



Machine Learning

Anomaly detection

Problem
motivation

Anomaly detection example

Aircraft engine features:

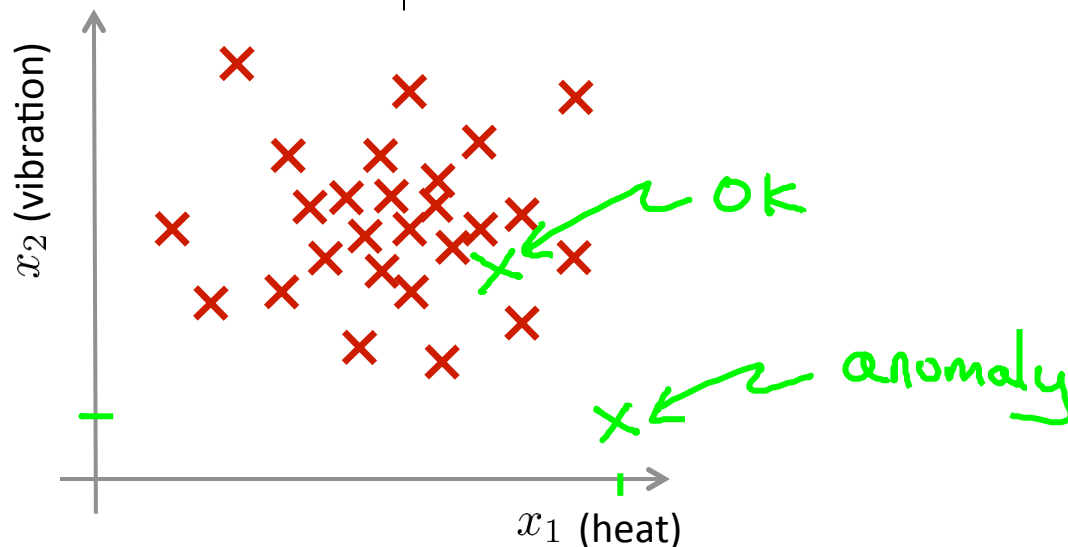
→ x_1 = heat generated

→ x_2 = vibration intensity

...

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

New engine: x_{test}

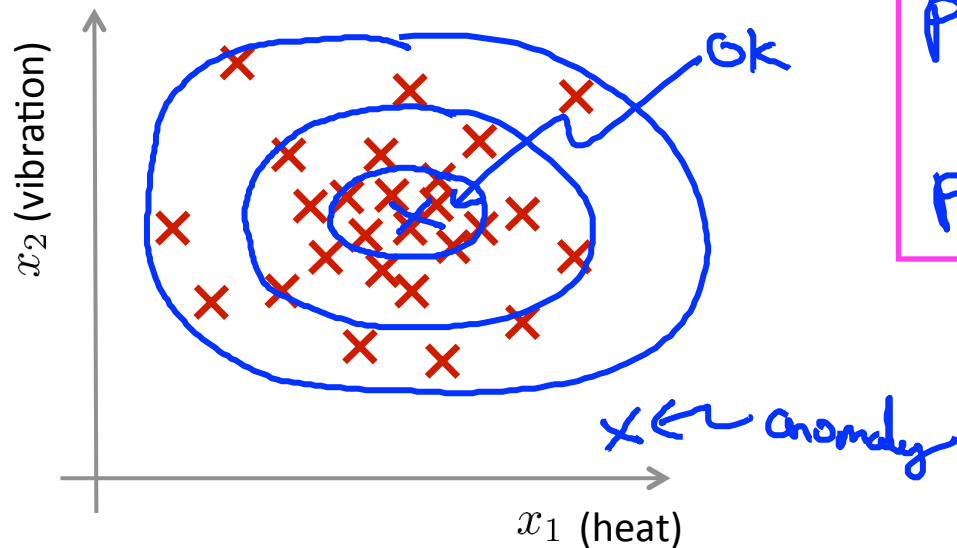


Density estimation

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

→ Is x_{test} anomalous?

Model $p(x)$.



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

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

Anomaly detection example

→ Fraud detection:

x_1
 x_2
 x_3
 x_4 $p(x)$

→ $x^{(i)}$ = 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.

...

$p(x) < \epsilon$



Machine Learning

Anomaly detection

Gaussian
distribution

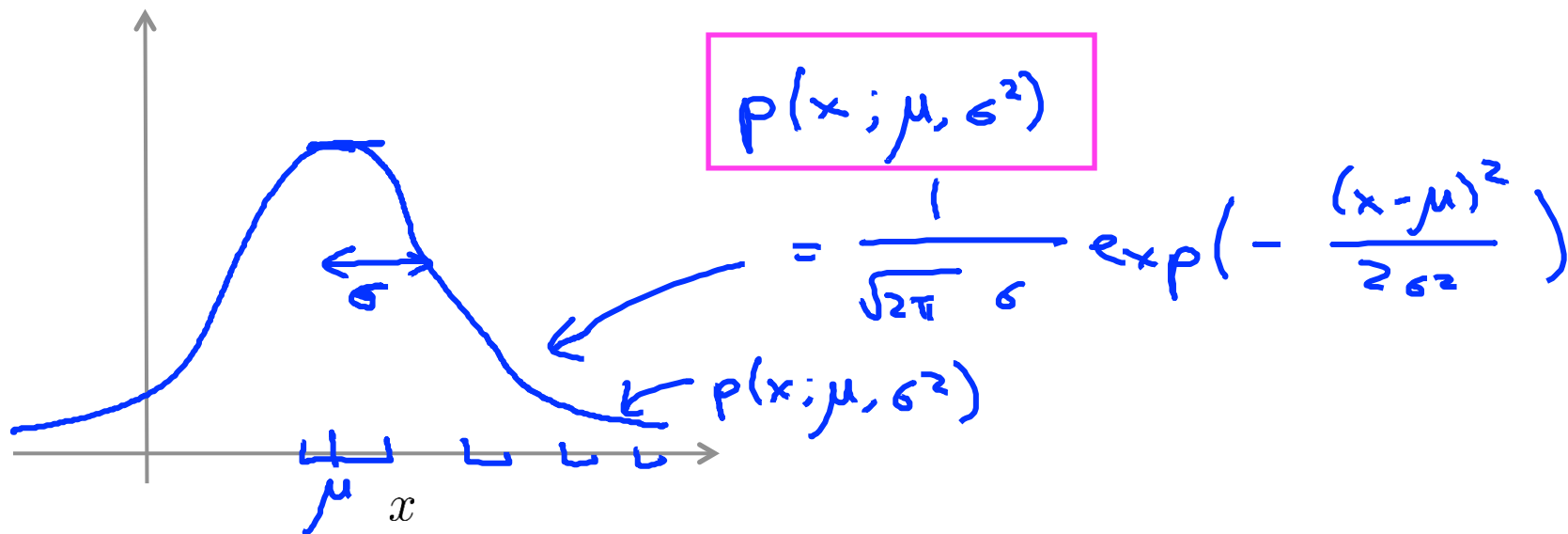
Gaussian (Normal) distribution

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

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

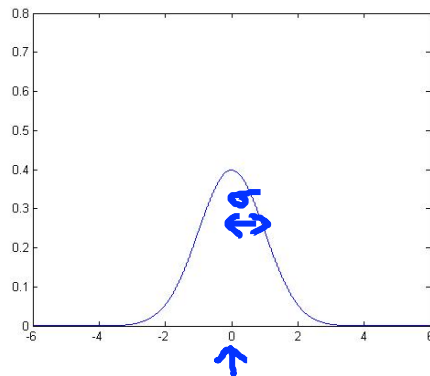
↑ "distributed as"

σ standard deviation



Gaussian distribution example

→ $\mu = 0, \sigma = 1$

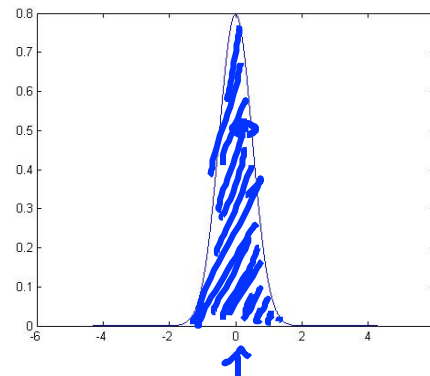


→ $\mu = 0, \sigma = 2$

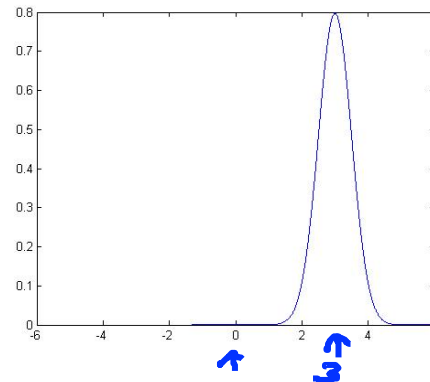


→ $\mu = 0, \sigma = \underline{0.5}$

$\sigma^2 = 0.25$

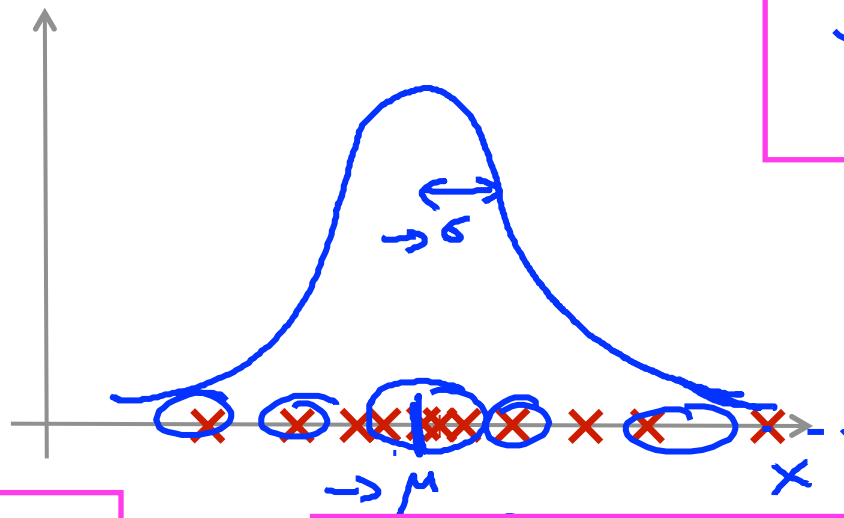


→ $\mu = 3, \sigma = 0.5$



Parameter estimation

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



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

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

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



Machine Learning

Anomaly detection

Algorithm

→ Density estimation

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

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

→ $p(x)$

$$= \left[p(x_1; \mu_1, \sigma_1^2) p(x_2; \mu_2, \sigma_2^2) p(x_3; \mu_3, \sigma_3^2) \dots p(x_n; \mu_n, \sigma_n^2) \right] \leftarrow$$

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

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

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

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

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

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

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 $\mu_1, \dots, \mu_n, \sigma_1^2, \dots, \sigma_n^2$

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

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

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

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

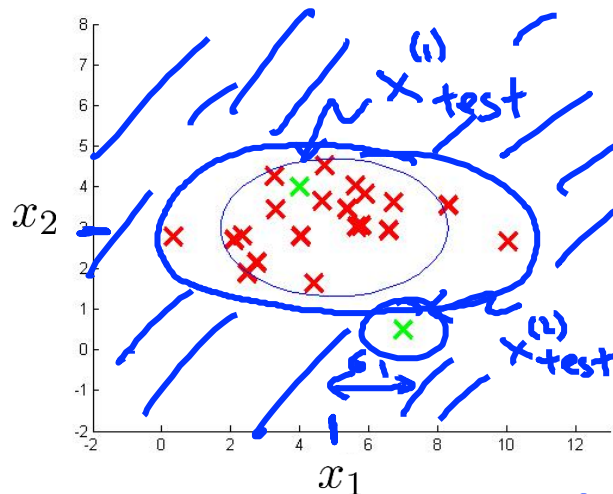
$$\sigma_j^2 = \frac{1}{m} \sum_{i=1}^m (x_j^{(i)} - \mu_j)^2$$

→ 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 $p(x) < \varepsilon$

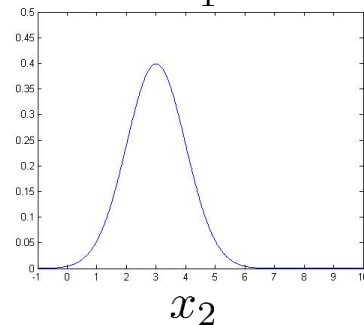
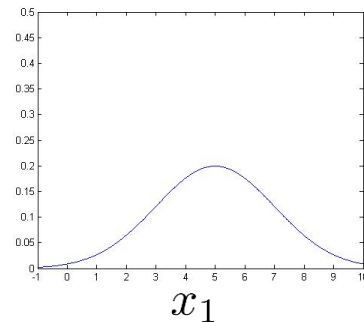
Anomaly detection example



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

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

$$\sigma_1^2 = 4$$



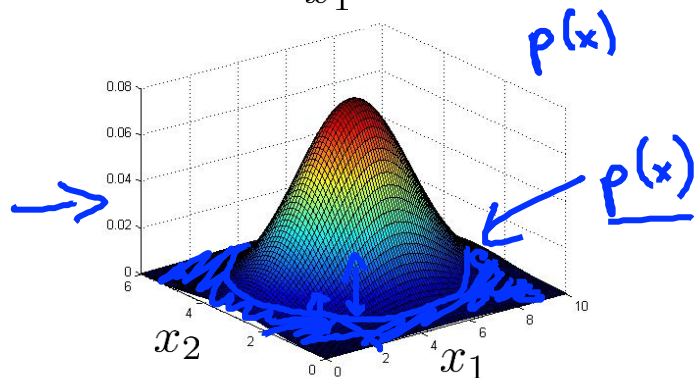
$$p(x_1; \mu_1, \sigma_1^2)$$

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



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

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



$$\epsilon = 0.02$$

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

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



Machine Learning

Anomaly detection

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

Better

- 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 ε ←



Machine Learning

Anomaly detection

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

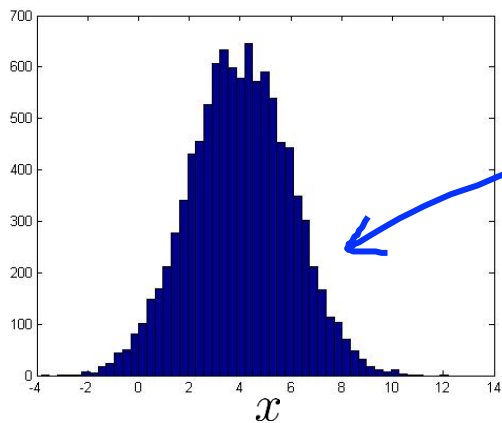
Anomaly detection

Choosing what
features to use

Non-gaussian features

Transformation

Techniques



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

hist

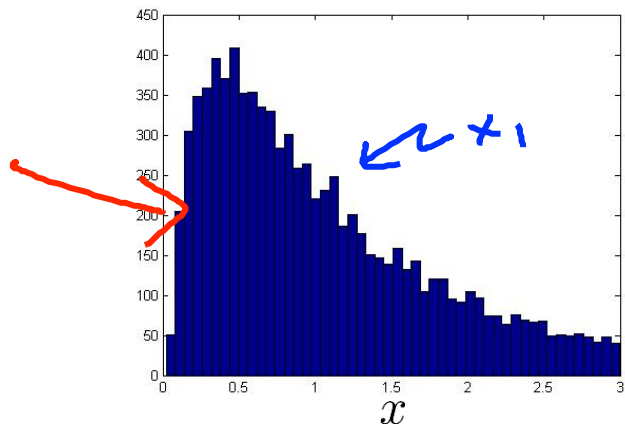
$$x_1 \leftarrow \frac{\log(x_i)}{\log(x_i+1)}$$

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

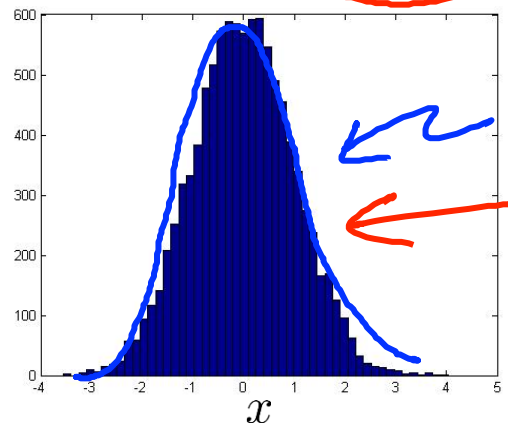
$$x_3 \leftarrow \sqrt{x_3} = x_3^{\frac{1}{2}}$$

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

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



$$\log(x)$$

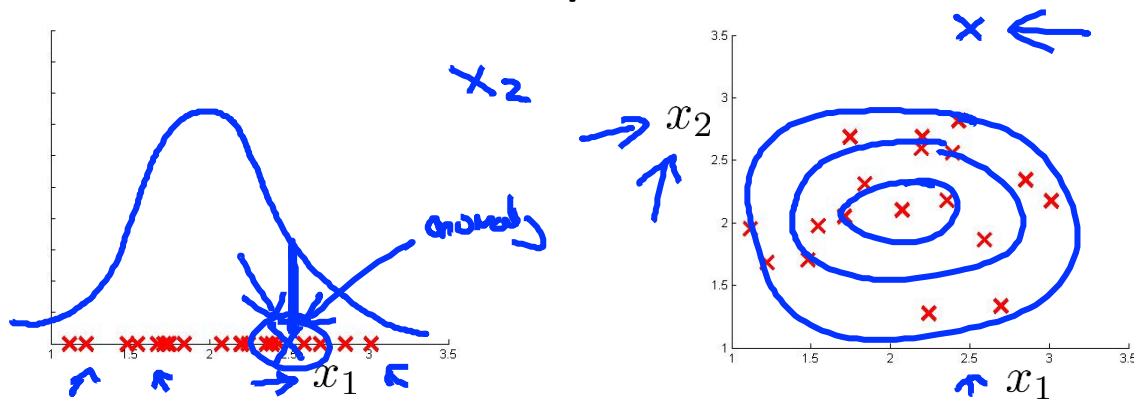


→ Error analysis for anomaly detection

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 ←

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

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

Can also create new features artificially.

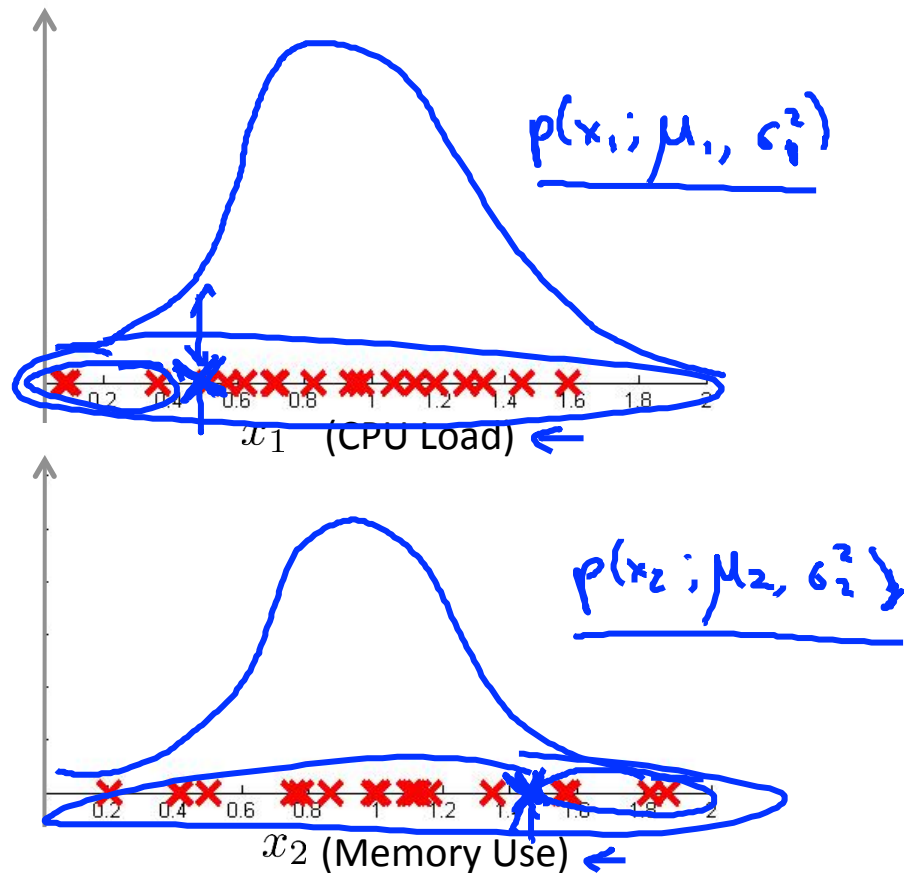


Machine Learning

Anomaly detection

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)

Centre

Covariance Matrix

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

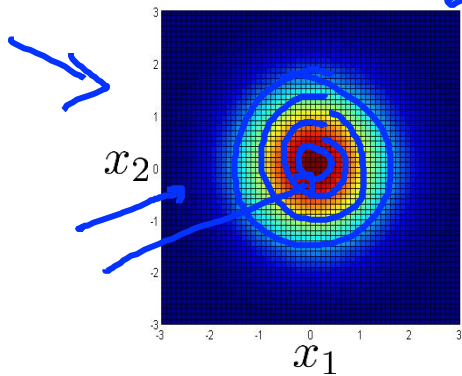
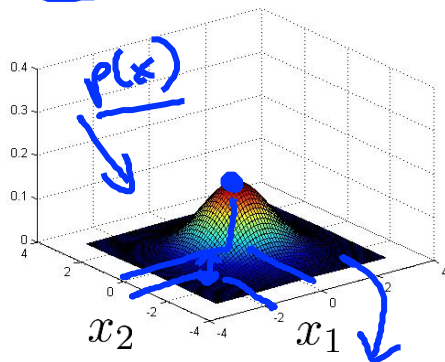
$$\frac{1}{(2\pi)^{n/2} |\Sigma|^{1/2}}$$

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

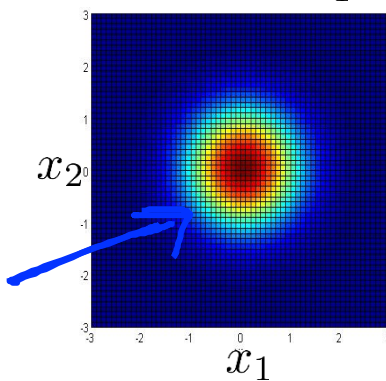
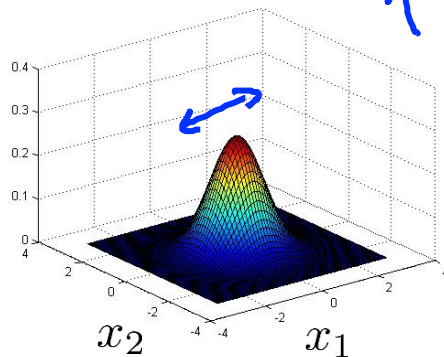
$$|\Sigma| = \text{determinant of } \Sigma \quad \left| \det(\text{Sigma}) \right|$$

Multivariate Gaussian (Normal) examples

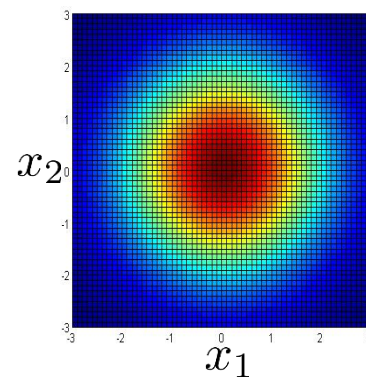
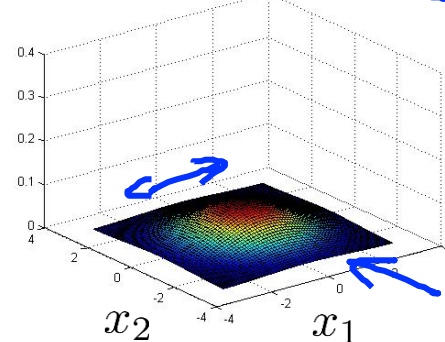
$$\mu = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad \Sigma = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$



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

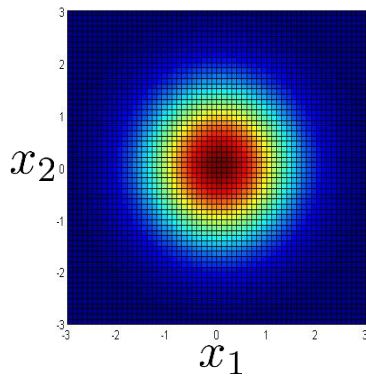
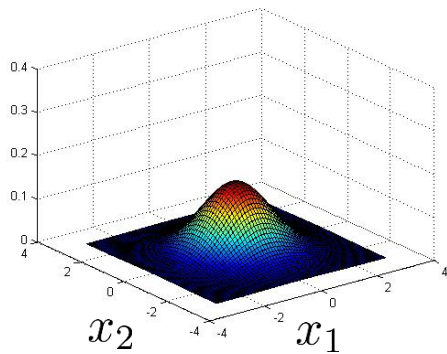


$$\mu = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad \Sigma = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix}$$

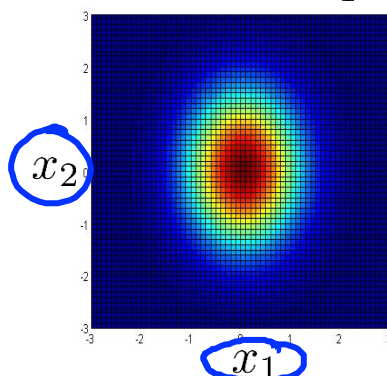


Multivariate Gaussian (Normal) examples

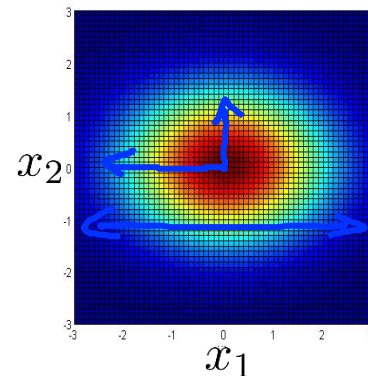
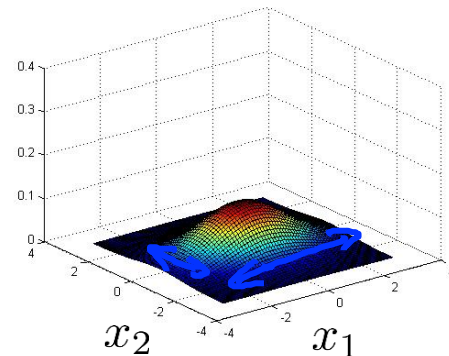
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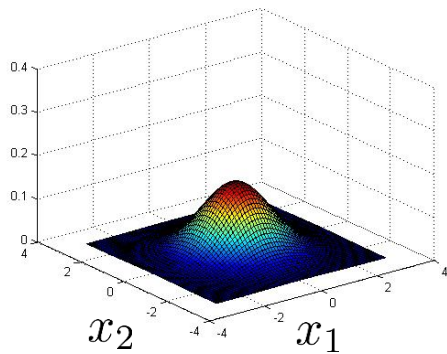


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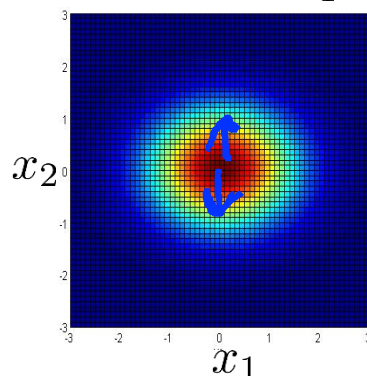


Multivariate Gaussian (Normal) examples

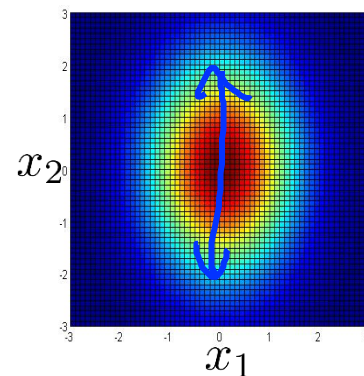
$$\mu = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad \Sigma = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$



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

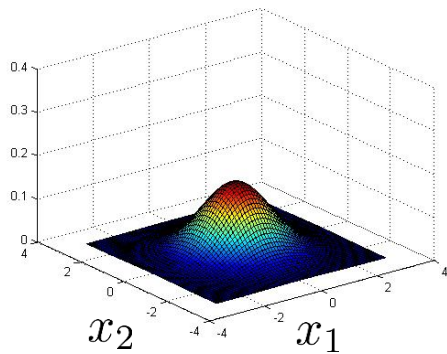


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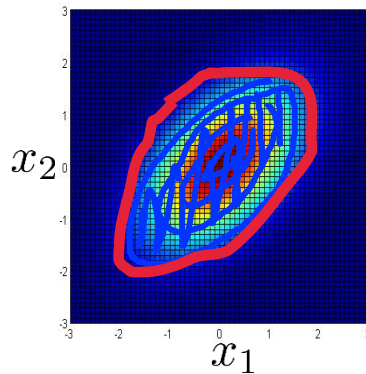
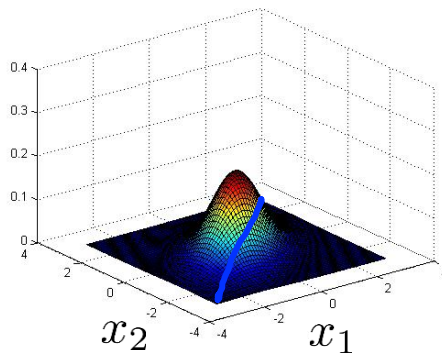


Multivariate Gaussian (Normal) examples

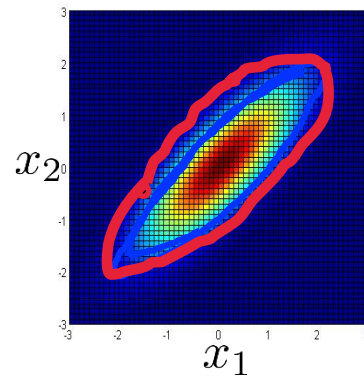
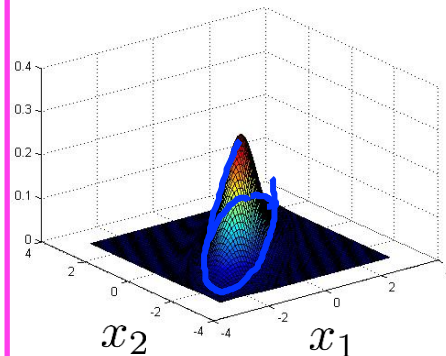
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$$\mu = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad \Sigma = \begin{bmatrix} 1 & 0.5 \\ 0.5 & 1 \end{bmatrix}$$



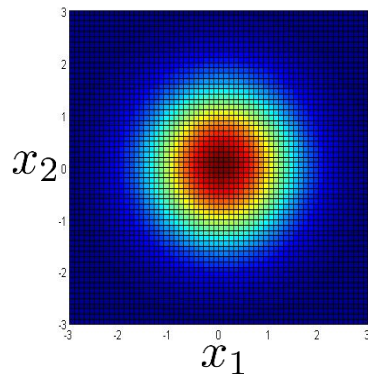
$$\mu = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad \Sigma = \begin{bmatrix} 1 & 0.8 \\ 0.8 & 1 \end{bmatrix}$$



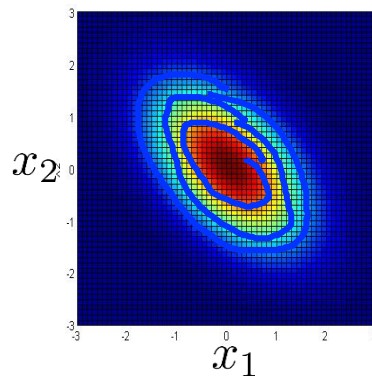
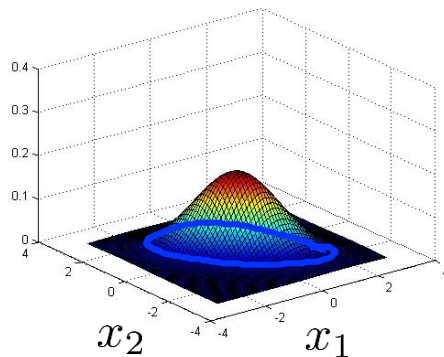
Multivariate Gaussian (Normal) examples

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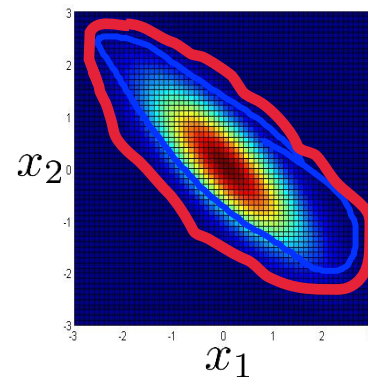
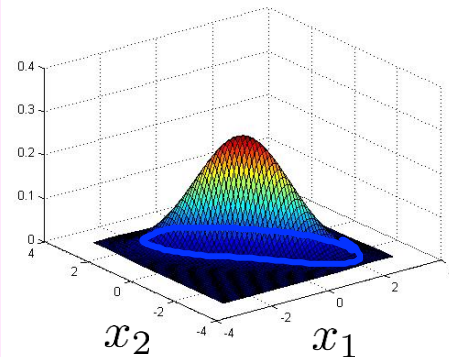
↑



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



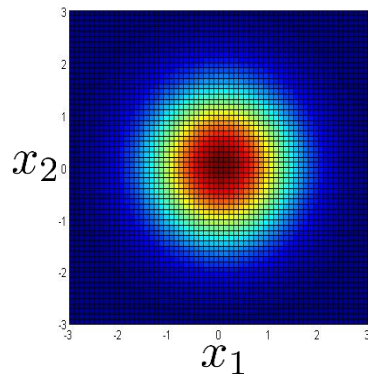
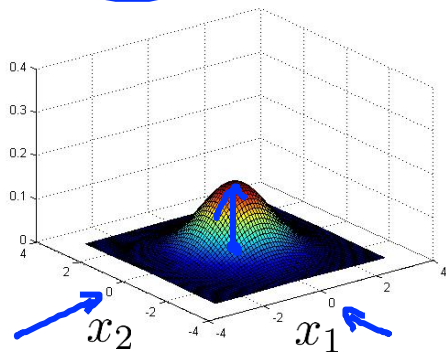
$$\mu = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad \Sigma = \begin{bmatrix} 1 & -0.8 \\ -0.8 & 1 \end{bmatrix}$$



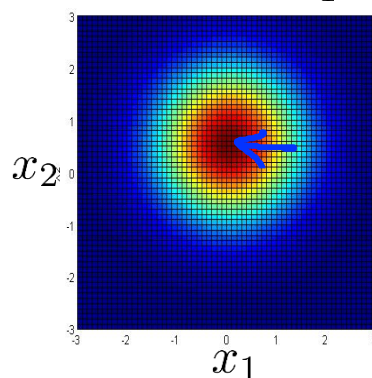
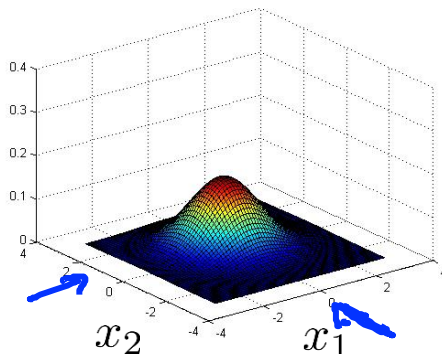
Multivariate Gaussian (Normal) examples

Changing the Centre point

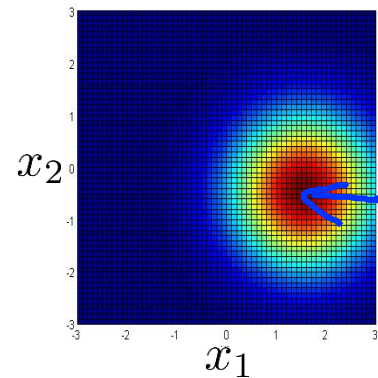
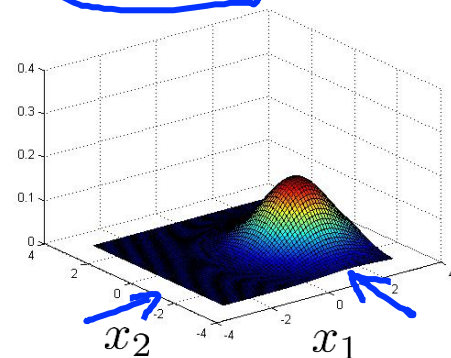
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$$\mu = \begin{bmatrix} 0 \\ 0.5 \end{bmatrix} \quad \Sigma = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$



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





Machine Learning

Anomaly detection

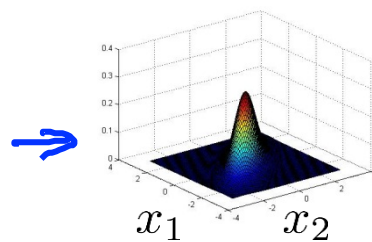
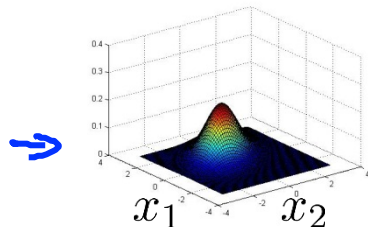
Anomaly detection using
the multivariate
Gaussian distribution

Multivariate Gaussian (Normal) distribution

Parameters μ, Σ

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

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



Parameter fitting:

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

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

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

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

Anomaly detection with the multivariate Gaussian

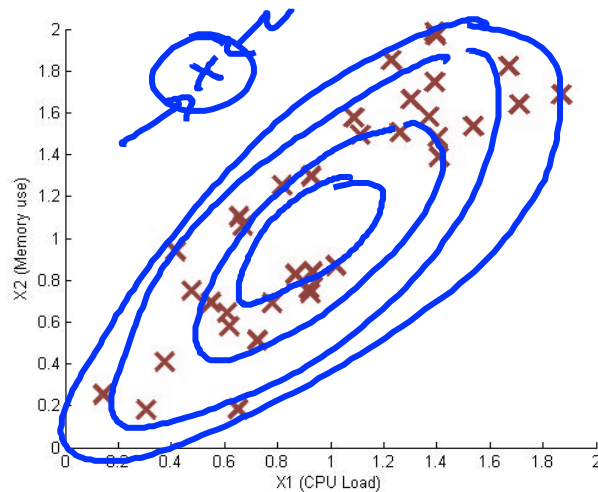
1. Fit model $p(x)$ by setting

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

2. Given a new example x , compute

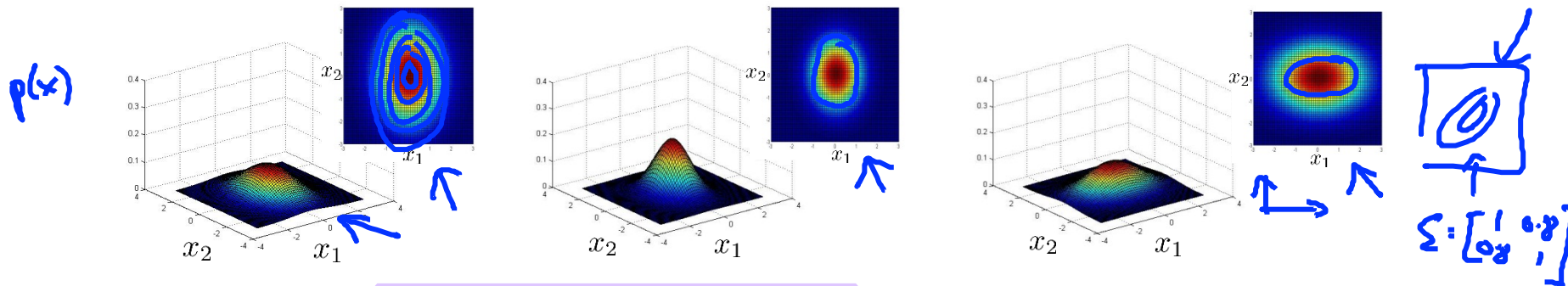
$$p(x) = \frac{1}{(2\pi)^{\frac{n}{2}} |\Sigma|^{\frac{1}{2}}} \exp \left(-\frac{1}{2} (x - \mu)^T \Sigma^{-1} (x - \mu) \right)$$

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

$$\Sigma = \begin{bmatrix} \sigma_1^2 & \rho \sigma_1 \sigma_2 & \dots \\ \rho \sigma_1 \sigma_2 & \sigma_2^2 & \dots \\ \vdots & \vdots & \ddots \end{bmatrix}$$

→ 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 $n=10,000, \quad n=100,000$)

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

$$\rightarrow \Sigma \sim \frac{1}{2} n^2$$

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

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