



Machine Learning

# Anomaly detection

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Problem  
motivation



# Anomaly detection example

Aircraft engine features:

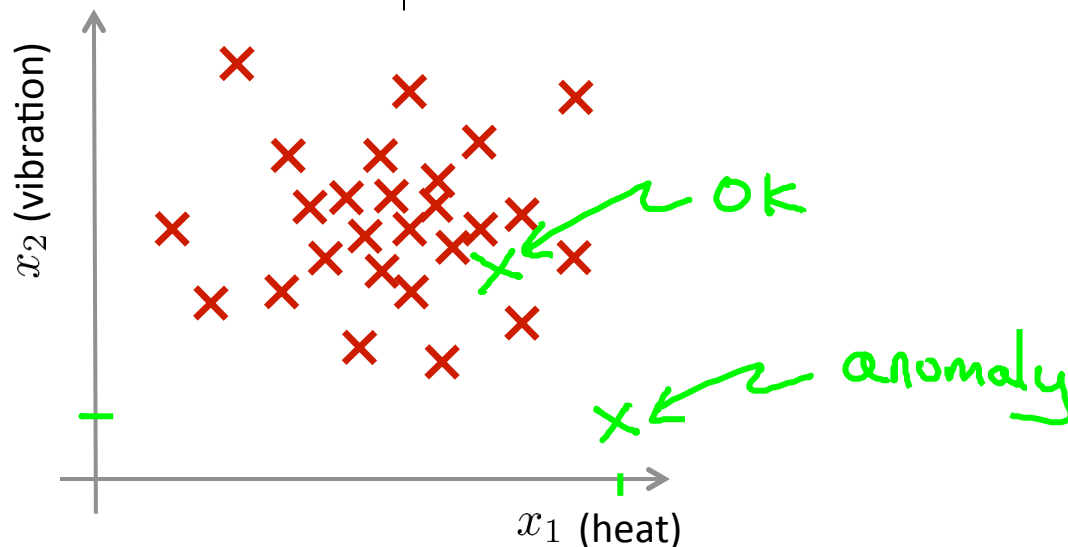
→  $x_1$  = heat generated

→  $x_2$  = vibration intensity

...

Dataset:  $\{x^{(1)}, x^{(2)}, \dots, x^{(m)}\}$

New engine:  $x_{test}$

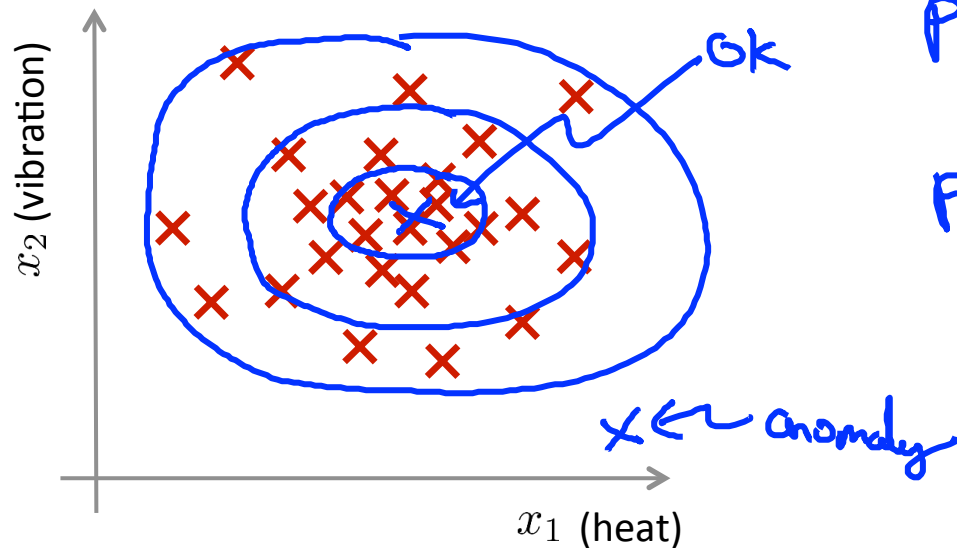


# Density estimation

→ Dataset:  $\{x^{(1)}, x^{(2)}, \dots, x^{(m)}\}$

→ Is  $x_{test}$  anomalous?

Model  $p(x)$ .



$p(x_{test}) < \varepsilon \rightarrow$  flag anomaly

$p(x_{test}) \geq \varepsilon \rightarrow$  OK

# Anomaly detection example

→ Fraud detection:

→  $x^{(i)}$  = features of user  $i$ 's activities

→ Model  $p(x)$  from data.

→ Identify unusual users by checking which have  $p(x) < \epsilon$

→ Manufacturing

→ Monitoring computers in a data center.

→  $x^{(i)}$  = features of machine  $i$

$x_1$  = memory use,  $x_2$  = number of disk accesses/sec,

$x_3$  = CPU load,  $x_4$  = CPU load/network traffic.

...

$p(x) < \epsilon$

$x_1$   
 $x_2$   
 $x_3$   
 $x_4$        $p(x)$



Machine Learning

# Anomaly detection

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## Gaussian distribution

# Gaussian (Normal) distribution

Say  $x \in \mathbb{R}$ . If  $x$  is a distributed Gaussian with mean  $\mu$ , variance  $\sigma^2$ .

$$x \sim \mathcal{N}(\mu, \sigma^2)$$

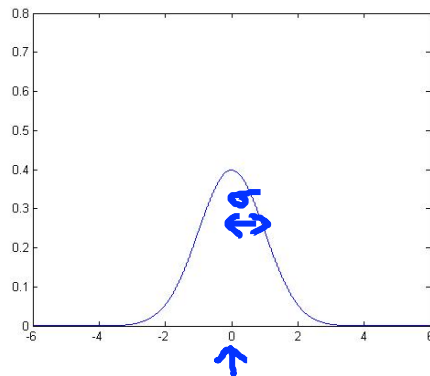
↑ "distributed as"

$\sigma$  standard deviation



# Gaussian distribution example

→  $\mu = 0, \sigma = 1$

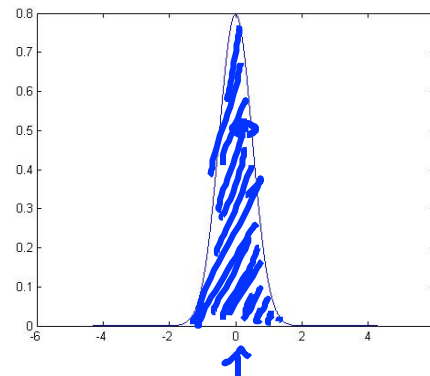


→  $\mu = 0, \sigma = 2$

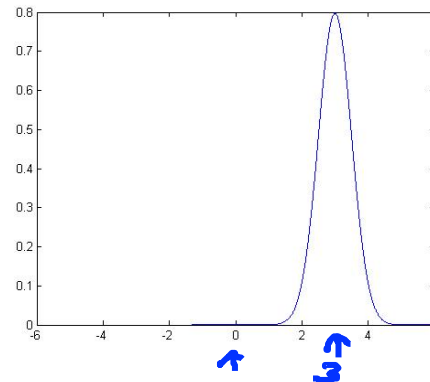


→  $\mu = 0, \sigma = \underline{0.5}$

$\sigma^2 = 0.25$



→  $\mu = 3, \sigma = 0.5$

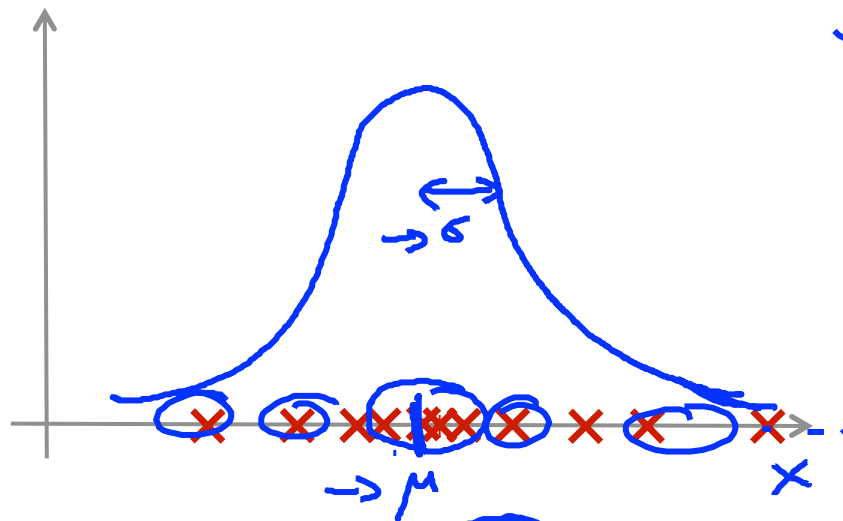


# Parameter estimation

→ Dataset:  $\{x^{(1)}, x^{(2)}, \dots, x^{(m)}\}$   $x^{(i)} \in \mathbb{R}$

$$x^{(i)} \sim \mathcal{N}(\mu, \sigma^2)$$

↑   ↑



$$\rightarrow \mu = \frac{1}{m} \sum_{i=1}^m x^{(i)}$$

$$\rightarrow \sigma^2 = \left( \frac{1}{m} \right) \sum_{i=1}^m \underbrace{(x^{(i)} - \mu)^2}_{\frac{1}{m-1} \leftarrow}$$





Machine Learning

# Anomaly detection

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# Algorithm

## → Density estimation

→ Training set:  $\{x^{(1)}, \dots, x^{(m)}\}$

Each example is  $x \in \mathbb{R}^n$

→  $p(x)$

$$= \boxed{p(x_1; \mu_1, \sigma_1^2) p(x_2; \mu_2, \sigma_2^2) p(x_3; \mu_3, \sigma_3^2) \dots p(x_n; \mu_n, \sigma_n^2)} \leftarrow$$

$$= \prod_{j=1}^n p(x_j; \mu_j, \sigma_j^2)$$

$$x_1 \sim \mathcal{N}(\mu_1, \sigma_1^2)$$

$$x_2 \sim \mathcal{N}(\mu_2, \sigma_2^2)$$

$$x_3 \sim \mathcal{N}(\mu_3, \sigma_3^2)$$

$$\sum_{i=1}^n i = 1 + 2 + 3 + \dots + n$$

$$\prod_{i=1}^n i = 1 \times 2 \times 3 \times \dots \times n$$

# Anomaly detection algorithm

→ 1. Choose features  $x_i$  that you think might be indicative of anomalous examples.  $\{x^{(1)}, \dots, x^{(m)}\}$

→ 2. Fit parameters  $\mu_1, \dots, \mu_n, \sigma_1^2, \dots, \sigma_n^2$

→ 
$$\mu_j = \frac{1}{m} \sum_{i=1}^m x_j^{(i)}$$

→ 
$$\sigma_j^2 = \frac{1}{m} \sum_{i=1}^m (x_j^{(i)} - \mu_j)^2$$

$$p(x_j; \mu_j, \sigma_j^2)$$

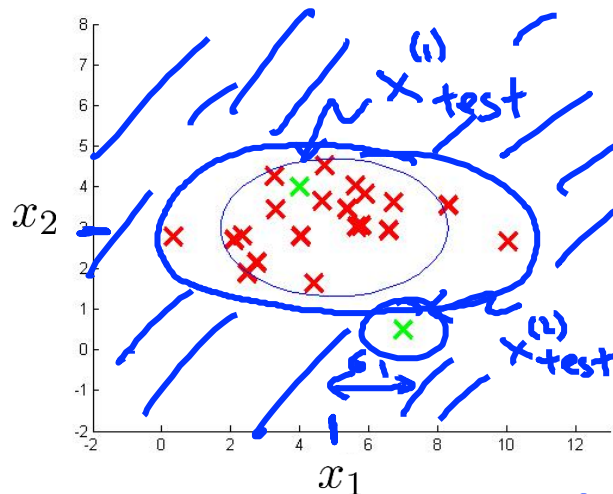
$$\mu = \begin{bmatrix} \mu_1 \\ \mu_2 \\ \vdots \\ \mu_n \end{bmatrix} = \frac{1}{m} \sum_{i=1}^m x^{(i)}$$

→ 3. Given new example  $x$ , compute  $p(x)$ :

$$p(x) = \prod_{j=1}^n p(x_j; \mu_j, \sigma_j^2) = \prod_{j=1}^n \frac{1}{\sqrt{2\pi}\sigma_j} \exp\left(-\frac{(x_j - \mu_j)^2}{2\sigma_j^2}\right)$$

Anomaly if  $p(x) < \varepsilon$

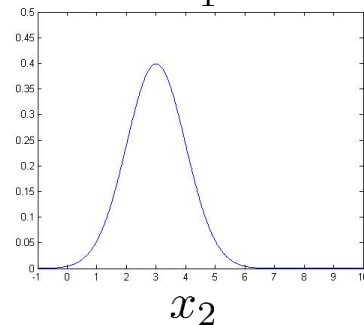
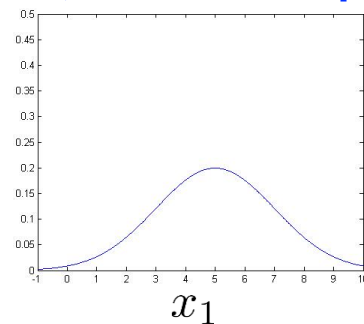
# Anomaly detection example



$$\mu_1 = 5, \sigma_1 = 2$$

$$\mu_2 = 3, \sigma_2 = 1$$

$$\sigma_1^2 - \sigma_2^2 = 4$$

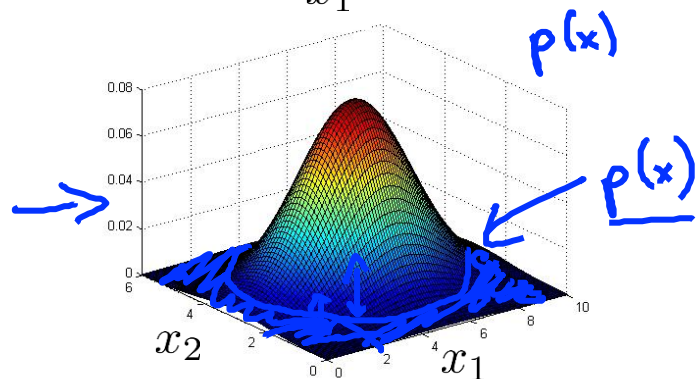


$$p(x_1; \mu_1, \sigma_1^2) \cdot p(x_2; \mu_2, \sigma_2^2)$$

$$p(x_1; \mu_1, \sigma_1^2)$$



$$p(x_2; \mu_2, \sigma_2^2)$$



$$\epsilon = 0.02$$

$$p(x_{test}^{(1)}) = 0.0426 \geq \epsilon$$

$$p(x_{test}^{(2)}) = 0.0021 < \epsilon$$



Machine Learning

# Anomaly detection

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Developing and  
evaluating an anomaly  
detection system

## The importance of real-number evaluation

When developing a learning algorithm (choosing features, etc.), making decisions is much easier if we have a way of evaluating our learning algorithm.

- Assume we have some labeled data, of anomalous and non-anomalous examples. ( $y = 0$  if normal,  $y = 1$  if anomalous).
- Training set:  $x^{(1)}, x^{(2)}, \dots, x^{(m)}$  (assume normal examples/not anomalous)
- Cross validation set:  $(x_{cv}^{(1)}, y_{cv}^{(1)}), \dots, (x_{cv}^{(m_{cv})}, y_{cv}^{(m_{cv})})$
- Test set:  $(x_{test}^{(1)}, y_{test}^{(1)}), \dots, (x_{test}^{(m_{test})}, y_{test}^{(m_{test})})$

$y=1$

## Aircraft engines motivating example

- 10000 good (normal) engines
- 20 flawed engines (anomalous) 2-50  $y=1$
- Training set: 6000 good engines ( $y=0$ )  $\mu_1, \sigma_1^2, \dots, \mu_n, \sigma_n^2$   $p(x) = p(x_1; \mu_1, \sigma_1^2) \dots p(x_n; \mu_n, \sigma_n^2)$
- CV: 2000 good engines ( $y=0$ ), 10 anomalous ( $y=1$ )
- Test: 2000 good engines ( $y=0$ ), 10 anomalous ( $y=1$ )

Alternative:

Training set: 6000 good engines

- CV: 4000 good engines ( $y=0$ ), 10 anomalous ( $y=1$ )
- Test: 4000 good engines ( $y=0$ ), 10 anomalous ( $y=1$ )

## Algorithm evaluation

- Fit model  $p(x)$  on training set  $\{x^{(1)}, \dots, x^{(m)}\}$
- On a cross validation/test example  $x$ , predict

$$y = \begin{cases} 1 & \text{if } p(x) < \varepsilon \text{ (anomaly)} \\ 0 & \text{if } p(x) \geq \varepsilon \text{ (normal)} \end{cases}$$

$(x_{\text{test}}^{(i)}, y_{\text{test}}^{(i)})$   
↑

$y = 0$

Possible evaluation metrics:

- - True positive, false positive, false negative, true negative
- - Precision/Recall
- -  $F_1$ -score ←

CV

Test set

Can also use cross validation set to choose parameter  $\varepsilon$  ←





Machine Learning

# Anomaly detection

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Anomaly detection  
vs. supervised  
learning

## Anomaly detection

- Very small number of positive examples ( $y = 1$ ). (0-20 is common).
- Large number of negative ( $y = 0$ ) examples.  $p(x)$  ←
- Many different “types” of anomalies. Hard for any algorithm to learn from positive examples what the anomalies look like;
- future anomalies may look nothing like any of the anomalous examples we've seen so far.

vs.

## Supervised learning

Large number of positive and negative examples. ←

Enough positive examples for algorithm to get a sense of what positive examples are like, future positive examples likely to be similar to ones in training set. ←

Spam ←

## Anomaly detection

vs.

## Supervised learning

- • Fraud detection  $y=1$
- • Manufacturing (e.g. aircraft engines)
- • Monitoring machines in a data center

⋮

- Email spam classification ←
- Weather prediction (sunny/~~rainy~~/etc). ←
- Cancer classification ←

⋮



Machine Learning

# Anomaly detection

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Choosing what  
features to use

# Non-gaussian features



$$p(x; \mu, \sigma^2)$$

hist

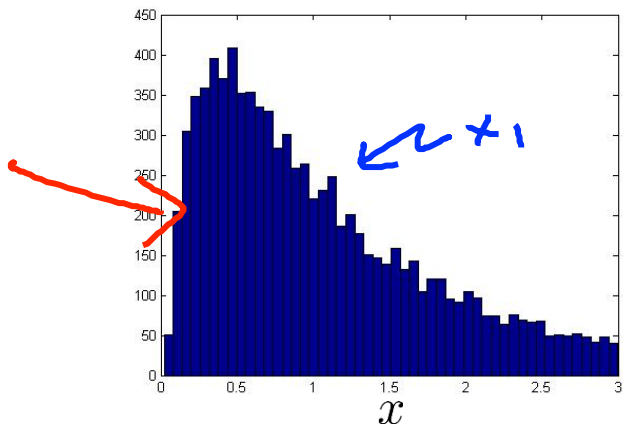
$$x_1 \leftarrow \frac{\log(x_1)}{\log(x_2+1)}$$

$$x_2 \leftarrow \log(x_2+1)$$

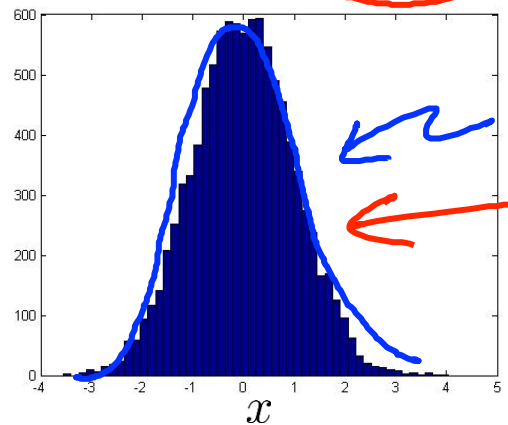
$$x_3 \leftarrow \sqrt{x_3} = x_3^{\frac{1}{2}}$$

$$x_4 \leftarrow x_4^{\frac{1}{3}}$$

$$\log(x_2 + \odot)$$



$$\log(x)$$

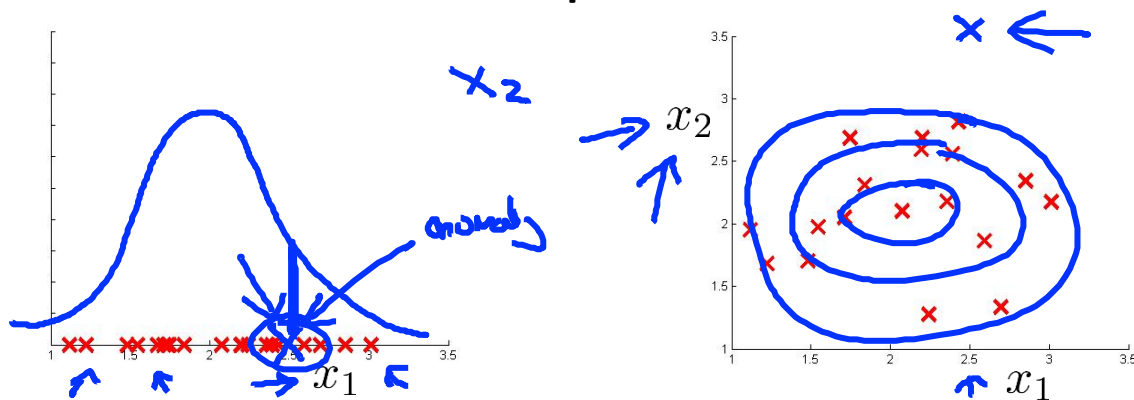


## → Error analysis for anomaly detection

Want  $p(x)$  large for normal examples  $x$ .  
 $p(x)$  small for anomalous examples  $x$ .

Most common problem:

$p(x)$  is comparable (say, both large) for normal  
and anomalous examples



- **Monitoring computers in a data center**
- Choose features that might take on unusually large or small values in the event of an anomaly.
  - $x_1$  = memory use of computer
  - $x_2$  = number of disk accesses/sec
  - $x_3$  = CPU load ←
  - $x_4$  = network traffic ←

$$\underline{x_5 = \frac{\text{CPU load}}{\text{network traffic}}}$$

$$\underline{x_6 = \frac{(\text{CPU load})^2}{\text{network traffic}}}$$



Machine Learning

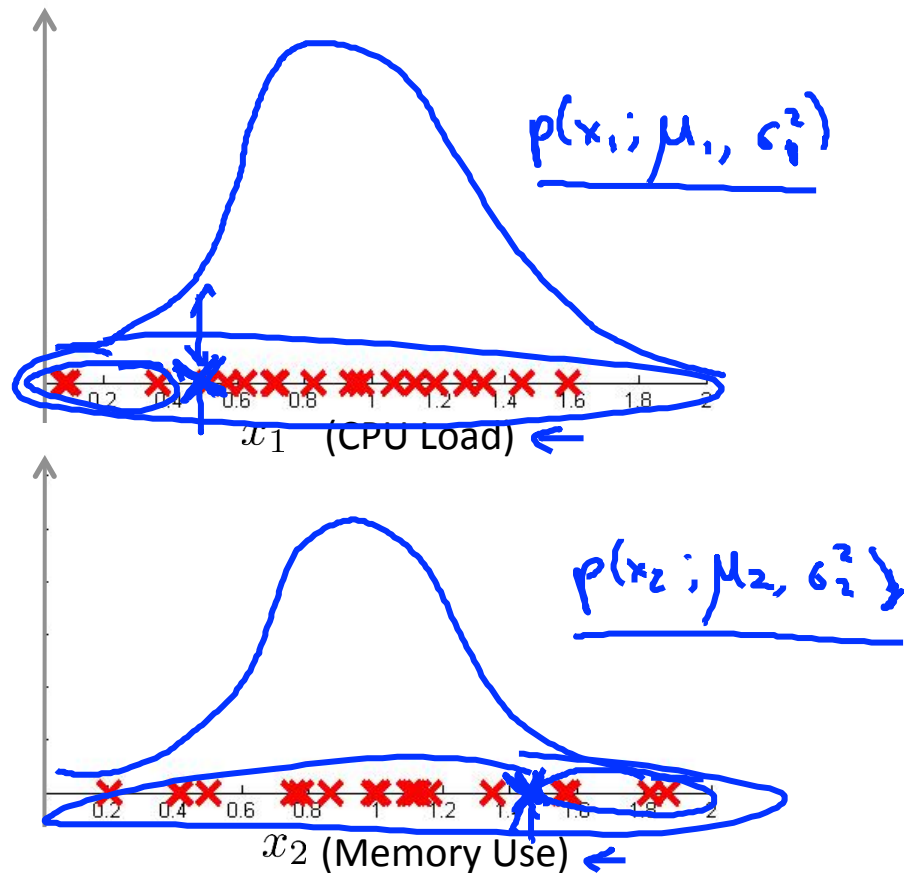
# Anomaly detection

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Multivariate  
Gaussian distribution



# Motivating example: Monitoring machines in a data center



# Multivariate Gaussian (Normal) distribution

→  $x \in \mathbb{R}^n$ . Don't model  $p(x_1), p(x_2), \dots$ , etc. separately.

Model  $p(x)$  all in one go.

Parameters:  $\mu \in \mathbb{R}^n$ ,  $\Sigma \in \mathbb{R}^{n \times n}$  (covariance matrix)

$$p(x; \mu, \Sigma) =$$

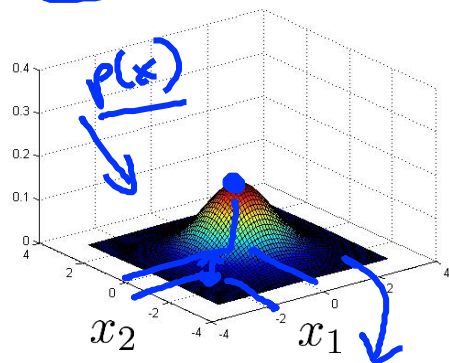
$$\frac{1}{(2\pi)^{n/2} |\Sigma|^{1/2}}$$

$$\exp\left(-\frac{1}{2} (x-\mu)^\top \Sigma^{-1} (x-\mu)\right)$$

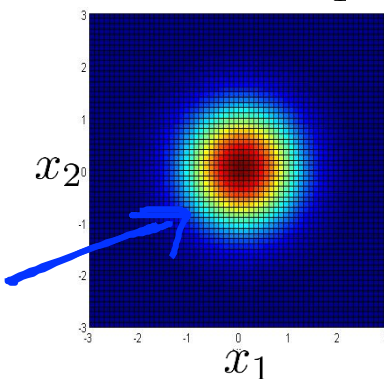
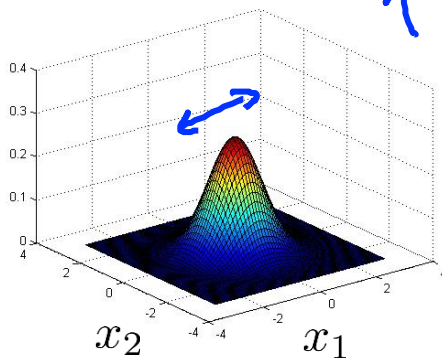
$$|\Sigma| = \text{determinant of } \Sigma \quad \left| \det(\text{Sigma}) \right|$$

# Multivariate Gaussian (Normal) examples

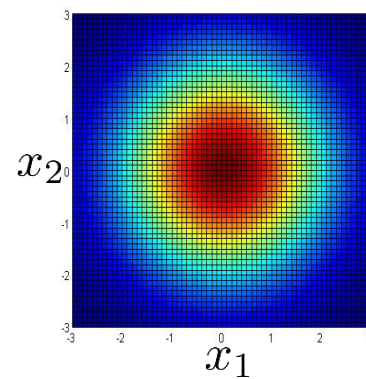
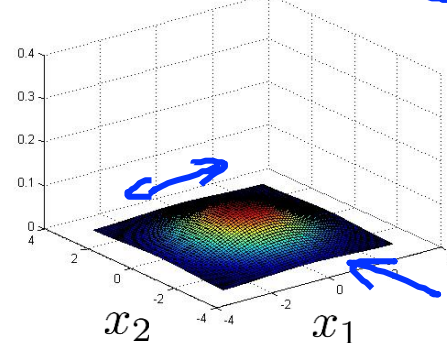
$$\mu = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad \Sigma = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$



$$\mu = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad \Sigma = \begin{bmatrix} 0.6 & 0 \\ 0 & 0.6 \end{bmatrix}$$

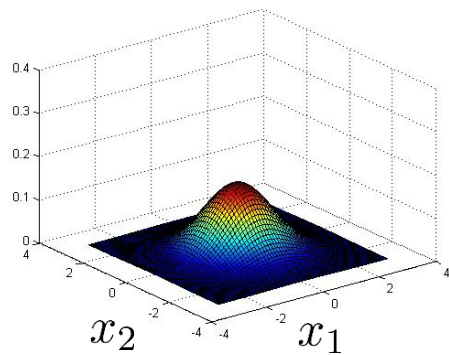


$$\mu = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad \Sigma = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix}$$

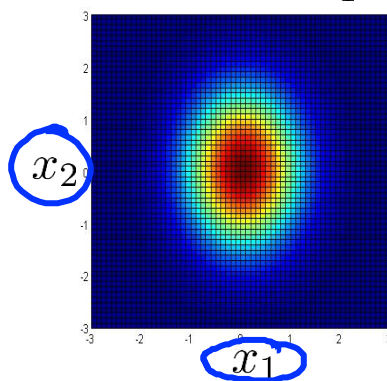
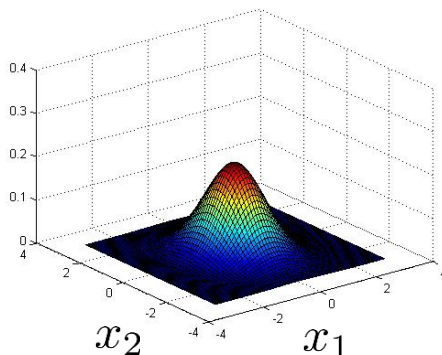


# Multivariate Gaussian (Normal) examples

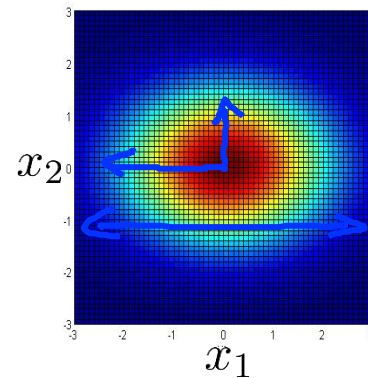
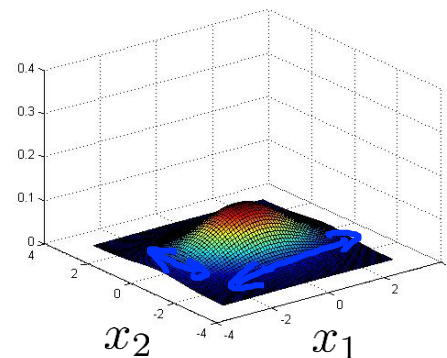
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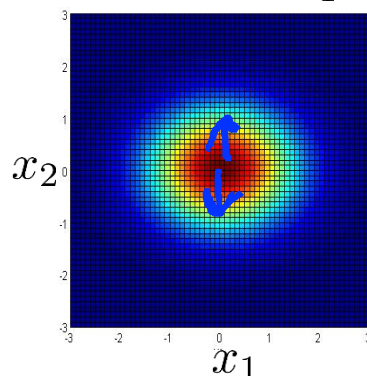


# Multivariate Gaussian (Normal) examples

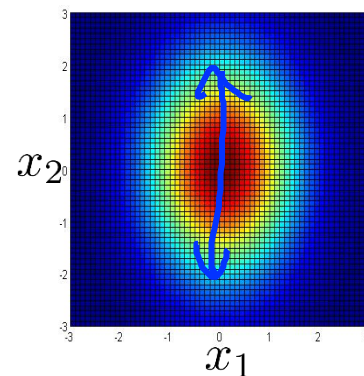
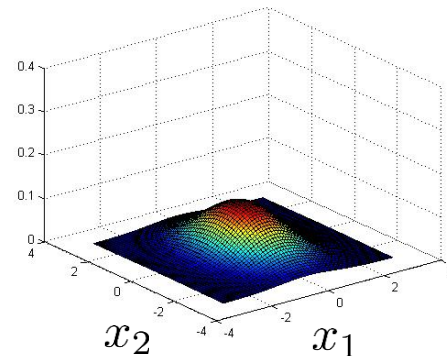
$$\mu = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad \Sigma = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$



$$\mu = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad \Sigma = \begin{bmatrix} 1 & 0 \\ 0 & 0.6 \end{bmatrix}$$

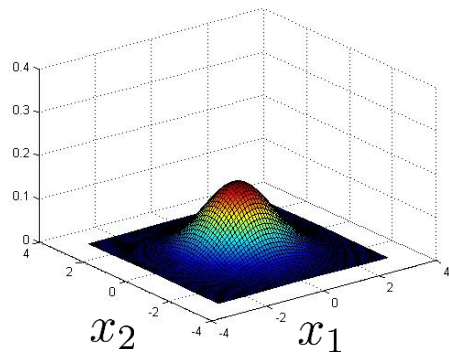


$$\mu = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad \Sigma = \begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix}$$

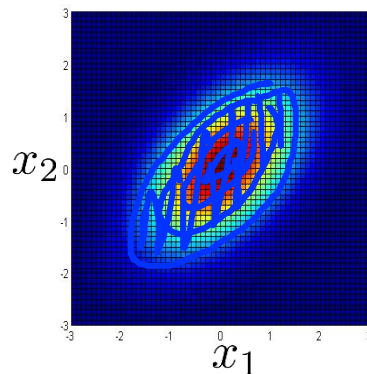
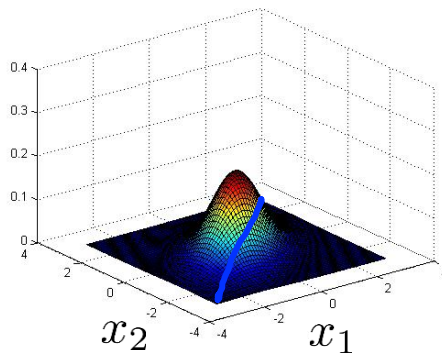


# Multivariate Gaussian (Normal) examples

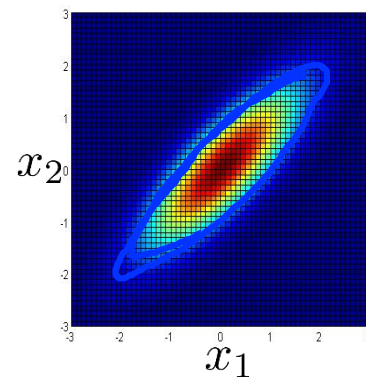
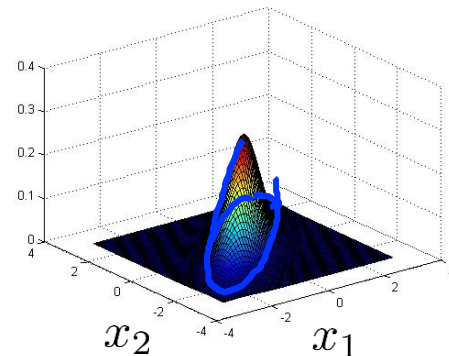
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$$\mu = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad \Sigma = \begin{bmatrix} 1 & 0.5 \\ 0.5 & 1 \end{bmatrix}$$



$$\mu = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad \Sigma = \begin{bmatrix} 1 & 0.8 \\ 0.8 & 1 \end{bmatrix}$$





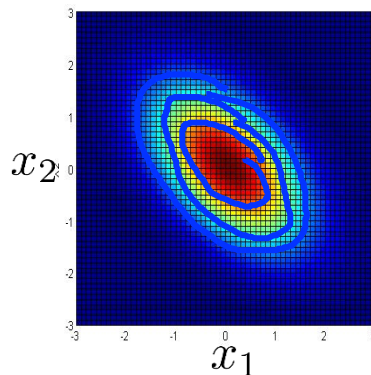
# Multivariate Gaussian (Normal) examples

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

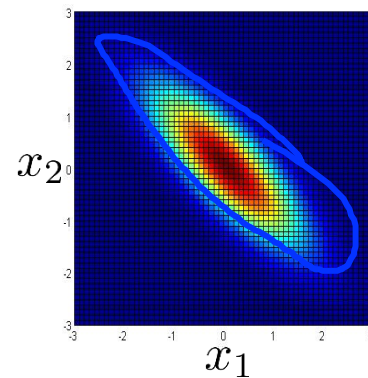
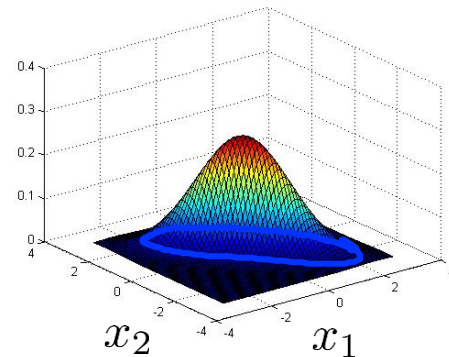
↑



$$\mu = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad \Sigma = \begin{bmatrix} 1 & -0.5 \\ -0.5 & 1 \end{bmatrix}$$

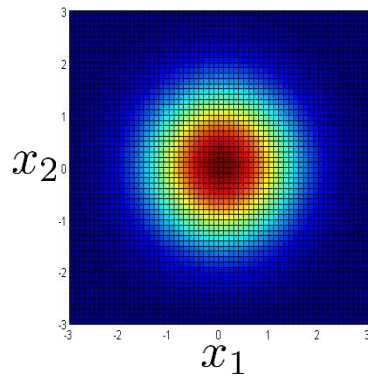


$$\mu = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad \Sigma = \begin{bmatrix} 1 & -0.8 \\ -0.8 & 1 \end{bmatrix}$$

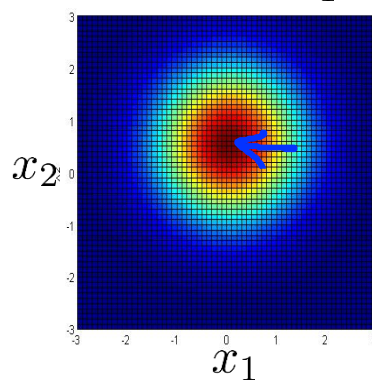
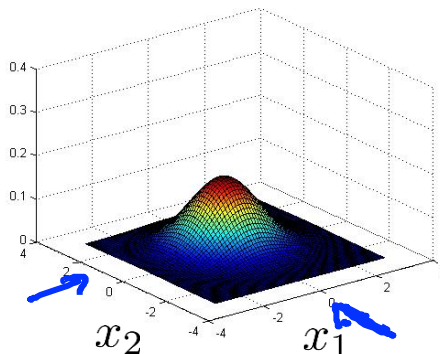


# Multivariate Gaussian (Normal) examples

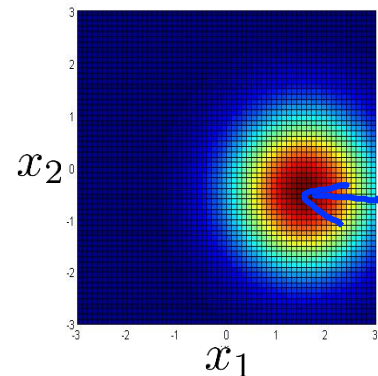
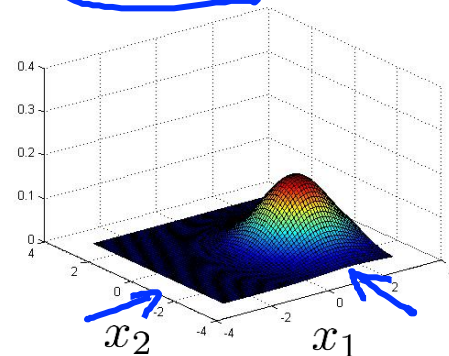
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$$\mu = \begin{bmatrix} 0 \\ 0.5 \end{bmatrix} \quad \Sigma = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$



$$\mu = \begin{bmatrix} 1.5 \\ -0.5 \end{bmatrix} \quad \Sigma = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$







Machine Learning

# Anomaly detection

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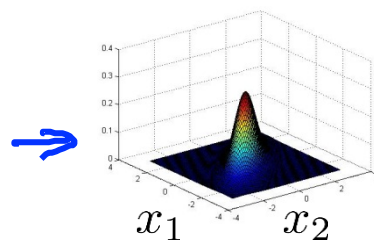
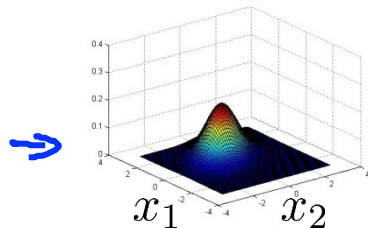
Anomaly detection using  
the multivariate  
Gaussian distribution

# Multivariate Gaussian (Normal) distribution

Parameters  $\mu, \Sigma$

$$\mu \in \mathbb{R}^n \quad \Sigma \in \mathbb{R}^{n \times n}$$

$$\rightarrow p(x; \mu, \Sigma) = \frac{1}{(2\pi)^{\frac{n}{2}} |\Sigma|^{\frac{1}{2}}} \exp \left( -\frac{1}{2} (x - \mu)^T \Sigma^{-1} (x - \mu) \right)$$



Parameter fitting:

Given training set  $\{x^{(1)}, x^{(2)}, \dots, x^{(m)}\}$  ←

$$x \in \mathbb{R}^n$$

$$\rightarrow \boxed{\mu} = \frac{1}{m} \sum_{i=1}^m x^{(i)} \quad \rightarrow \boxed{\Sigma} = \frac{1}{m} \sum_{i=1}^m (x^{(i)} - \mu)(x^{(i)} - \mu)^T$$

# Anomaly detection with the multivariate Gaussian

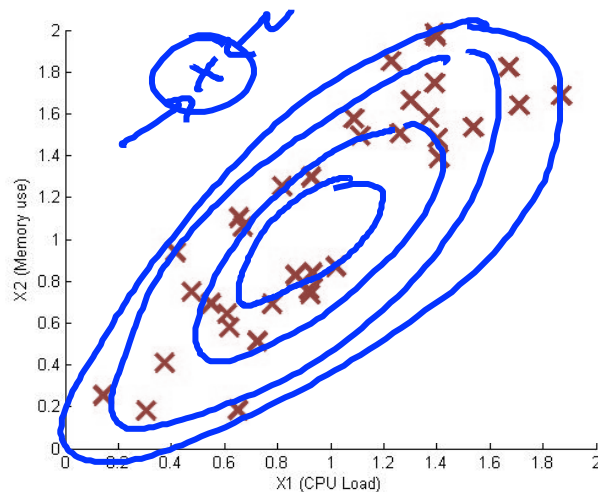
1. Fit model  $p(x)$  by setting

$$\begin{cases} \mu = \frac{1}{m} \sum_{i=1}^m x^{(i)} \\ \Sigma = \frac{1}{m} \sum_{i=1}^m (x^{(i)} - \mu)(x^{(i)} - \mu)^T \end{cases}$$

2. Given a new example  $x$ , compute

$$p(x) = \frac{1}{(2\pi)^{\frac{n}{2}} |\Sigma|^{\frac{1}{2}}} \exp \left( -\frac{1}{2} (x - \mu)^T \Sigma^{-1} (x - \mu) \right)$$

Flag an anomaly if  $p(x) < \varepsilon$



## Relationship to original model

Original model:  $p(x) = p(x_1; \mu_1, \sigma_1^2) \times p(x_2; \mu_2, \sigma_2^2) \times \cdots \times p(x_n; \mu_n, \sigma_n^2)$



Corresponds to multivariate Gaussian

$$\rightarrow p(x; \mu, \Sigma) = \frac{1}{(2\pi)^{\frac{n}{2}} |\Sigma|^{\frac{1}{2}}} \exp \left( -\frac{1}{2} (x - \mu)^T \Sigma^{-1} (x - \mu) \right)$$

where

$$\Sigma = \begin{bmatrix} \sigma_1^2 & \dots & \sigma_{1n} \\ \vdots & \ddots & \vdots \\ \sigma_{n1} & \dots & \sigma_n^2 \end{bmatrix}$$

## → Original model

$$p(x_1; \mu_1, \sigma_1^2) \times \cdots \times p(x_n; \mu_n, \sigma_n^2)$$

Manually create features to capture anomalies where  $\underline{x_1}, \underline{x_2}$  take unusual combinations of values.

$$\rightarrow x_3 = \frac{x_1}{x_2} = \frac{\text{CPU load}}{\text{memory}}$$

→ Computationally cheaper (alternatively, scales better to large  $n=10,000, \quad n=100,000$ )

OK even if  $m$  (training set size) is small

## vs. → Multivariate Gaussian

$$p(x; \mu, \Sigma) = \frac{1}{(2\pi)^{\frac{n}{2}} |\Sigma|^{\frac{1}{2}}} \exp \left( -\frac{1}{2} (x - \mu)^T \Sigma^{-1} (x - \mu) \right)$$

→ Automatically captures correlations between features

$$\Sigma \in \mathbb{R}^{n \times n}$$

$$\Sigma^{-1}$$

Computationally more expensive

$$\rightarrow \Sigma \sim \frac{n^2}{2}$$

Must have  $m > n$  or else  $\Sigma$  is non-invertible. →  $m \geq 10n$

$$\left[ \begin{array}{l} \rightarrow x_1 = \cancel{x_2} \\ \cancel{x_3} = x_4 + x_5 \end{array} \right]$$