ITCS 6156/8156 Fall 2023
Machine Learning

Generative Models for Classification

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Some content in the slides is based on Dr. Raquel Urtasun’s lecture

Classification

- Given inputs $\mathbf{x}$ and classes y we can do classification in several ways. How?

(features)

$\mathbf{x}$

e.g:
- height
- weight
- color

(class label)

y

elefant

bear

Discriminative Classifiers

- **Discriminative** classifiers try to either:
  - learn mappings directly from the space of inputs $\mathcal{X}$ to class labels $\{0, 1, 2, \ldots, K\}$

(features) (class label)

$\mathbf{x} \longrightarrow y$

e.g:
- height
- weight
- color

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For example:

- Linear regression (as a classifier)
- Neural Networks

Discriminative Classifiers

- **Discriminative** classifiers try to either:
  - or try to learn $p(y|\mathbf{x})$ directly

(features)

$\mathbf{x}$

e.g:
- height
- weight
- color

(class probability)

$p(y|\mathbf{x})$

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bear

For example:

- Logistic Regression

Generative Classifiers

How about this approach: build a model of "how data for a class looks like"

- **Generative** classifiers try to model $p(\mathbf{x}|y)$
- Classification via Bayes rule (thus also called Bayes classifiers)

(prob. of features given label) (class label)

$$p(\mathbf{x}|y) \longleftarrow y$$

e.g:
- height
- weight
- color

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Tries to model:
- How does data look like for a class?

Classification (How?)

Generative vs Discriminative

Two approaches to classification:

- Discriminative classifiers estimate parameters of decision boundary/class separator directly from labeled examples
  - learn $p(y|\mathbf{x})$ directly (logistic regression models)
  - learn mappings from inputs to classes (least-squares, neural nets)

- Generative approach: model the distribution of inputs characteristic of the class (Bayes classifier)
  - Build a model of $p(\mathbf{x}|y)$
  - Apply Bayes Rule

Probability Formulas

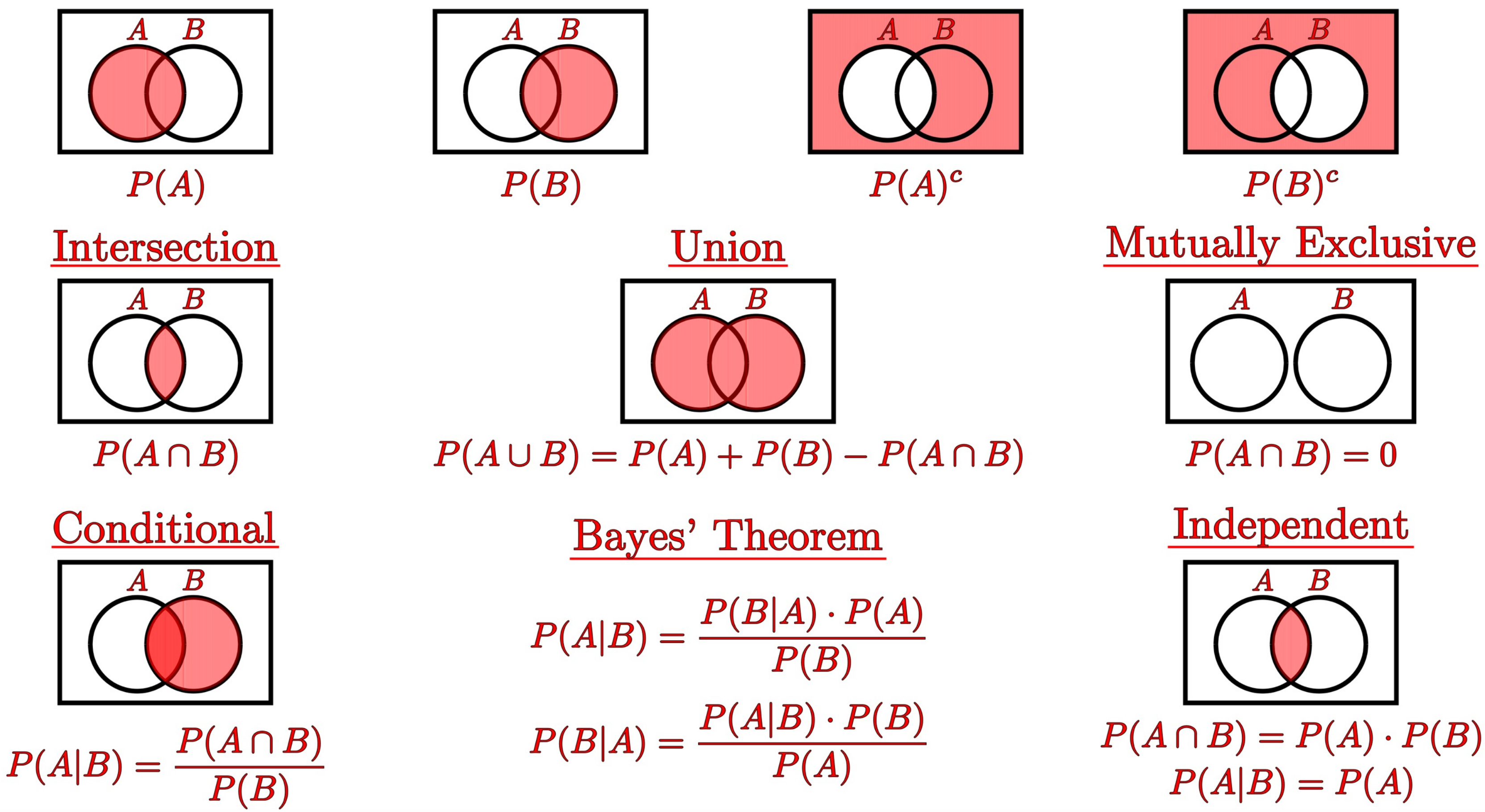


Image from: https://theacetutors.com/blog/

Bayes Classifier

- Aim to diagnose whether patient has diabetes: classify into one of two classes (yes C=1; no C=0)
- Run battery of tests on the patients, get $\mathbf{x}$ for each patient
- Given patient's results: $\mathbf{x} = [x_1, x_2, \cdots, x_d]^T$ we want to compute class probabilities using Bayes Rule:

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

- More formally

$$\text{posterior} = \frac{\text{Class likelihood} \times \text{prior}}{\text{Evidence}}$$

- How can we compute $p(\mathbf{x})$ for the two class case?

$$p(\mathbf{x}) = p(\mathbf{x}|C=0)p(C=0) + p(\mathbf{x}|C=1)p(C=1)$$

- To compute $p(C|\mathbf{x})$ we need: $p(\mathbf{x}|C)$ and $p(C)$

A Discrete Example

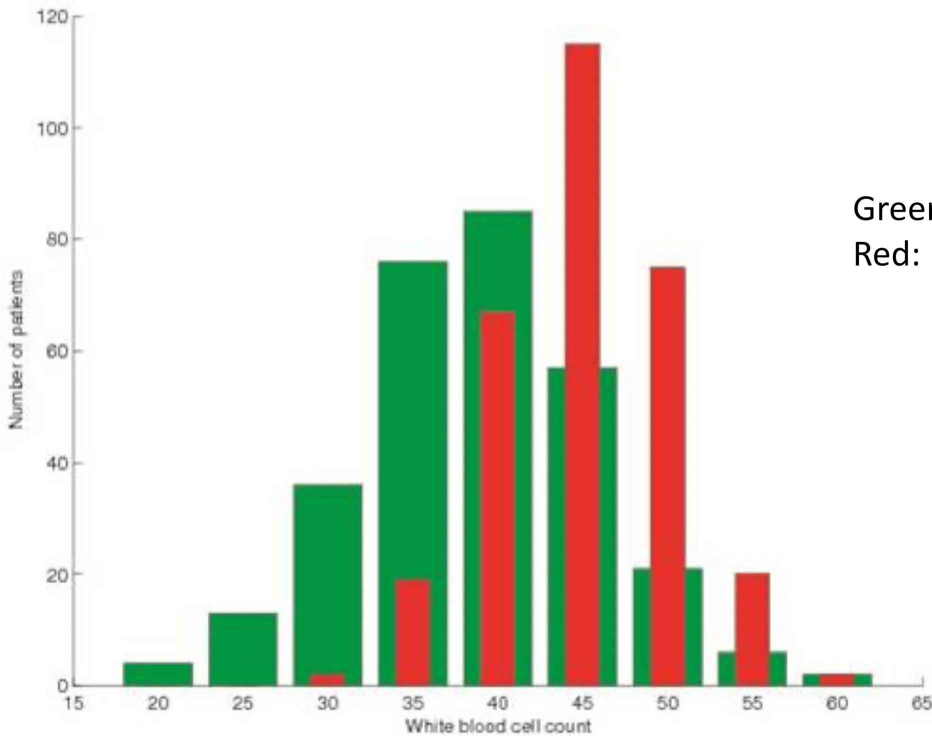
- For a genetic defect test we have the following information:
  - 1% of people have a certain genetic defect;
  - For people who have genetic defects, 90% of tests show positive results;
  - For people who have no genetic defects, 90% tests show negative results.
- If a person gets a positive test result, what is the probability he/she actually have the genetic defect?

- Solution:

$$P(G=1|T=1) = \frac{P(T=1|G=1)P(G=1)}{P(T=1)}$$
$$= \frac{P(T=1|G=1)P(G=1)}{P(T=1|G=1)P(G=1) + P(T=1|G=0)P(G=0)}$$
$$= \frac{0.9 * 0.01}{0.9 * 0.01 + 0.1 * 0.99} = 8.33\%$$

Classification: Diabetes Example

- Let's start with the simplest case where the input is only 1-dimensional, for example: white blood cell count (this is our x)
- We need to choose a probability distribution $p(x|C)$ that makes sense



Green: No Diabetes
Red: Diabetes

Figure : Our example (showing counts of patients for input value): What distribution to choose?

Gaussian Bayes Classifier

- Our first generative classifier assumes that $p(\mathbf{x}|y)$ is distributed according to a multivariate normal (Gaussian) distribution
- This classifier is called Gaussian Discriminant Analysis
- Let's first continue our simple case when inputs are just 1-dim and have a Gaussian distribution:

$$p(x|C) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(x-\mu_C)^2}{2\sigma_C^2}\right)$$

with $\mu \in \Re$ and $\sigma^2 \in \Re^+$

- Notice that we have different parameters for different classes
- How can I fit a Gaussian distribution to my data?

MLE for Gaussians

- Let's assume that the class-conditional densities are Gaussian

$$p(x|C) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(x-\mu_C)^2}{2\sigma_C^2}\right)$$

with $\mu \in \Re$ and $\sigma^2 \in \Re^+$

- How can I fit a Gaussian distribution to my data?
- We are given a set of training examples $\{x^{(n)}, t^{(n)}\}_{n=1,\cdots,N}$ with $t^{(n)} \in \{0, 1\}$ and we want to estimate the model parameters $\{(\mu_0, \sigma_0), (\mu_1, \sigma_1)\}$
- First divide the training examples into two classes according to $t^{(n)}$, and for each class take all the examples and fit a Gaussian to model $p(x|C)$
- Let's try maximum likelihood estimation (MLE)

MLE for Gaussians

(note: we are dropping subscript C for simplicity of notation)

- We assume that the data points that we have are independent and identically distributed

$$p(x^{(1)}, \cdots, x^{(N)}|C) = \prod_{n=1}^{N} p(x^{(n)}|C) = \prod_{n=1}^{N} \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(x^{(n)} - \mu)^2}{2\sigma^2}\right)$$

- Now we want to maximize the likelihood, or minimize its negative (if you think in terms of a loss)

$$\begin{aligned} \ell_{log-loss} &= -\ln p(x^{(1)}, \cdots, x^{(N)}|C) = -\ln\left(\prod_{n=1}^{N} \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(x^{(n)} - \mu)^2}{2\sigma^2}\right)\right) \\ &= \sum_{n=1}^{N} \ln(\sqrt{2\pi}\sigma) + \sum_{n=1}^{N} \frac{(x^{(n)} - \mu)^2}{2\sigma^2} = \frac{N}{2} \ln\left(2\pi\sigma^2\right) + \sum_{n=1}^{N} \frac{(x^{(n)} - \mu)^2}{2\sigma^2} \end{aligned}$$

Computing the Mean

- (let's try to find a) Closed-form solution: Write $\frac{d\ell_{log-loss}}{d\mu}$ and $\frac{d\ell_{log-loss}}{d\sigma^2}$ and equal it to 0 to find the parameters μ and σ^2

$$
\begin{aligned}
\frac{\partial \ell_{log-loss}}{\partial \mu} &= \frac{\partial\left(\frac{N}{2}\ln\left(2\pi\sigma^2\right) + \sum_{n=1}^{N}\frac{(x^{(n)}-\mu)^2}{2\sigma^2}\right)}{\partial \mu} = \frac{d\left(\sum_{n=1}^{N}\frac{(x^{(n)}-\mu)^2}{2\sigma^2}\right)}{d\mu} \\
&= \frac{-\sum_{n=1}^{N} 2(x^{(n)}-\mu)}{2\sigma^2} = -\sum_{n=1}^{N}\frac{(x^{(n)}-\mu)}{\sigma^2} = \frac{N\mu - \sum_{n=1}^{N} x^{(n)}}{\sigma^2}
\end{aligned}
$$

- And equating to zero we have

$$
\frac{d\ell_{log-loss}}{d\mu} = 0 = \frac{N\mu - \sum_{n=1}^{N} x^{(n)}}{\sigma^2}
$$

Thus

$$
\boxed{\mu = \frac{1}{N}\sum_{n=1}^{N} x^{(n)}}
$$

Computing the Variance

- And for σ^2:

$$\frac{d\ell_{log-loss}}{d\sigma^2} = \frac{d\left(\frac{N}{2}\ln\left(2\pi\sigma^2\right) + \sum_{n=1}^{N}\frac{(x^{(n)}-\mu)^2}{2\sigma^2}\right)}{d\sigma^2}$$

$$= \frac{N}{2}\frac{1}{2\pi\sigma^2}2\pi + \frac{\sum_{n=1}^{N}(x^{(n)}-\mu)^2}{2}\left(\frac{-1}{\sigma^4}\right)$$

$$= \frac{N}{2\sigma^2} - \frac{\sum_{n=1}^{N}(x^{(n)}-\mu)^2}{2\sigma^4}$$

- And equating to zero we have

$$\frac{d\ell_{log-loss}}{d\sigma^2} = 0 = \frac{N}{2\sigma^2} - \frac{\sum_{n=1}^{N}(x^{(n)}-\mu)^2}{2\sigma^4} = \frac{N\sigma^2 - \sum_{n=1}^{N}(x^{(n)}-\mu)^2}{2\sigma^4}$$

- Thus:

$$\boxed{\sigma^2 = \frac{1}{N}\sum_{n=1}^{N}(x^{(n)}-\mu)^2}$$

MLE of a Gaussian

- In summary, we can compute the parameters of a Gaussian distribution in closed form for each class by taking the training points that belong to that class

MLE estimates of parameters for a Gaussian distribution:

$$\mu = \frac{1}{N}\sum_{n=1}^{N} x^{(n)}$$

$$\sigma^2 = \frac{1}{N}\sum_{n=1}^{N}(x^{(n)} - \mu)^2$$

Posterior Probability

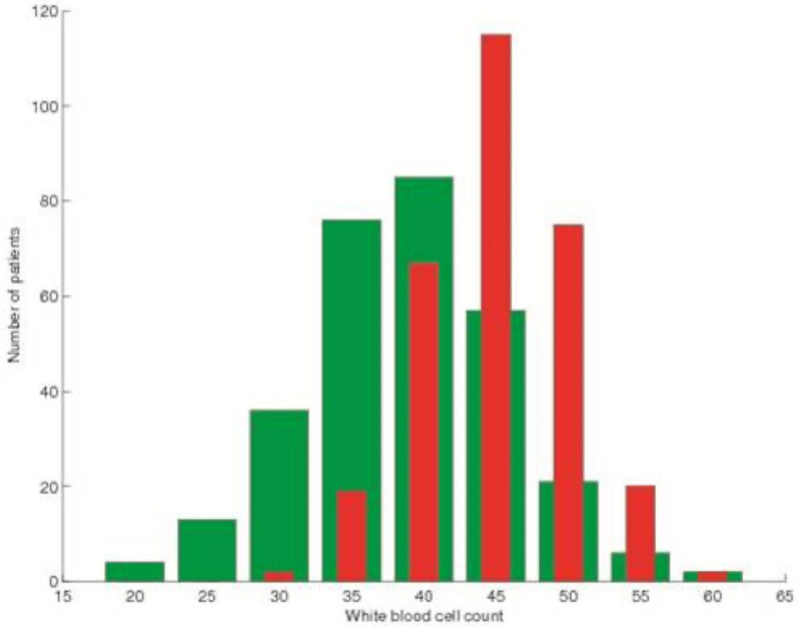
- We now have $p(x|C)$
- In order to compute the posterior probability:

$$
\begin{aligned}
p(C|x) &= \frac{p(x|C)p(C)}{p(x)} \\
&= \frac{p(x|C)p(C)}{p(x|C=0)p(C=0) + p(x|C=1)p(C=1)}
\end{aligned}
$$

  given a new observation, we still need to compute the **prior**

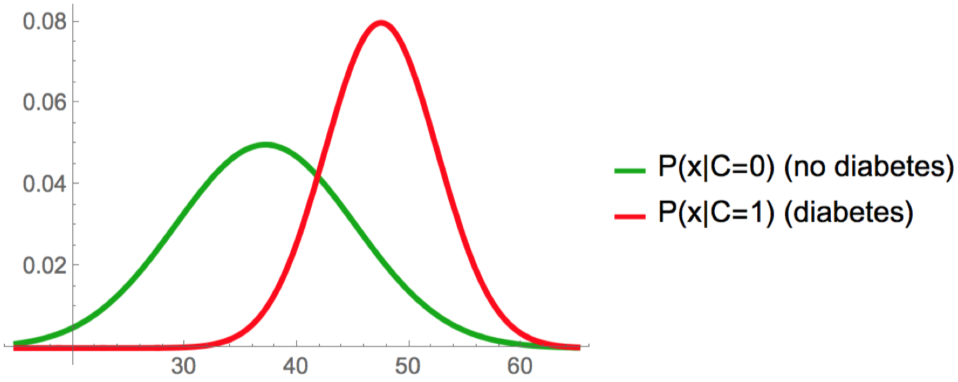
- Prior: In the absence of any observation, what do I know about the problem?

Diabetes Example



- Doctor has a prior $p(C = 0) = 0.8$, how?
- A new patient comes in, the doctor measures $x = 48$
- Does the patient have diabetes?

Diabetes Example



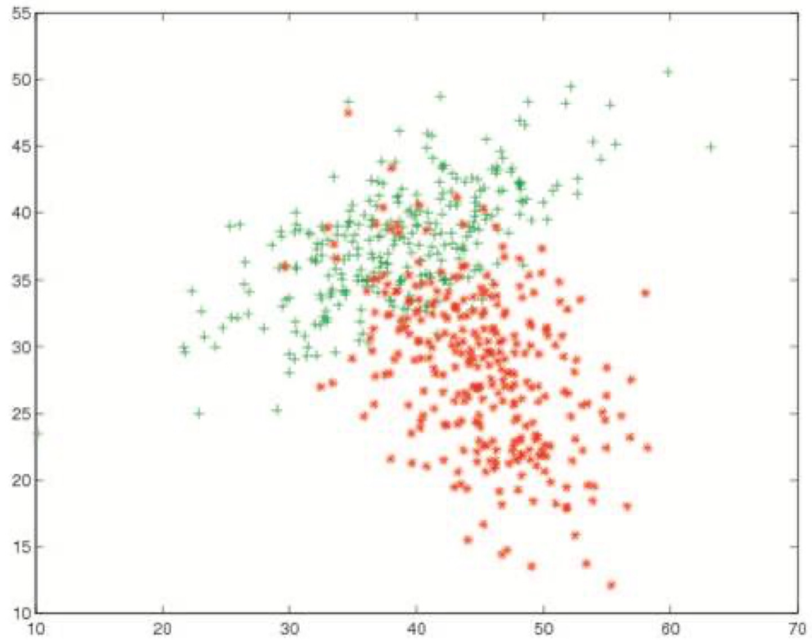
- Compute $p(x = 48|C = 0)$ and $p(x = 48|C = 1)$ via our estimated Gaussian distributions
- Compute posterior $p(C = 0|x = 48)$ via Bayes rule using the prior (how can we get $p(C = 1|x = 48)$?)
- How can we decide on diabetes/non-diabetes?

Bayes Classifier

- Use Bayes classifier to classify new patients (unseen test examples)
- Simple Bayes classifier: estimate posterior probability of each class
- What should the decision criterion be?
- The optimal decision is the one that minimizes the expected number of mistakes

Multiple-dimensional Inputs

- Add second observation: Plasma glucose value
- Now our input **x** is 2-dimensional



Gaussian Bayes Classifier

- Gaussian Discriminant Analysis in its general form assumes that $p(\mathbf{x}|t)$ is distributed according to a multivariate normal (Gaussian) distribution
- Multivariate Gaussian distribution:

$$p(\mathbf{x}|t=k) = \frac{1}{(2\pi)^{d/2}|\Sigma_k|^{1/2}} \exp\left[-(\mathbf{x}-\boldsymbol{\mu}_k)^T \Sigma_k^{-1}(\mathbf{x}-\boldsymbol{\mu}_k)\right]$$

  where $|\Sigma_k|$ denotes the determinant of the matrix, and d is dimension of $\mathbf{x}$
- Each class k has associated mean vector $\boldsymbol{\mu}_k$ and covariance matrix Σ_k
- Typically the classes share a single covariance matrix Σ ("share" means that they have the same parameters; the covariance matrix in this case): $\Sigma = \Sigma_1 = \cdots = \Sigma_k$

Multivariate Data

- Multiple measurements (sensors)
- d inputs/features/attributes
- N instances/observations/examples

$$\mathbf{X} = \begin{bmatrix} x_1^{(1)} & x_2^{(1)} & \cdots & x_d^{(1)} \\ x_1^{(2)} & x_2^{(2)} & \cdots & x_d^{(2)} \\ \vdots & \vdots & \ddots & \vdots \\ x_1^{(N)} & x_2^{(N)} & \cdots & x_d^{(N)} \end{bmatrix}$$

Multivariate Parameters

- Mean

$$\mathbb{E}[\mathbf{x}] = [\mu_1, \cdots, \mu_d]^T$$

- Covariance

$$\Sigma = Cov(\mathbf{x}) = \mathbb{E}[(\mathbf{x} - \mu)^T(\mathbf{x} - \mu)] = \begin{bmatrix} \sigma_1^2 & \sigma_{12} & \cdots & \sigma_{1d} \\ \sigma_{12} & \sigma_2^2 & \cdots & \sigma_{2d} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{d1} & \sigma_{d2} & \cdots & \sigma_d^2 \end{bmatrix}$$

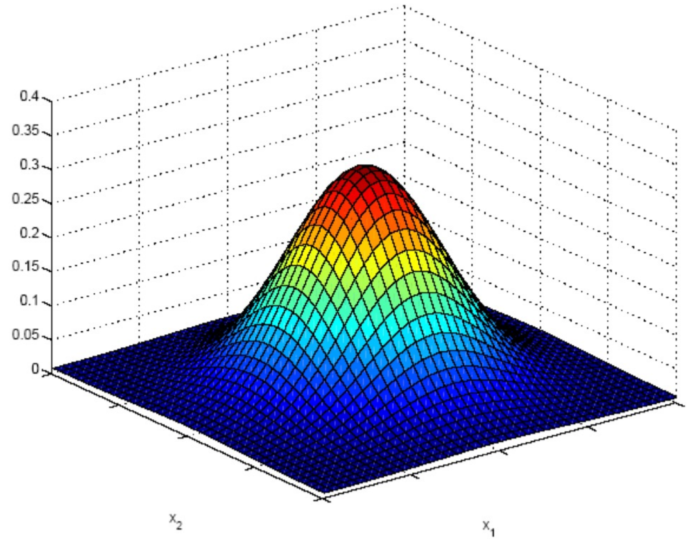
- Correlation $= Corr(\mathbf{x})$ is the covariance divided by the product of standard deviation

$$\rho_{ij} = \frac{\sigma_{ij}}{\sigma_i \sigma_j}$$

Multivariate Gaussian Distribution

- $\mathbf{x} \sim \mathcal{N}(\mu, \Sigma)$, a Gaussian (or normal) distribution defined as

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



- Mahalanobis distance $(\mathbf{x}-\mu_k)^T\Sigma^{-1}(\mathbf{x}-\mu_k)$ measures the distance from $\mathbf{x}$ to μ in terms of Σ
- It normalizes for difference in variances and correlations

Simplifying the Model

What if $\mathbf{x}$ is high-dimensional?

- For Gaussian Bayes Classifier, if input $\mathbf{x}$ is high-dimensional, then covariance matrix has many parameters
- Save some parameters by using a shared covariance for the classes
- Any other idea you can think of?

Naive Bayes

- Given patient's results: $\mathbf{x} = [x_1, x_2, \cdots, x_d]^T$ we want to update class probabilities using Bayes Rule:

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

- More formally

$$\text{posterior} = \frac{\text{Class likelihood} \times \text{prior}}{\text{Evidence}}$$

- **Naive Bayes** is an alternative generative model: Assumes features independent given the class

$$p(\mathbf{x}|t = k) = \prod_{i=1}^{d} p(x_i|t = k)$$

Naive Bayes Classifier

Given

- prior $p(t = k)$
- assuming features are conditionally independent given the class
- likelihood $p(x_i | t = k)$ for each x_i

The decision rule

$$y = arg\max_k p(t = k) \prod_{i=1}^{d} p(x_i | t = k)$$

- If the assumption of conditional independence holds, NB is the optimal classifier
- If not, a heavily regularized version of generative classifier

- Note: NB's assumptions (cond. independence) typically do not hold in practice. However, the resulting algorithm still works well on many problems, and it typically serves as a decent baseline for more sophisticated models

A Discrete Example

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
x (1)	1	1	1	1	1	2	2	2	2	2	3	3	3	3	3
x (2)	S	M	M	S	S	S	M	M	L	L	L	M	M	L	L
y	-1	-1	1	1	-1	-1	1	1	1	1	1	1	1	1	-1

x(1): Humidity (level 1, 2, 3);
x(2): Wind intensity (Low, Mediate, Strong);
y: Rain (1) or not (-1).

- Will it rain when humidity is at level 2 and wind intensity is strong?

$$P(y=1|H=2,W=S) = \frac{P(y=1)P(H=2,W=S|y=1)}{P(H=2,W=s)} = \frac{P(y=1)P(H=2|y=1)P(W=S|y=1)}{P(H=2,W=s)} = \frac{\frac{10}{15}*\frac{4}{10}*\frac{1}{10}}{P(H=2,W=s)} = \frac{\frac{2}{75}}{P(H=2,W=s)}$$

$$P(y=0|H=2,W=S) = \frac{P(y=0)P(H=2,W=S|y=0)}{P(H=2,W=s)} = \frac{P(y=0)P(H=2|y=0)P(W=S|y=0)}{P(H=2,W=s)} = \frac{\frac{5}{15}*\frac{1}{5}*\frac{3}{5}}{P(H=2,W=s)} = \frac{\frac{3}{75}}{P(H=2,W=s)}$$

- It will probably not rain.

Questions?

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