Multivariate Data

- Previous methods on sample: $\mathcal{X} = \{x^t\}_{t=1}^N$ $\mathcal{X} = \{x^t, r^t\}_{t=1}^N$
- Several measurements generate observation vector. Sample as a data matrix

$$\mathbf{X} = \begin{bmatrix} X_1^1 & X_2^1 & \cdots & X_d^1 \\ X_1^2 & X_2^2 & \cdots & X_d^2 \\ \vdots & & & \\ X_1^N & X_2^N & \cdots & X_d^N \end{bmatrix}$$

- Nxd matrix
- d columns: d variables
- N rows: N instances
    - Independent and identically distributed (i.i.d)

Multivariate Data – Parameter Estimation

Mean vector $E[\boldsymbol{x}] = \boldsymbol{\mu} = [\mu_1, \ldots, \mu_d]^T$

The variance of X_i σ_i^2

The covariance of two variables X_i and X_j $\sigma_{ij} \equiv \mathrm{Cov}(X_i, X_j) = E[(X_i - \mu_i)(X_j - \mu_j)]$

Covariance matrix

$$\boldsymbol{\Sigma} = \begin{bmatrix} \sigma_1^2 & \sigma_{12} & \cdots & \sigma_{1d} \\ \sigma_{21} & \sigma_2^2 & \cdots & \sigma_{2d} \\ \vdots & & & \\ \sigma_{d1} & \sigma_{d2} & \cdots & \sigma_d^2 \end{bmatrix}$$

Linear dependence:
> 0
< 0
= 0

$$\boldsymbol{\Sigma} \equiv \mathrm{Cov}(\boldsymbol{X}) = E[(\boldsymbol{X} - \boldsymbol{\mu})(\boldsymbol{X} - \boldsymbol{\mu})^T]$$

Multivariate Data – Parameter Estimation

Covariance matrix

$$\Sigma = \begin{bmatrix} \sigma_1^2 & \sigma_{12} & \cdots & \sigma_{1d} \\ \sigma_{21} & \sigma_2^2 & \cdots & \sigma_{2d} \\ \vdots & & & \\ \sigma_{d1} & \sigma_{d2} & \cdots & \sigma_d^2 \end{bmatrix}$$

$$\Sigma \equiv \mathrm{Cov}(\boldsymbol{X}) = E[(\boldsymbol{X} - \boldsymbol{\mu})(\boldsymbol{X} - \boldsymbol{\mu})^T]$$

Correlation

$$\mathrm{Corr}(X_i, X_j) \equiv \rho_{ij} = \frac{\sigma_{ij}}{\sigma_i \sigma_j}$$

Two variables independent $\rightarrow$ covariance = correlation = 0

Covariance = 0 $\not\rightarrow$ two variables independent

Multivariate Data – Parameter Estimation

Sample mean $$\boldsymbol{m} = \frac{\sum_{t=1}^{N} \boldsymbol{x}^t}{N} \text{ with } m_i = \frac{\sum_{t=1}^{N} x_i^t}{N}, i = 1, \ldots, d$$

Sample covariance matrix $$s_i^2 = \frac{\sum_{t=1}^{N} (x_i^t - m_i)^2}{N}$$
$$s_{ij} = \frac{\sum_{t=1}^{N} (x_i^t - m_i)(x_j^t - m_j)}{N}$$

Multivariate Data – Estimating missing values

- Fill-in missing entries by estimating them: **imputation**
  - Mean imputation
  - Imputation by regression

	sex	race	educ_r	r_age	earnings	police
[91,]	1	3	3	31	NA	0
[92,]	2	1	2	37	135.00	1
[93,]	2	3	2	40	NA	1
[94,]	1	1	3	42	3.00	1
[95,]	1	3	1	24	0.00	NA

Multivariate Data – Normal distribution

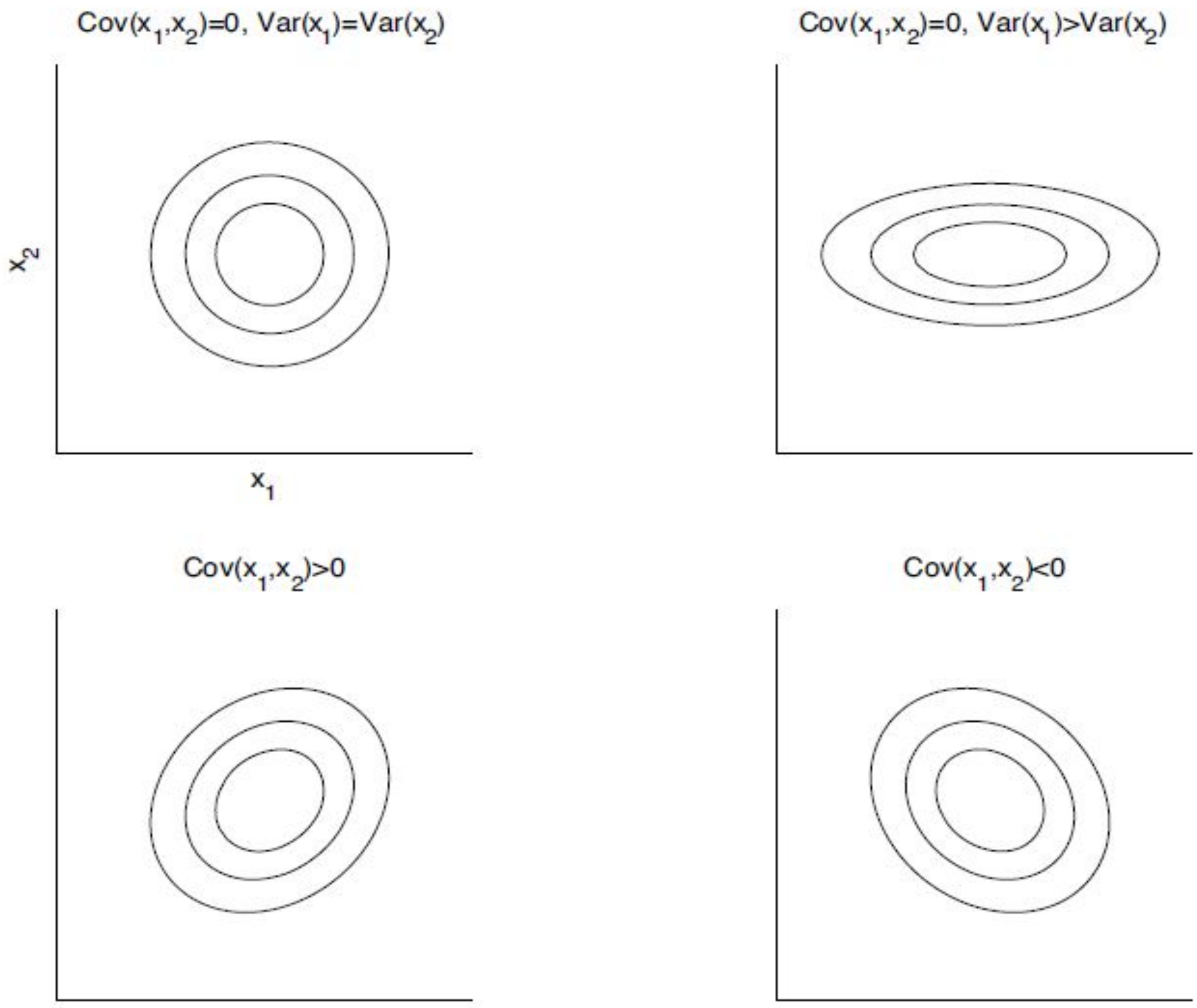
$$\boldsymbol{x} \sim \mathcal{N}_d(\boldsymbol{\mu}, \Sigma)$$

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

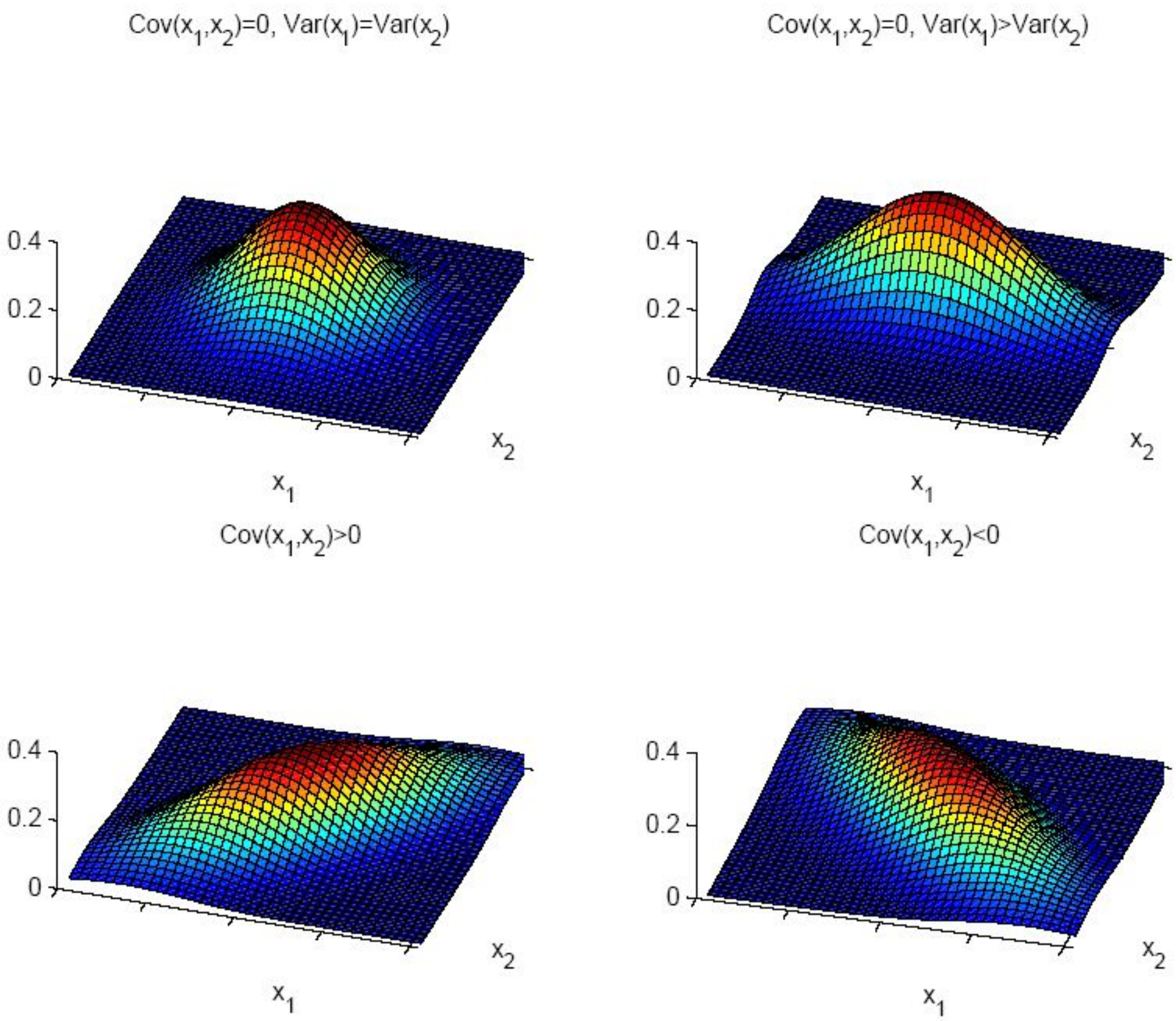
Mahalanobis distance
(standardizes all variables
to unit variance and eliminate
correlations)

Univariate case: $\frac{(x-\mu)^2}{\sigma^2} = (x-\mu)(\sigma^2)^{-1}(x-\mu)$

Multivariate Data – Normal distribution



Multivariate Data – Normal distribution



Multivariate Data – Classification

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

$$g_i(\boldsymbol{x}) = -\frac{d}{2}\log 2\pi - \frac{1}{2}\log|\boldsymbol{\Sigma}_i| - \frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu}_i)^T\boldsymbol{\Sigma}_i^{-1}(\boldsymbol{x}-\boldsymbol{\mu}_i) + \log P(C_i)$$

Using maximum likelihood:

$$\begin{aligned}
\hat{P}(C_i) &= \frac{\sum_t r_i^t}{N} \\
\boldsymbol{m}_i &= \frac{\sum_t r_i^t \boldsymbol{x}^t}{\sum_t r_i^t} \\
\mathbf{S}_i &= \frac{\sum_t r_i^t (\boldsymbol{x}^t - \boldsymbol{m}_i)(\boldsymbol{x}^t - \boldsymbol{m}_i)^T}{\sum_t r_i^t}
\end{aligned}$$

Multivariate Data – Classification

- Use common covariance matrix for each class
- Assume all off-diagonals of covariance matrix be 0
- Product of individual univariate densities...

- All variances equal – Mahalanobis distance to Euclidean distance
- All priors are equal

Multivariate Data – Classification

- Use common covariance matrix for each class
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Naive Bayes' classifier

$$g_i(\boldsymbol{x}) = -\frac{1}{2}\sum_{j=1}^{d}\left(\frac{x_j^t - m_{ij}}{s_j}\right)^2 + \log \hat{P}(C_i)$$

- All variances equal – Mahalanobis distance to Euclidean distance
- All priors are equal

Nearest mean classifier

$$g_i(\boldsymbol{x}) = -\|\boldsymbol{x} - \boldsymbol{m}_i\|^2$$

Multivariate Data – Linear Regression

Minimize sum of squared errors:

$$E(w_0, w_1, \ldots, w_d | \mathcal{X}) = \frac{1}{2} \sum_t (r^t - w_0 - w_1 x_1^t - w_2 x_2^t - \cdots - w_d x_d^t)^2$$

Take derivatives:

$$\begin{aligned}
\sum_t r^t &= N w_0 + w_1 \sum_t x_1^t + w_2 \sum_t x_2^t + \cdots + w_d \sum_t x_d^t \\
\sum_t x_1^t r^t &= w_0 \sum_t x_1^t + w_1 \sum_t (x_1^t)^2 + w_2 \sum_t x_1^t x_2^t + \cdots + w_d \sum_t x_1^t x_d^t \\
\sum_t x_2^t r^t &= w_0 \sum_t x_2^t + w_1 \sum_t x_1^t x_2^t + w_2 \sum_t (x_2^t)^2 + \cdots + w_d \sum_t x_2^t x_d^t \\
&\vdots \\
\sum_t x_d^t r^t &= w_0 \sum_t x_d^t + w_1 \sum_t x_d^t x_1^t + w_2 \sum_t x_d^t x_2^t + \cdots + w_d \sum_t (x_d^t)^2
\end{aligned}$$

Linear regression, higher order polynomial

$$\mathbf{A}\boldsymbol{w} = \boldsymbol{y}$$

$$\mathbf{A} = \begin{bmatrix} N & \sum_t x^t & \sum_t (x^t)^2 & \cdots & \sum_t (x^t)^k \\ \sum_t x^t & \sum_t (x^t)^2 & \sum_t (x^t)^3 & \cdots & \sum_t (x^t)^{k+1} \\ \vdots & & & & \\ \sum_t (x^t)^k & \sum_t (x^t)^{k+1} & \sum_t (x^t)^{k+2} & \cdots & \sum_t (x^t)^{2k} \end{bmatrix}$$

$$\boldsymbol{w} = \begin{bmatrix} w_0 \\ w_1 \\ w_2 \\ \vdots \\ w_k \end{bmatrix}, \boldsymbol{y} = \begin{bmatrix} \sum_t r^t \\ \sum_t r^t x^t \\ \sum_t r^t (x^t)^2 \\ \vdots \\ \sum_t r^t (x^t)^k \end{bmatrix}$$

We can write $\mathbf{A} = \mathbf{D}^T\mathbf{D}$ and $\boldsymbol{y} = \mathbf{D}^T\boldsymbol{r}$ where

$$\mathbf{D} = \begin{bmatrix} 1 & x^1 & (x^1)^2 & \cdots & (x^1)^k \\ 1 & x^2 & (x^2)^2 & \cdots & (x^2)^k \\ \vdots & & & & \\ 1 & x^N & (x^N)^2 & \cdots & (x^N)^k \end{bmatrix}, \boldsymbol{r} = \begin{bmatrix} r^1 \\ r^2 \\ \vdots \\ r^N \end{bmatrix}$$

and we can then solve for the parameters as

$$\boldsymbol{w} = (\mathbf{D}^T\mathbf{D})^{-1}\mathbf{D}^T\boldsymbol{r}$$

Multivariate Data – Linear Regression

$$\mathbf{X} = \begin{bmatrix} 1 & x_1^1 & x_2^1 & \cdots & x_d^1 \\ 1 & x_1^2 & x_2^2 & \cdots & x_d^2 \\ \vdots & & & & \\ 1 & x_1^N & x_2^N & \cdots & x_d^N \end{bmatrix}, \boldsymbol{w} = \begin{bmatrix} w_0 \\ w_1 \\ \vdots \\ w_d, \end{bmatrix}, \boldsymbol{r} = \begin{bmatrix} r^1 \\ r^2 \\ \vdots \\ r^N \end{bmatrix}$$

Then the normal equations can be written as

$$\mathbf{X}^T\mathbf{X}\boldsymbol{w} = \mathbf{X}^T\boldsymbol{r}$$

and we can solve for the parameters as

$$\boldsymbol{w} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\boldsymbol{r}$$