Covariance matrix

Obtain: $p(\mathbf{x}|t = 0/1; \mu_{0/1}, \Sigma) \quad p(t; \phi)$

Prediction: $\arg\max_t p(t|\mathbf{x}_{te}) = \arg\max_t p(\mathbf{x}_{te}|t)p(t)$

$$p(\mathbf{x}_{te}|t = 0)p(t = 0) \textbf{ vs } p(\mathbf{x}_{te}|t = 1)p(t = 1)$$

Training: GDA with MLE

Input: Giving a set of N data points $\{(x_n, t_n)\}_{n=1}^{N}$ from two classes

Step 0: Model the likelihood of each class of data points as a Gaussian distribution

Step 1: Estimate the mean and covariance of two Gaussian distributions

$$\mu_i = \frac{\sum_{n=1}^{N} 1_{[t_n=i]} \cdot \mathbf{x}_n}{\sum_{n=1}^{N} 1_{[t_n=i]}},\ i \in \{0, 1\}$$

$$\Sigma = \frac{1}{N} \sum_{n=1}^{N} \left(\mathbf{x}_n - \mu_{t_n}\right)\left(\mathbf{x}_n - \mu_{t_n}\right)^T$$

Step 2: Estimate the prior p(t=k) as the fraction of training samples with label t=k

$$p(t = k) = \phi_k = \frac{1}{N} \sum_{n=1}^{N} 1_{[t_n=k]}$$

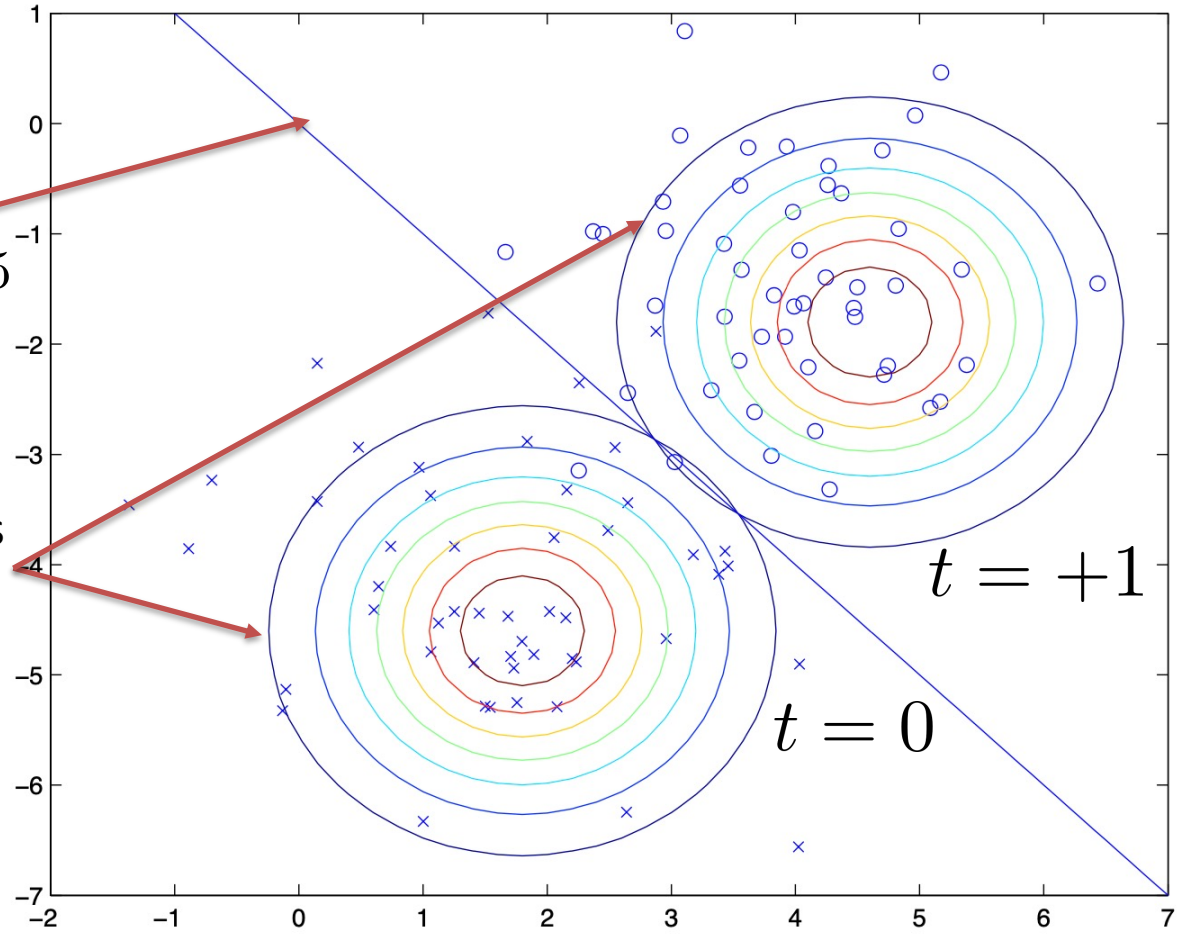
An Example

Decision boundary

$$p(t=1|\mathbf{x}) = p(t=0|\mathbf{x}) = 0.5$$

Contours of two gaussian dists fit to the data for two classes

Same shape and orientation due to the same cov. matrix



$$p(\mathbf{x}_{te}|t=0)p(t=0) \textbf{ vs } p(\mathbf{x}_{te}|t=1)p(t=1)$$

Naive Bayes Classifier (NBC): Discrete Random Variables

Motivating Example: Spam Filtering

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Keywords: English, Literature, Science, Economics, Engineering, Management, Agriculture, Horticulture, Environment .....

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New Email

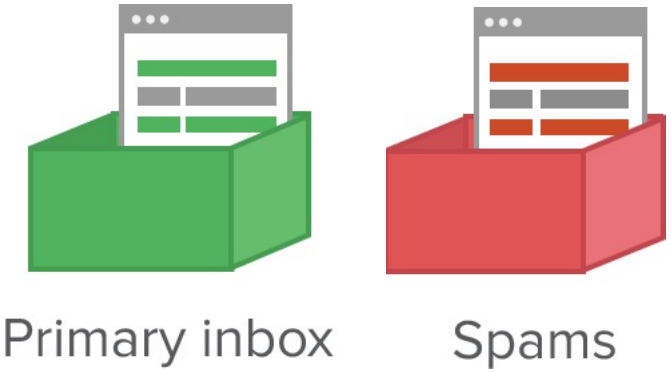
Classifier

Predict

Is Spam

Train

Binary classification



Primary inbox

Spams

Emails with Labels

Motivating Example: Spam Filtering

Represent an email via a feature vector whose length is equal to the **number of words** in the dictionary

If an email contains the i-th word of the dictionary, then we will set xi = 1; otherwise, we let xi = 0

$$x = \begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{bmatrix} \begin{matrix} \text{a} \\ \text{aardvark} \\ \text{aardwolf} \\ \vdots \\ \text{buy} \\ \vdots \\ \text{zygmurgy} \end{matrix} \in \{0,1\}^{50,000}$$

Now we build a generative model to learn p(**x**|t)

How many parameters to learn p(**x**|t) ?

$$2 \cdot 2^{50,000}$$

Computationally infeasible

Naïve Bayes Assumption

Naïve Bayes Assumption: All features are ***independent*** given the class label t

$$p(x_1, x_2, x_{50000}|t) = \prod_{i=1}^{50000} p(x_i|t) \qquad \#\ \text{paras.:}\ 2 \cdot 50,000$$

Strong assumption but works well in practice!

E.g., , if t = 1 (spam), “buy” is word 100 and “price” is word 800.

If I tell you t = 1, knowing the value of x100 (whether “buy” or not) has no effect on your beliefs about the value of x800 (whether “price” appears)

$$p(x_{100}, x_{800}|t) = p(x_{100}|t) \cdot p(x_{800}|t, x_{100}) = p(x_{100}|t) \cdot p(x_{800}|t)$$

Note: This is different from that x100 and x800 are independent

$$p(x_{100}) = p(x_{100}|x_{800})$$

Naïve Bayes Model: Binary Random Variables

Binary random variable per feature: $x_i \in \{0,1\}\ \forall i$

$$x_i|t = k \sim \text{Ber}(\phi_{i|t=k}) \qquad p(x_i|t = k; \phi_{i|t=k}) = \phi_{i|t=k}^{x_i}(1 - \phi_{i|t=k})^{1-x_i}$$

Binary/multiclass classification t ∈ {0,1}/{1,…K}

Binary classification

$$t \sim \text{Ber}(\phi) \qquad p(t; \phi) = \phi^t(1 - \phi)^{1-t}$$

Multiclass classification

$$t \sim \text{Multi}(\{\phi_k\}_{k=1}^K) \qquad p(t; \{\phi_k\}) = \phi_1^{1_{y=1}} \phi_2^{1_{y=2}} \cdot \phi_K^{1_{y=K}}$$

$$\sum_k \phi_k = 1$$

Parameters: $\{\phi_{i|t=k}\}, \phi(\phi_k)$

(Log-) Likelihood of Data: Binary Classification

Given N independent data samples $\{(x_n, t_n)\}_{n=1}^N$, the likelihood is defined as

$$\max \ell(\phi, \{\phi_{i|t=k}\}) = \log \prod_{n=1}^{N} p(\mathbf{x}_n, t_n) = \sum_{n=1}^{N} \log p(\mathbf{x}_n, t_n)$$

$$= \sum_{n=1}^{N} \log p(\mathbf{x}_n | t_n) + \sum_{n=1}^{N} \log p(t_n)$$

Naïve Bayes assumption

$$= \sum_{n=1}^{N} \sum_{i=1}^{d} \log p(x_{n,i} | t_n) + \sum_{n=1}^{N} \log p(t_n)$$

$$\text{subject to } \sum_{t \in \{0,1\}} p(t) = 1, \quad p(t) \geq 0$$

$$\sum_{x_i \in \{0,1\}} p(x_i|t) = 1,\ p(x_i|t) \geq 0, \forall i \in \{1, 2, \cdots, d\},\ t \in \{0, 1\}$$

Lagrangian

$$\max \ell(\phi, \{\phi_{i|t}\}; \alpha, \beta) = \sum_{n=1}^{N} \sum_{i=1}^{d} \log p(x_{n,i}|t_n) + \sum_{n=1}^{N} \log p(t_n) + \alpha \Big(1 - \sum_{t \in \{0,1\}} p(t)\Big) + \sum_{t \in \{0,1\}} \sum_{i=1}^{n} \beta_i \Big(1 - \sum_{x_i \in \{0,1\}} p(x_i|t)\Big)\Big)$$

Maximum Likelihood Estimation (MLE)

$$\frac{\partial \ell}{\partial \phi} = 0 \qquad \phi = \frac{1}{N}\sum_{n=1}^{N} 1_{[t_n=1]}$$

Fraction of data points belonging to class *1*

$$\frac{\partial \ell}{\partial \phi_{i|t=0}} = 0 \qquad \phi_{i|t=0} = \frac{\sum_{n=1}^{N} 1_{[t_n=0 \& x_{n,i}=1]}}{\sum_{n=1}^{N} 1_{[t_n=0]}}$$

$$\frac{\partial \ell}{\partial \phi_{i|t=1}} = 0 \qquad \phi_{i|t=1} = \frac{\sum_{n=1}^{N} 1_{[t_n=1 \& x_{n,i}=1]}}{\sum_{n=1}^{N} 1_{[t_n=1]}}$$

Fraction of data points belonging to class *0/1,* AND their i-th feature is 1

Obtain: $p(\mathbf{x}|t) = \prod_{i=1}^{d} p(x_i|t;\phi_{i|t}) \qquad p(t;\phi)$

Prediction: $\arg\max_t p(t|\mathbf{x}_{te}) = \arg\max_t p(\mathbf{x}_{te}|t)p(t)$

$$p(\mathbf{x}_{te}|t=0)p(t=0) \textbf{ vs } p(\mathbf{x}_{te}|t=1)p(t=1)$$

Maximum Likelihood Estimation (Details)

$$\max \ell(\phi, \{\phi_{i|t}\}; \alpha, \beta) = \sum_{n=1}^{N}\sum_{i=1}^{d} \log p(x_{n,i}|t_n) + \sum_{n=1}^{N} \log p(t_n) + \alpha\Big(1 - \sum_{t\in\{0,1\}} p(t)\Big) + \sum_{t\in\{0,1\}}\sum_{i=1}^{n} \beta_i\Big(1 - \sum_{x_i\in\{0,1\}} p(x_i|t)\Big)$$

$$\frac{\partial \ell}{\partial p(t)} = \sum_{n:t_n=t} \frac{\partial \log p(t)}{\partial p(t)} - \alpha = \sum_{n:t_n=t} \frac{1}{p(t)} - \alpha = \frac{\sum_n 1_{[t_n=t]}}{p(t)} - \alpha = 0$$

Fraction of data points belonging to class *1*

$$\Rightarrow \quad p(t) = \frac{\sum_{n=1}^{N} 1_{[t_n=t]}}{\alpha}$$

$$\sum_t p(t) = 1 \quad \Rightarrow \quad \alpha = N \quad \Rightarrow \quad p(t) = \frac{1}{N}\sum_{n=1}^{N} 1_{[t_n=t]} \quad \Rightarrow \quad \phi = p(t=1) = \frac{1}{N}\sum_{n=1}^{N} 1_{[t_n=1]}$$

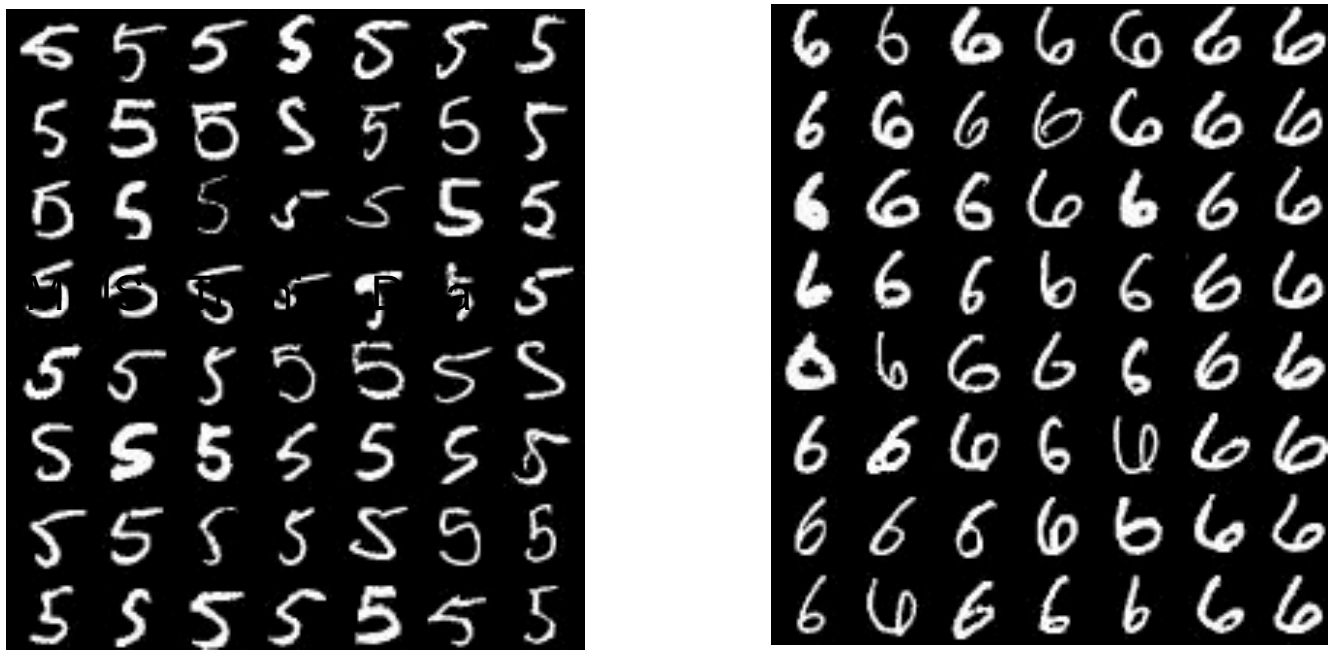
$$\frac{\partial \ell}{\partial p(x_i|t)} = \sum_{n:x_{n,i}=x_i, t_n=t} \frac{\partial \log p(x_i|t)}{\partial p(x_i|t)} - \beta_i = \frac{\sum_n 1_{[x_{n,i}=x_i \& t_n=t]}}{p(x_i|t)} - \beta_i = 0$$

Fraction of data points belonging to a class *k*, AND their i-th feature is 1

$$\Rightarrow \quad p(x_i|t) = \frac{\sum_n 1_{[t_n=t \& x_{n,i}=x_i]}}{\beta_i}$$

$$\sum_{x_i} p(x_i|t) = 1, \forall t \quad \Rightarrow \quad \beta_i = \sum_n 1_{[t_n=t]} \quad \Rightarrow \quad \phi_{x_i|t} = p(x_i|t) = \frac{\sum_{n=1}^{N} 1_{[t_n=t \& x_{n,i}=x_i]}}{\sum_{n=1}^{N} 1_{[t_n=t]}}$$

Example: Binary Digit Recognition

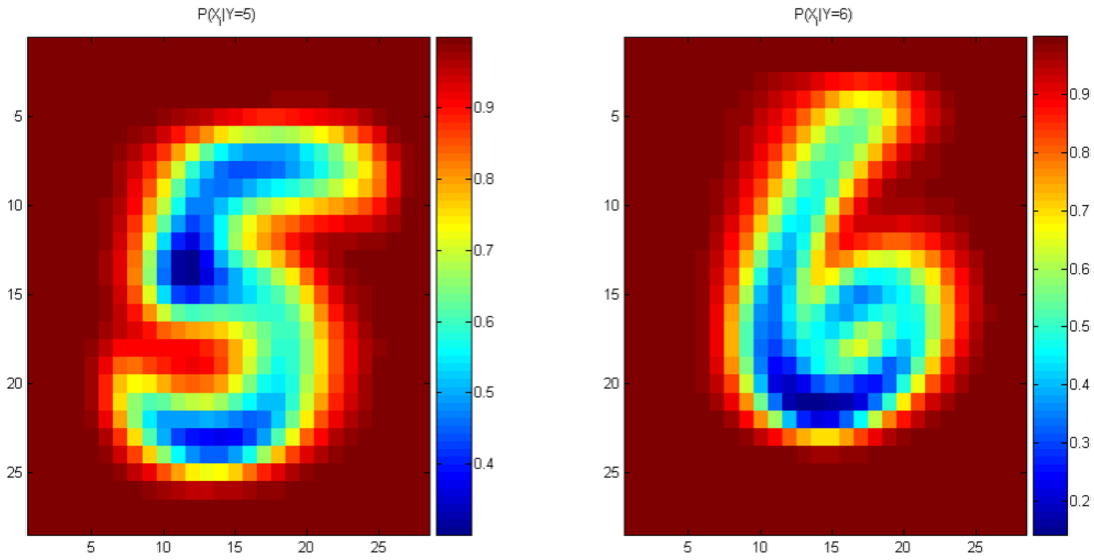


MNIST Training Data

Training: Naïve Bayes with MLE

Step 1: Estimate likelihood $P(X_i=0/1|t=k)$ as the fraction of training samples with $t=k$ for which $X_i=0/1$

$$p(x_i|t=k) = \phi_{x_i|t=k} = \frac{\sum_{n=1}^{N} 1_{[t_n=k \& x_{n,i}=x_i]}}{\sum_{n=1}^{N} 1_{[t_n=k]}}$$



Step 2: Estimate prior $P(t=k)$ as the fraction of training samples with label $t=k$

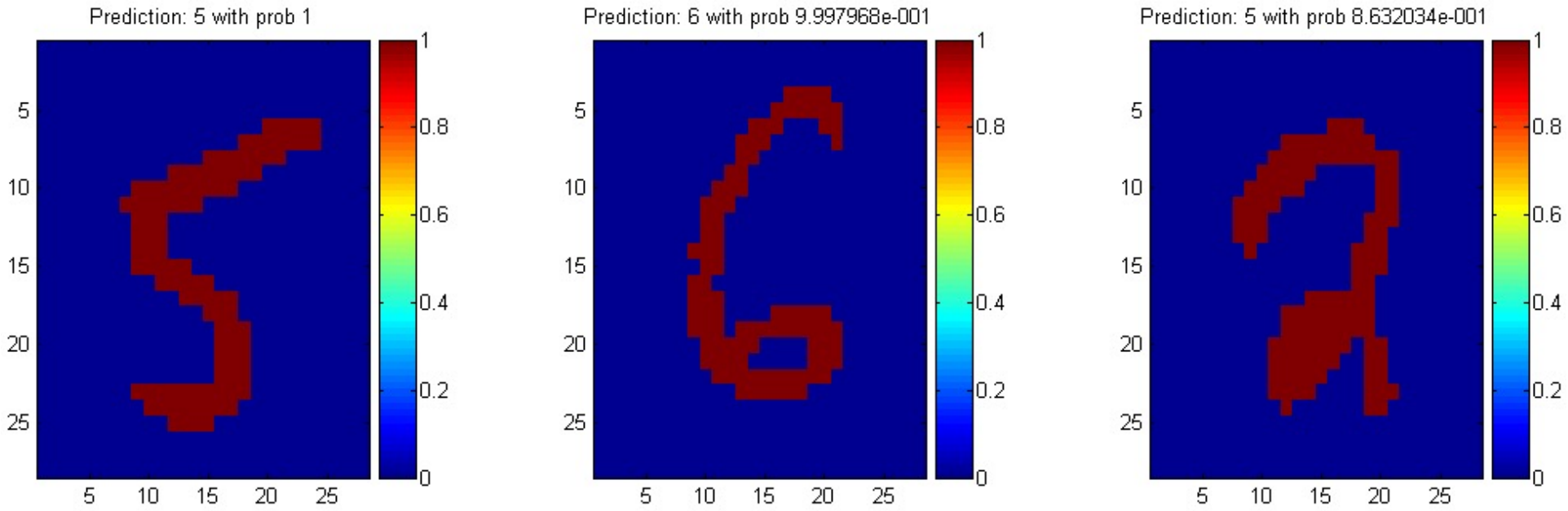
$$p(t=k) = \phi_k = \frac{1}{N}\sum_{n=1}^{N} 1_{[t_n=k]}$$

$$p(t = \text{“5”}) = p(t = \text{“6”}) = 0.5$$

Testing with New Samples

$$\arg\max_t p(t|\mathbf{x}_{te}) = \arg\max_t p(\mathbf{x}_{te}|t)p(t)$$

$$p(\mathbf{x}_{te}|t = \text{“5”})p(t = \text{“5”}) \quad \textbf{vs.} \quad p(\mathbf{x}_{te}|t = \text{“6”})p(t = \text{“6”})$$



Summary

- Probabilistic generative models
  - Model likelihood (class-conditional density) p(x|t) and class prior p(t)
  - Maximum likelihood estimation on joint distribution p(x, t)
  - Prediction: argmax p(t|x) <=> argmax p(x|t) p(t)
- Gaussian Discriminant Analysis
  - Continuous random variables
  - p(x|t): Gaussian distributions with shared covariance matrix
  - p(t): Bernoulli (Multinomial) distribution for binary (multi) class
- Naïve Bayes Classifier
  - Discrete random variables
  - Naïve Bayes assumption: p(x_i, x_j | t) = p(x_i | t) p(x_j | t), for all i,j
  - p(x_i|t) : Bernoulli distribution for binary features
  - p(t): Bernoulli (Multinomial) distribution for binary (multi) class

Comparison

Generative models

Learn the model that generates the observed data; 'Everything' are about the distribution

Pros

- Need less data due to prior knowledge of dist.
- Can work with missing data
- Can capture uncertainty, priors, etc
- Low variance

Cons

- High bias (underfitting): due to the generalization by assumed distribution
- Less accurate than discriminative models (when the distribution assumption is violated)

Discriminative models

Directly discriminative the observed data regardless of the underlying generation process

Pros

- Easy to model
- Low bias
- More accurate than generative models

Cons

- Need more data to avoid underfitting
- Not easy to work with missing data
- Cannot capture priors, uncertainty, etc.
- High variance (easy to overfitting)