



Machine Learning

# Anomaly detection

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Problem  
motivation

# Anomaly detection example

Aircraft engine features:

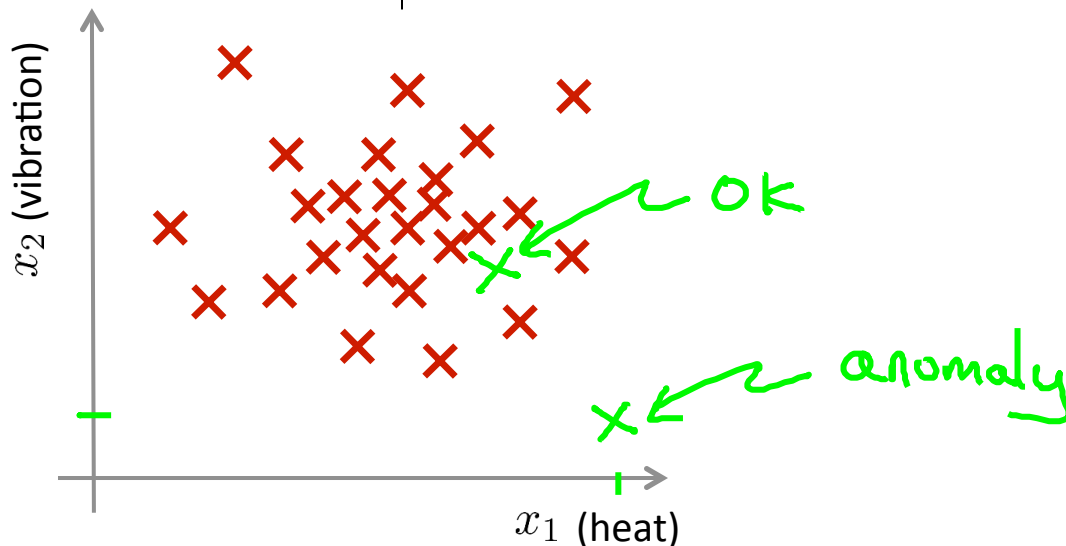
→  $x_1$  = heat generated

→  $x_2$  = vibration intensity

...

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

New engine:  $x_{test}$

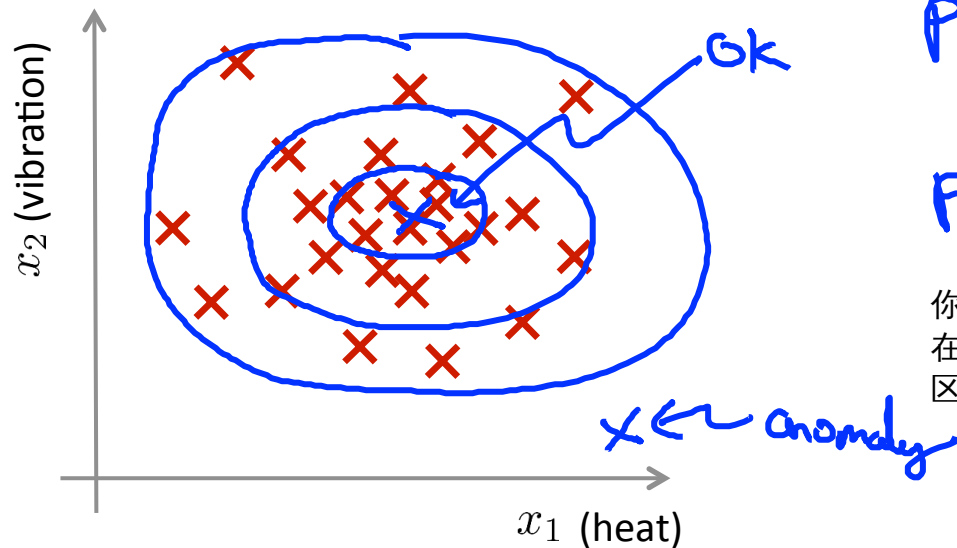


# Density estimation

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

→ Is  $x_{test}$  anomalous?

Model  $p(x)$ .



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

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

你将很可能发现飞机引擎 很可能发现模型 $p(x)$  将会认为在中心区域的这些点 有很大的概率值 而稍微远离中心区域的点概率会小一些

异常检测算法有如下应用案例

也许 $x_1$ 是用户登陆的频率  $x_2$ 也许是 用户访问 某个页面的次数 或者 交易次数 也许 $x_3$ 是 用户在论坛上发贴的次数  $x_4$ 是 用户的 打字速度

## Anomaly detection example

也许异常检测 最常见的应用是 是欺诈检测

→ Fraud detection:

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

→ Model  $p(x)$  from data.

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

异常检测的另一个例子是在工业生产领域 事实上 我们之前已经谈到过 飞机引擎的问题

→ Manufacturing

第三个应用是 数据中心的计算机监控

→ 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  $\sigma^2$ .

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

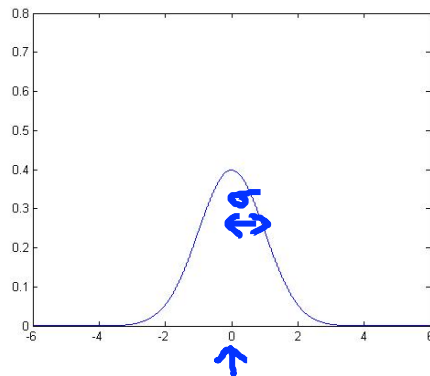
↑ "distributed as"

$\sigma$  standard deviation



# Gaussian distribution example

→  $\mu = 0, \sigma = 1$

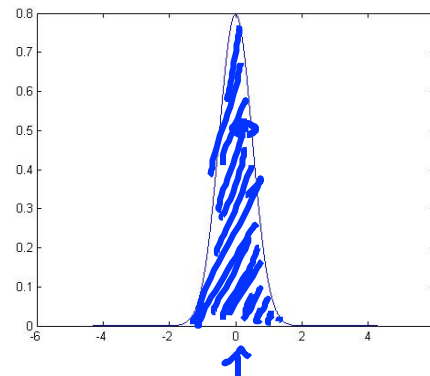


→  $\mu = 0, \sigma = 2$

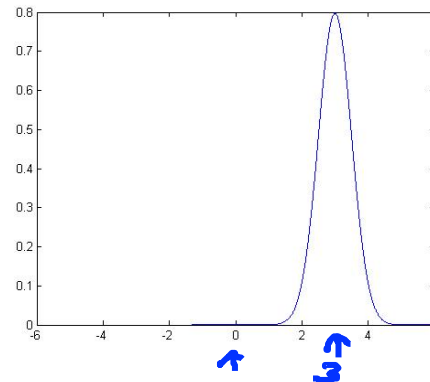


→  $\mu = 0, \sigma = \underline{0.5}$

$\sigma^2 = 0.25$



→  $\mu = 3, \sigma = 0.5$

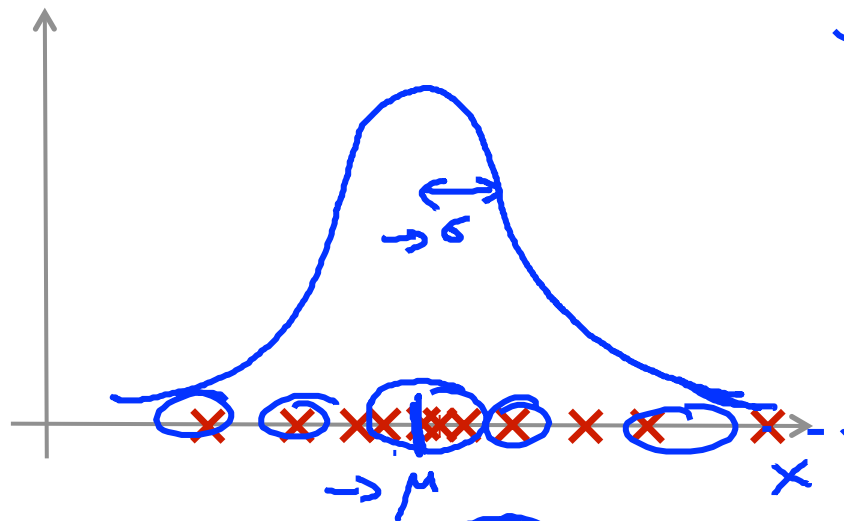


# Parameter estimation

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

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

↑   ↑



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

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

↑   ←

$m-1$     $\frac{1}{m-1}$

在实际使用中 到底是选择使用1/m还是1/(m-1)其实区别很小. 在机器学习领域大部分人更习惯使用1/m 这个版本的公式





Machine Learning

# Anomaly detection

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# Algorithm

## → Density estimation

假如说我们有一个无标签的训练集 共有  $m$  个训练样本

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

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

我们要从数据中 建立一个  $p(x)$  概率模型

→  $p(x)$  即使这个独立的假设不成立 这个算法的效果也还不错

假定  $x_1$  分布 服从高斯正态分布...

这就是我要说的模型

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

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

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

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

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

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

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

# Anomaly detection algorithm

這句話很misleading, 可以不看

→ 1. Choose features  $x_i$  that you think might be indicative of anomalous examples.

(要看的): 給出一組  $\{x^{(1)}, \dots, x^{(m)}\}$   
m 个无标签数据构成的训练集

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

j表示分量

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

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

$$\mu_1, \mu_2, \dots, \mu_n$$

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

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

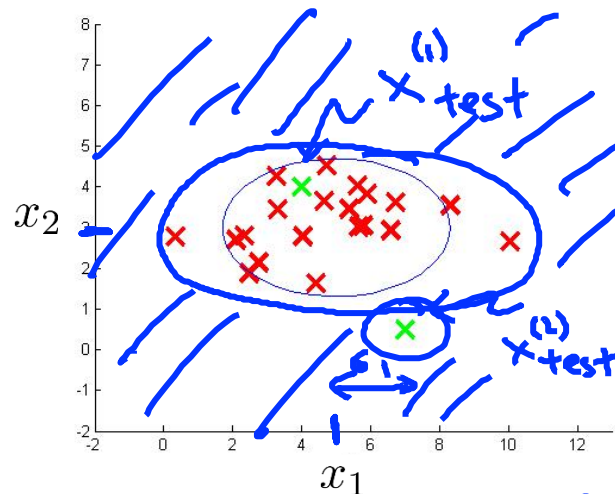
当给出一个新样本时, 你要知道是否出现异常

→ 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  $p(x) < \varepsilon$

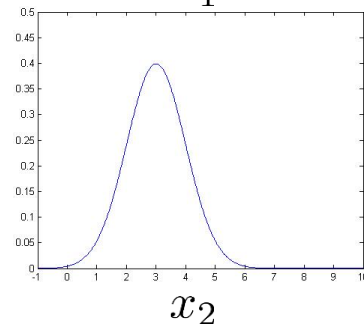
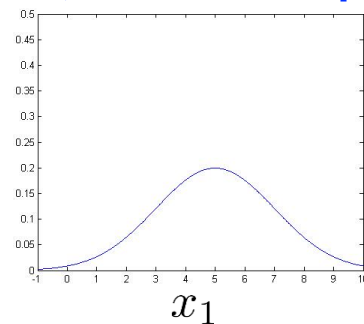
# Anomaly detection example



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

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

$$\sigma_1^2 = 4$$



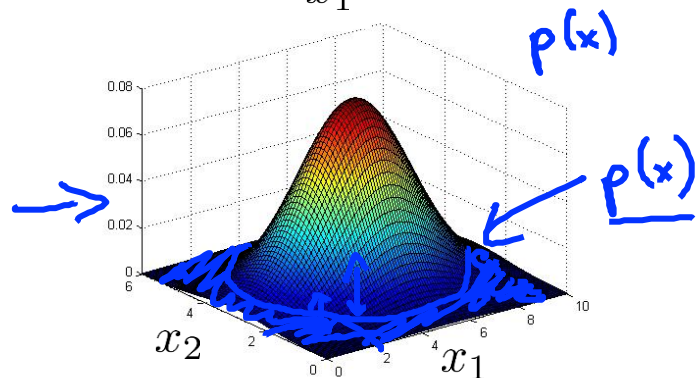
$$p(x_1; \mu_1, \sigma_1^2)$$

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



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

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



$$\epsilon = 0.02$$

我会在后面讲到如何选取  $\epsilon$  的值

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

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



Machine Learning

# Anomaly detection

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Developing and  
evaluating an anomaly  
detection system

## The importance of real-number evaluation 意思就是評價一個算法好不好

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

Alternative: 其实我真的不推荐这么分 但就有人喜欢这么分

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

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

↑

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

$$\underline{y = 0}$$

Possible evaluation metrics:

- 見 Lec 11 p11, p14 → - True positive, false positive, false negative, true negative
- - Precision/Recall
- -  $F_1$ -score ←

CV 一种选择参数  $\varepsilon$  的方法 就是你可以试一试 多个不同的  $\varepsilon$  的取值 然后选出一个 使得 F1-积分 的值最大的那个  $\varepsilon$  也就是在交叉验证集中表现最好的

Test set

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

更一般来说当 我们需要作出决定时 比如要包括哪些特征 或者说要确定参数  $\varepsilon$  取多大合适 我们就可以 不断地用交叉验证集来评价这个算法 然后决定





Machine Learning

# Anomaly detection

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Anomaly detection  
vs. supervised  
learning

为什么我们不直接用监督学习的方法呢？为什么不直接用逻辑回归或者神经网络的方法来直接学习这些带标签的数据从而给出预测  $y=1$  或  $y=0$  呢？

## Anomaly detection

vs.

## Supervised learning

- 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.

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  $y=1$

如果你掌握了大量的实施诈骗犯罪的人那么有时候欺诈检测的方法也可能会偏向于使用监督学习算法

- • Manufacturing (e.g. aircraft engines)

- • Monitoring machines in a data center

⋮

- Email spam classification

对于垃圾邮件的问题 我们通常有足够多的垃圾邮件的样本

- Weather prediction (sunny/rainy/etc).

- Cancer classification

⋮



Machine Learning

# Anomaly detection

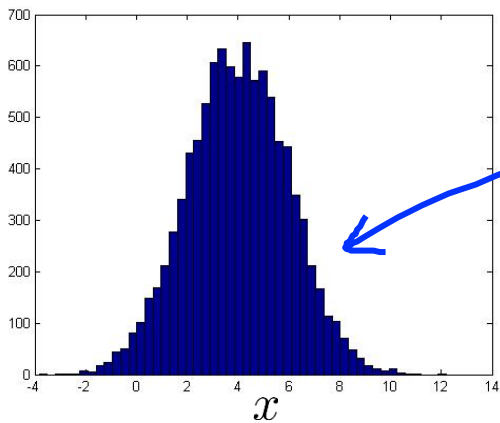
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Choosing what  
features to use

用异常检测时 对它的效率 影响最大的 因素之一是 你使用什么features

# Non-gaussian features

如果我有一个特征变量 比如  $x_1$  直方图是这样的 那么我就用  $x_1$  的对数  $\log(x_1)$  来替换掉  $x_1$  所以 经过替换 这就是我的新  $x_1$  我把它的直方图画在右边 这看起来更像高斯分布了



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

hist

除了取对数变换之外 还有别的一些方法 也可以用

$x_1 \leftarrow \log(x_1)$

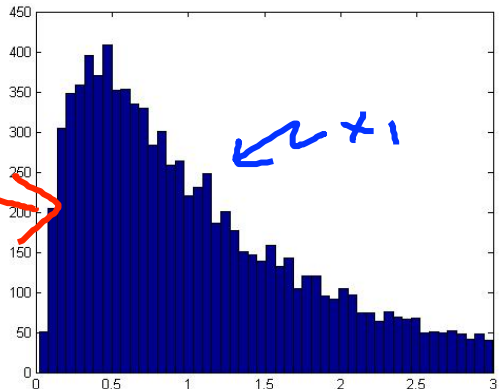
$x_2 \leftarrow \log(x_2 + 1)$

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

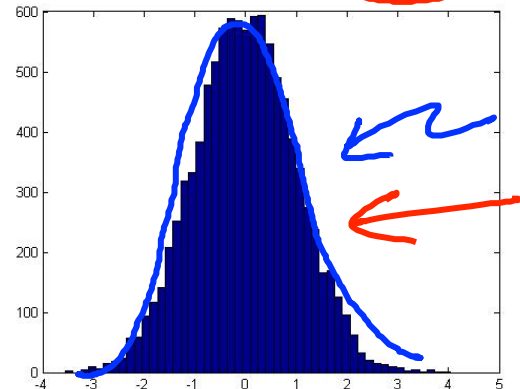
$x_4 \leftarrow x_4^{\frac{1}{3}}$

$\log(x_2 + 1)$

如果我的数据是这样的话 通常我要做的事情 是对数据进行一些不同的转换 来确保这些数据 看起来更像高斯分布 虽然通常来说你不这么做 算法也会运行地很好 但如果你使用一些转换方法 使你的数据更像高斯分布的话 你的算法会工作得更好



$\log(x)$



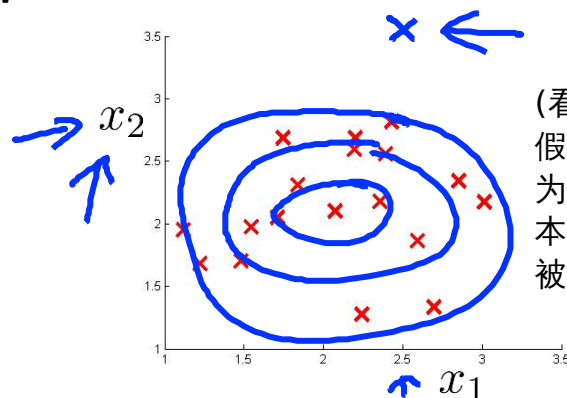
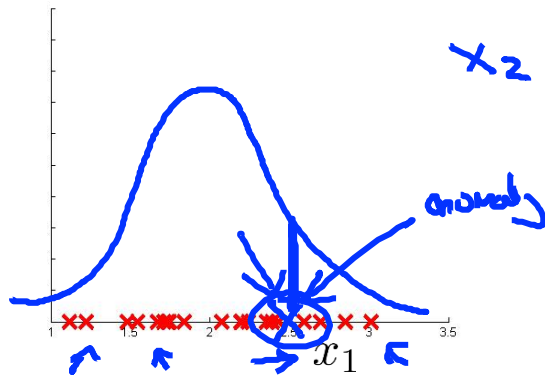
这跟我们之前学习监督学习算法时的 误差分析步骤是类似的 也就是说 我们先完整地训练出 一个学习算法 然后在一组交叉验证集上运行算法 然后找出那些预测出错的样本 然后再看看 我们能否找到一些其他的特征变量 来帮助学习算法 让它在那些交叉验证时判断出错的样本中表现更

## → 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



(看不清楚無所謂)  
假如我的异常样本中  $x$  的取值为 2.5 因此 我画出我的异常样本 你不难发现 它看起来就像被淹没在一堆正常样本中似的

能不能启发我 想出一个新的特征  $x_2$  来帮助算法区别出 不好的样本

## → 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 ←

$x_5$ 和 $x_6$ 都可以

我怀疑其中一个出错的情形  
是我的计算机在执行一个  
任务时 进入了一个死循环  
因此CPU负载升高  
但网络流量没有升高

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

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



Machine Learning

# Anomaly detection

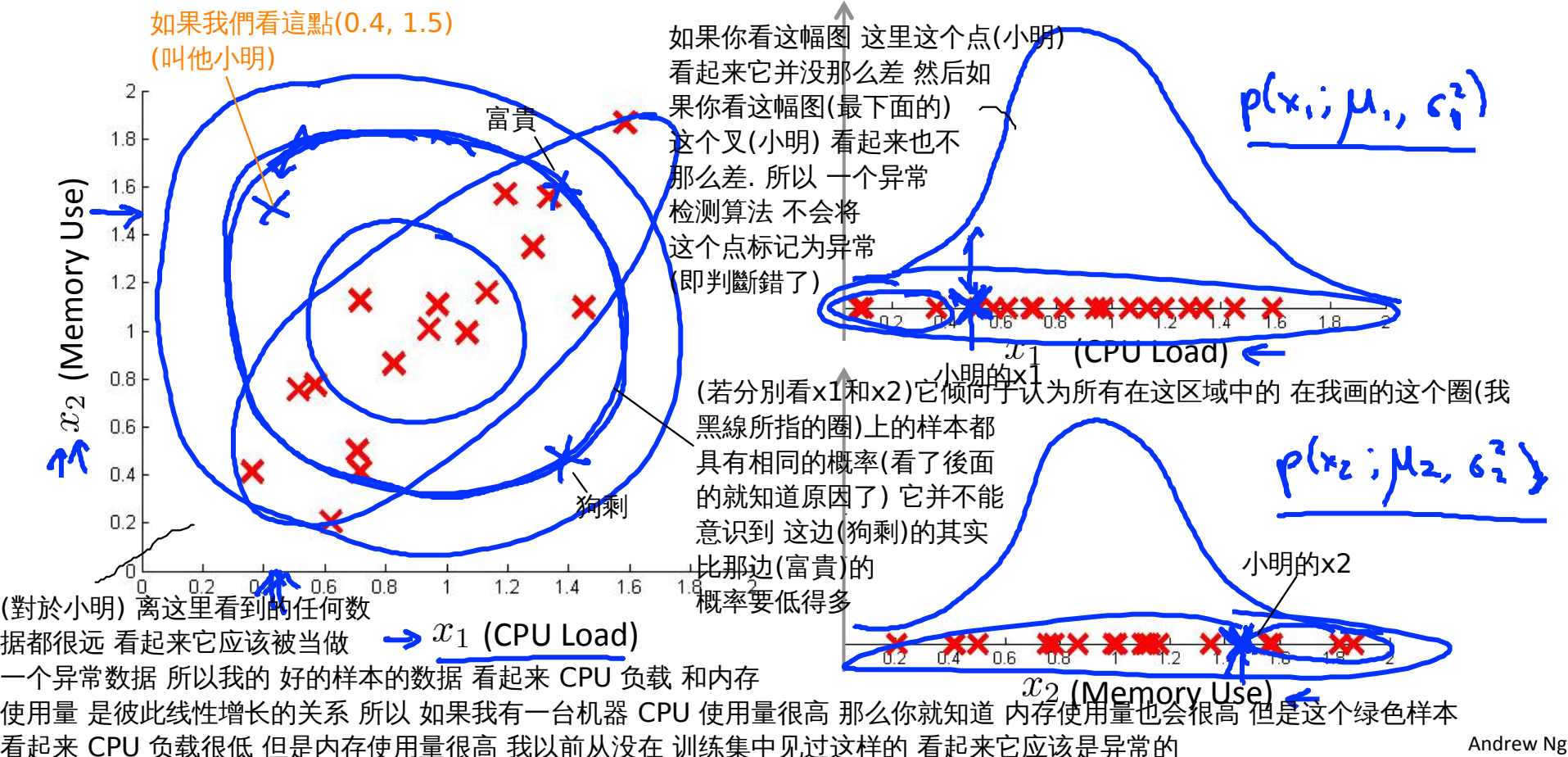
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Multivariate  
Gaussian distribution



multivariate Gaussian distribution 它有一些优势 也有一些劣势 它能捕捉到一些之前的算法检测不出来的异常

## Motivating example: Monitoring machines in a data center



所以 为了解决这个问题 我们要开发一种 改良版的异常检测算法 叫做多元高斯分布或者多元正态分布的东西

## 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)

$x, \mu$  都是  $n$  維向量,  $\Sigma$  是  $n \times n$  矩陣

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

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

$|\Sigma|$  = determinant of  $\Sigma$  |  $\det(\Sigma)$

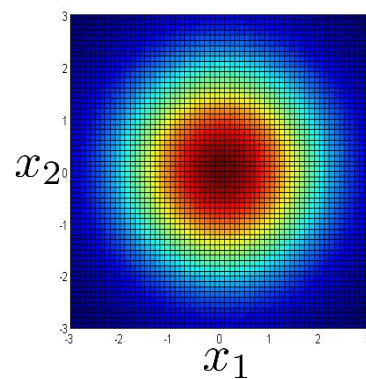
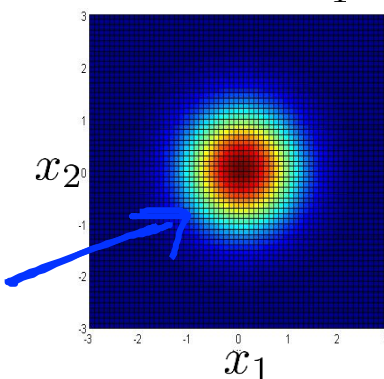
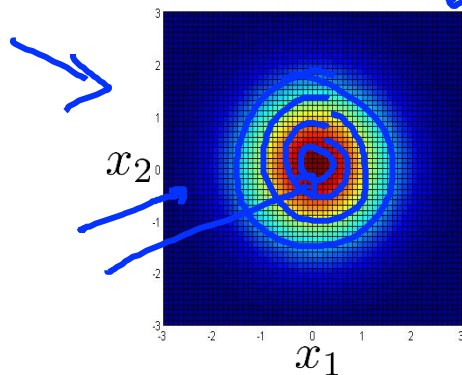
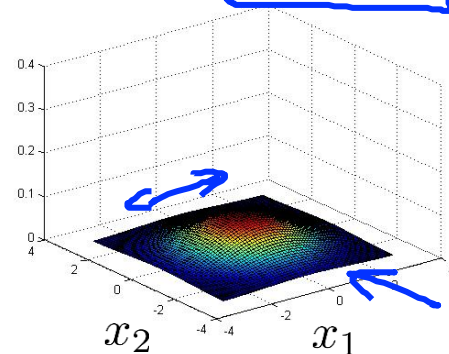
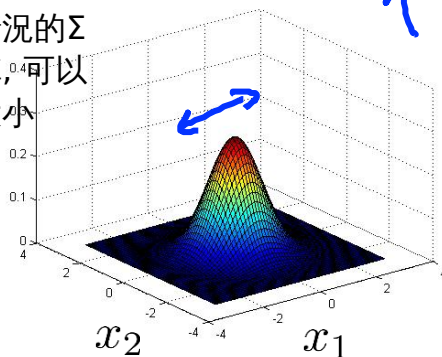
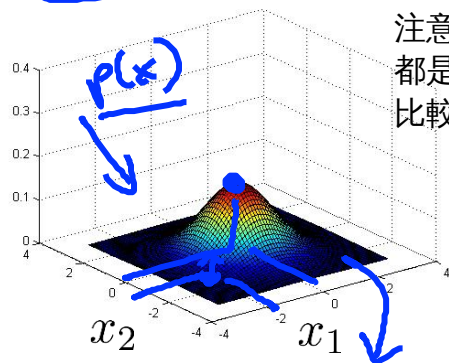
# Multivariate Gaussian (Normal) examples

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

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

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

注意這三種情況的 $\Sigma$ 都是單位矩陣, 可以比較其元素大小

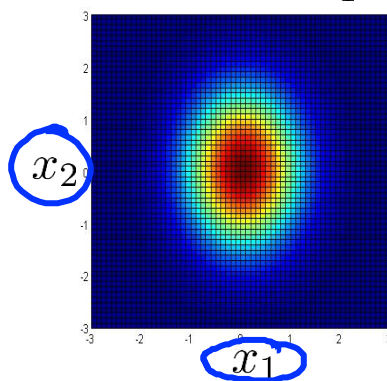


# Multivariate Gaussian (Normal) examples

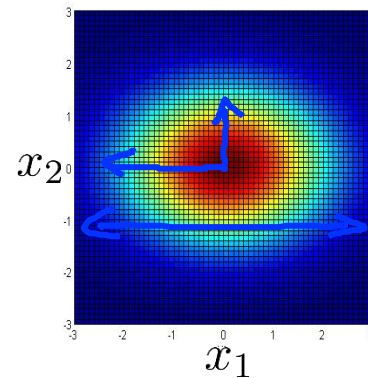
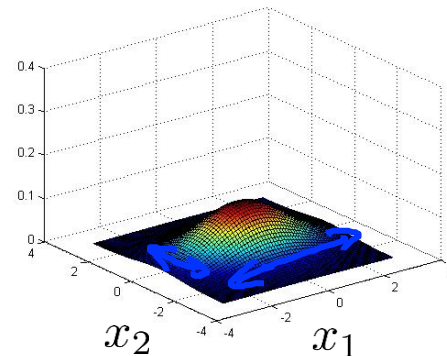
$$\mu = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad \Sigma = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$



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

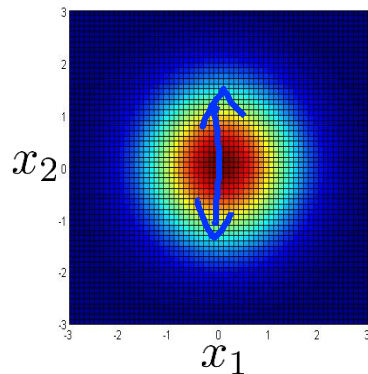


$$\mu = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad \Sigma = \begin{bmatrix} 2 & 0 \\ 0 & 1 \end{bmatrix}$$

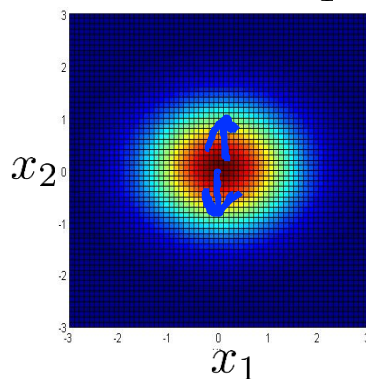


# Multivariate Gaussian (Normal) examples

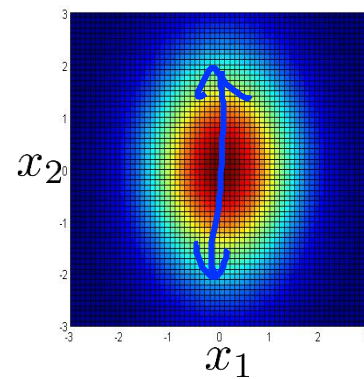
$$\mu = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad \Sigma = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$



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



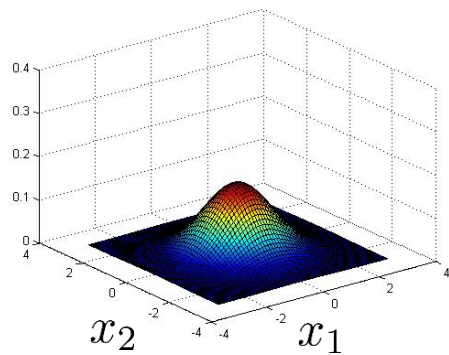
$$\mu = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad \Sigma = \begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix}$$



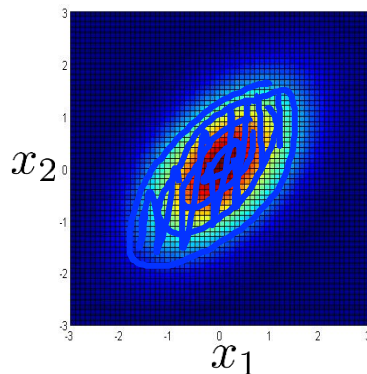
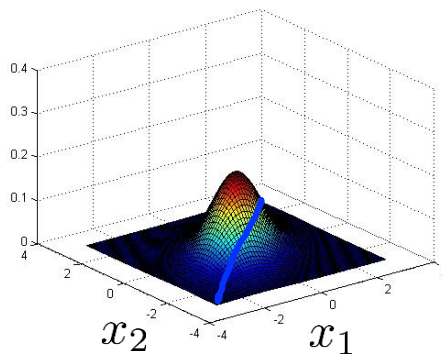


# Multivariate Gaussian (Normal) examples

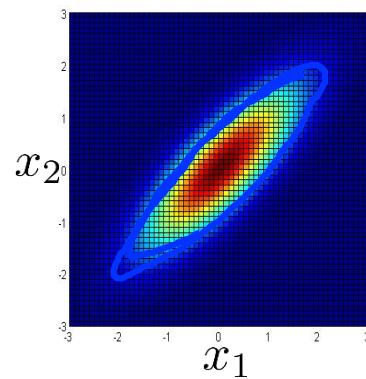
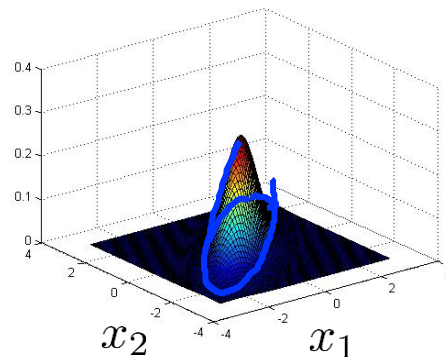
$$\mu = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad \Sigma = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$



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



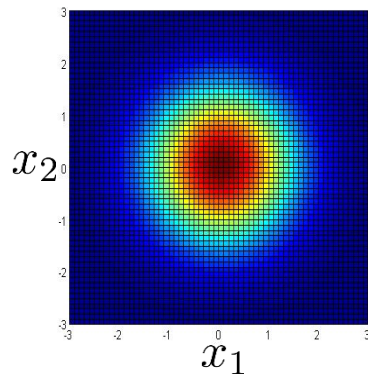
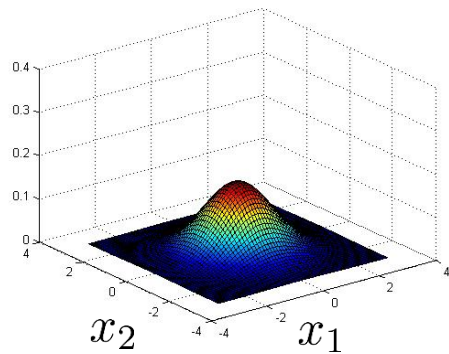
$$\mu = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad \Sigma = \begin{bmatrix} 1 & 0.8 \\ 0.8 & 1 \end{bmatrix}$$



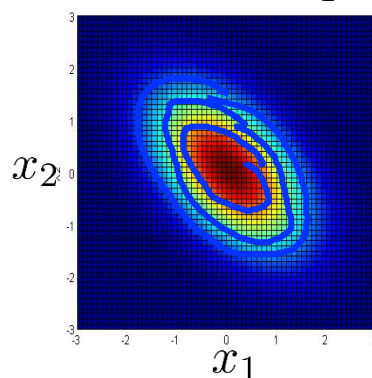
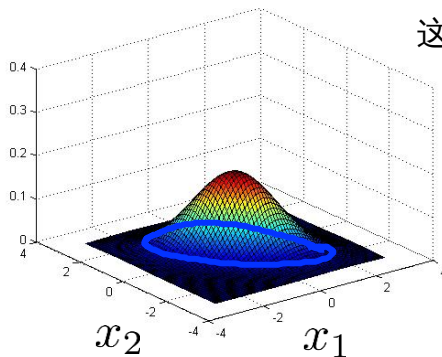
# Multivariate Gaussian (Normal) examples

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

↑

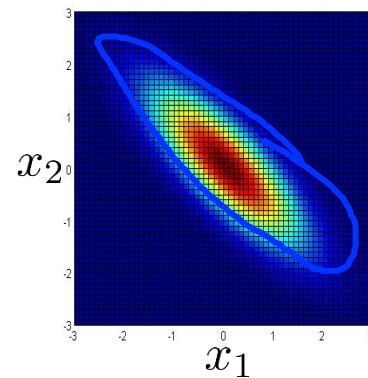
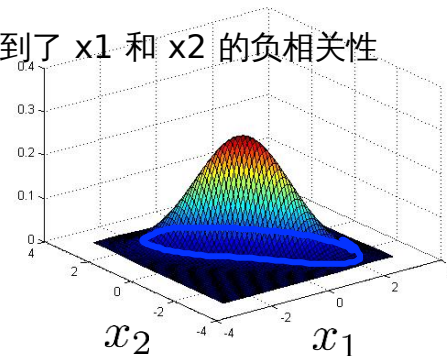


$$\mu = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad \Sigma = \begin{bmatrix} 1 & -0.5 \\ -0.5 & 1 \end{bmatrix}$$



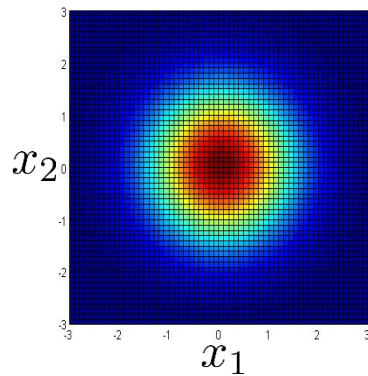
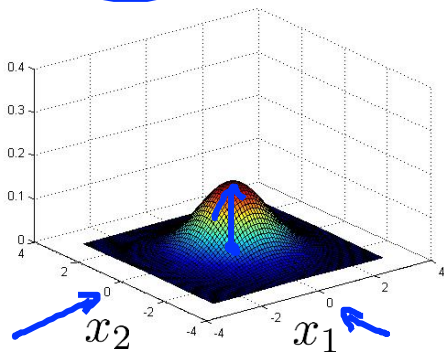
$$\mu = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad \Sigma = \begin{bmatrix} 1 & -0.8 \\ -0.8 & 1 \end{bmatrix}$$

这个捕捉到了  $x_1$  和  $x_2$  的负相关性

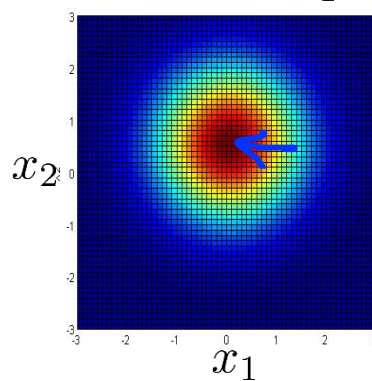
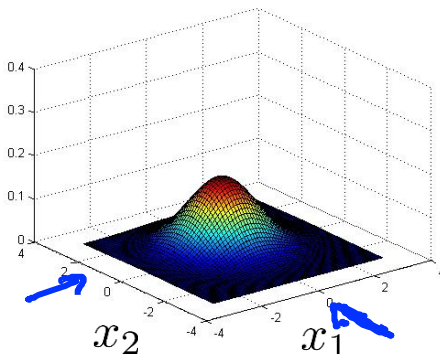


# Multivariate Gaussian (Normal) examples

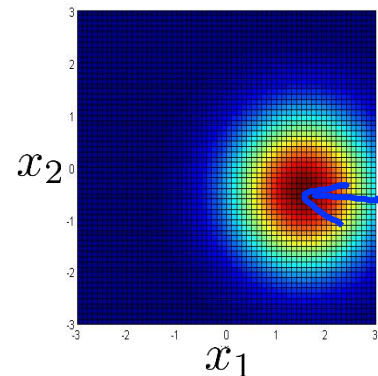
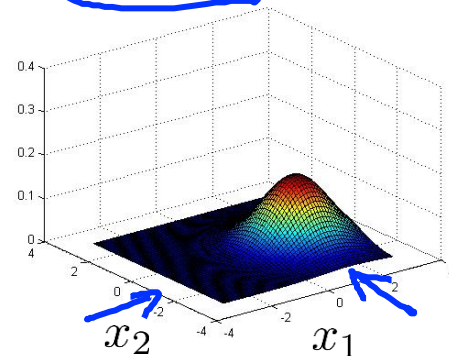
$$\mu = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad \Sigma = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$



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



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







Machine Learning

# Anomaly detection

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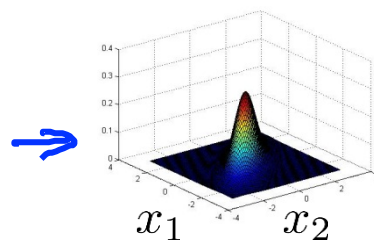
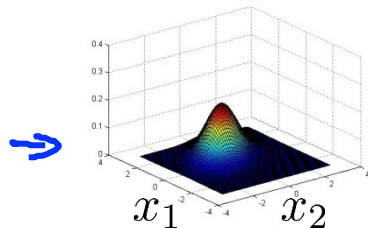
Anomaly detection using  
the multivariate  
Gaussian distribution

# 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

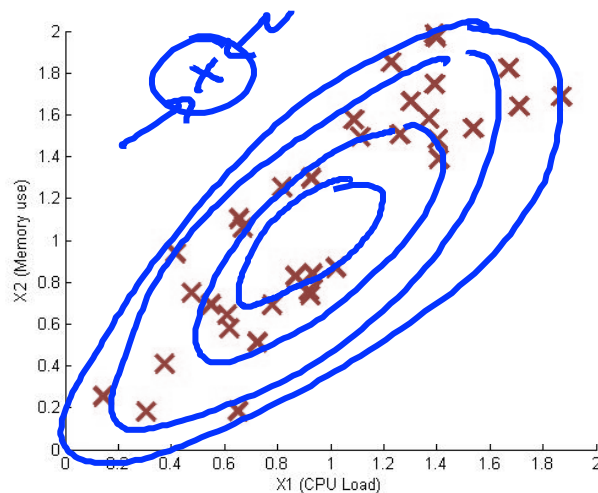
1. Fit model  $p(x)$  by setting

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

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

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

在实际应用当中 左边这个原来的模型比较常用

→ 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

典型的经验法则是 我\*\*只\*\*在当  $m$  远大于  $n$  的时候 使用多元高斯模型

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

Tao: 注意前面的例子中, CPU 负载和内存使用量是正相关的

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

$\Sigma^{-1}$

Computationally more expensive

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

$\rightarrow x_1 = \cancel{x_2} + \cancel{x_3} + x_4 + x_5$

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