Statistics: The Backbone of Statistical Learning

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Introduction to Machine Learning

CSCI-335

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Statistics

Standard deviation - a measure of data points differ from mean

Average of differences (w/ mean as reference point)

Higher standard deviation indicates higher spread, less consistency, and less "clustering/blobbing"

Sample standard deviation: $s = \sqrt{\frac{\sum\left(x - \bar{X}\right)^2}{n-1}}$

Mean (average): $\bar{X} = \left(\frac{1}{n}\right)\sum(x)$

Population standard deviation: $\sigma = \sqrt{\frac{\sum\left(x - \mu\right)^2}{N}}$

Expectation

X is univariate here!

$$\mathrm{E}[X] = \sum_{i=1}^{k} x_i\, p_i = x_1 p_1 + x_2 p_2 + \cdots + x_k p_k$$

Definition A *random vector* $\vec{X}$ is a vector $(X_1, X_2, \ldots, X_p)$ of jointly distributed random variables. As is customary in linear algebra, we will write vectors as column matrices whenever convenient.

Definition The expectation $E\vec{X}$ of a random vector $\vec{X} = [X_1, X_2, \ldots, X_p]^T$ is given by

$$E\vec{X} = \begin{bmatrix} EX_1 \\ EX_2 \\ \vdots \\ EX_p \end{bmatrix}.$$

$$\begin{aligned} E\vec{X} &= E\begin{bmatrix} X_1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} + E\begin{bmatrix} 0 \\ X_2 \\ \vdots \\ 0 \end{bmatrix} + \cdots + E\begin{bmatrix} 0 \\ 0 \\ \vdots \\ X_p \end{bmatrix} \\ &= \begin{bmatrix} EX_1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ EX_2 \\ \vdots \\ 0 \end{bmatrix} + \cdots + \begin{bmatrix} 0 \\ 0 \\ \vdots \\ EX_p \end{bmatrix} \\ &= \begin{bmatrix} EX_1 \\ EX_2 \\ \vdots \\ EX_p \end{bmatrix}. \end{aligned}$$

The linearity properties of the expectation can be expressed compactly by stating that for any $k \times p$-matrix A and any $1 \times j$-matrix B,

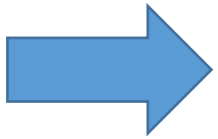
$$E(A\vec{X}) = AE\vec{X} \quad \text{and} \quad E(\vec{X}B) = (E\vec{X})B.$$

X is *p x 1* here!

X is *j x 1* here!

Covariance

- Variance and Covariance:
  - Measure of the “spread” of a set of points around their center of mass (mean)
- Variance:
  - Measure of deviation from mean for points in one dimension
- Covariance:
  - Measure of how much each of dimensions vary from mean with **respect to each other**



- **Covariance is measured between two dimensions**
- **Covariance → relation between two dimensions**
- **Covariance between one dimension is variance**

Variance-Covariance

Definition The *variance–covariance matrix* (or simply the *covariance matrix*) of a random vector $\vec{X}$ is given by:

$$\mathrm{Cov}(\vec{X}) = E\left[(\vec{X} - E\vec{X})(\vec{X} - E\vec{X})^T\right].$$

Proposition

$$\mathrm{Cov}(\vec{X}) = E[\vec{X}\vec{X}^T] - E\vec{X}(E\vec{X})^T.$$

Proposition

$$\mathrm{Cov}(\vec{X}) = \begin{bmatrix} \mathrm{Var}(X_1) & \mathrm{Cov}(X_1, X_2) & \cdots & \mathrm{Cov}(X_1, X_p) \\ \mathrm{Cov}(X_2, X_1) & \mathrm{Var}(X_2) & \cdots & \mathrm{Cov}(X_2, X_p) \\ \vdots & \vdots & \ddots & \vdots \\ \mathrm{Cov}(X_p, X_1) & \mathrm{Cov}(X_p, X_2) & \cdots & \mathrm{Var}(X_p) \end{bmatrix}.$$

Thus, $\mathrm{Cov}(\vec{X})$ *is a symmetric matrix, since* $\mathrm{Cov}(X, Y) = \mathrm{Cov}(Y, X)$.

Covariance Matrix

- Gives a measure of the dispersion of the data
- It is a D **x** D matrix
  - Element in position i,j is the covariance between the i^{th} and j^{th} variables.
    - Covariance between two variables x_i and x_j is defined as $E[(x_i-\mu_i)(y_i-\mu_j)]$
    - Can be positive or negative
  - If the variables are independent then the covariance is zero.
    - Then all matrix elements are zero except diagonal elements which represent the variances

The Gaussian Distribution

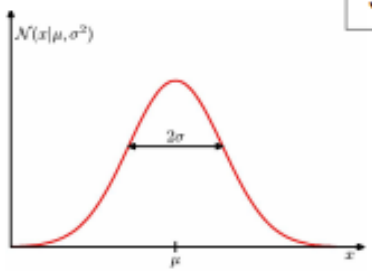
Carl Friedrich Gauss
1777-1855

- For single real-valued variable x

$$N(x \mid \mu, \sigma^2) = \frac{1}{(2\pi\sigma^2)^{1/2}} \exp\left\{-\frac{1}{2\sigma^2}(x-\mu)^2\right\}$$

68% of data lies within σ of mean
95% within 2σ

- Parameters:
  - Mean μ, variance σ^2,
- *Standard deviation* σ



- *Precision* $\beta = 1/\sigma^2$, $E[x] = \mu$, $Var[x] = \sigma^2$
- For D-dimensional vector $\mathbf{x}$, multivariate Gaussian

$$N(\mathbf{x} \mid \boldsymbol{\mu}, \Sigma) = \frac{1}{(2\pi)^{D/2}} \frac{1}{|\Sigma|^{1/2}} \exp\left\{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^T \Sigma^{-1} (\mathbf{x}-\boldsymbol{\mu})\right\}$$

$\boldsymbol{\mu}$ is a mean vector, Σ is a D x D covariance matrix, $|\Sigma|$ is the determinant of Σ

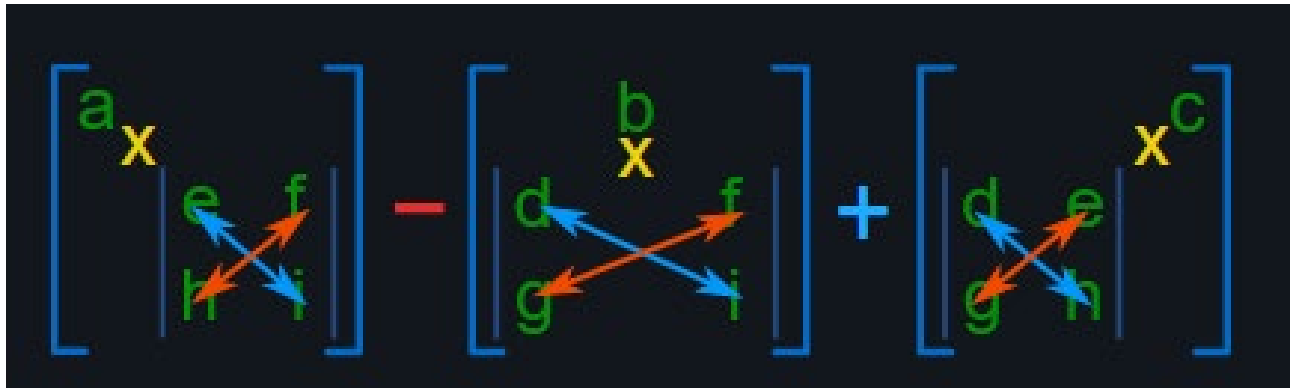
Σ^{-1} is also referred to as the precision matrix

Matrix Determinant

$$A = \begin{bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{bmatrix}$$

$$|A| = a(ei - fh) - b(di - fg) + c(dh - eg)$$

"The determinant of A equals ... etc"



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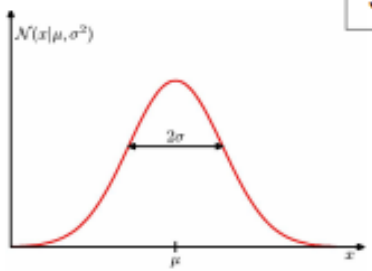

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The Multivariate Gaussian Distribution

A p-dimensional random vector $\vec{X}$ has the *multivariate normal distribution* if it has the density function

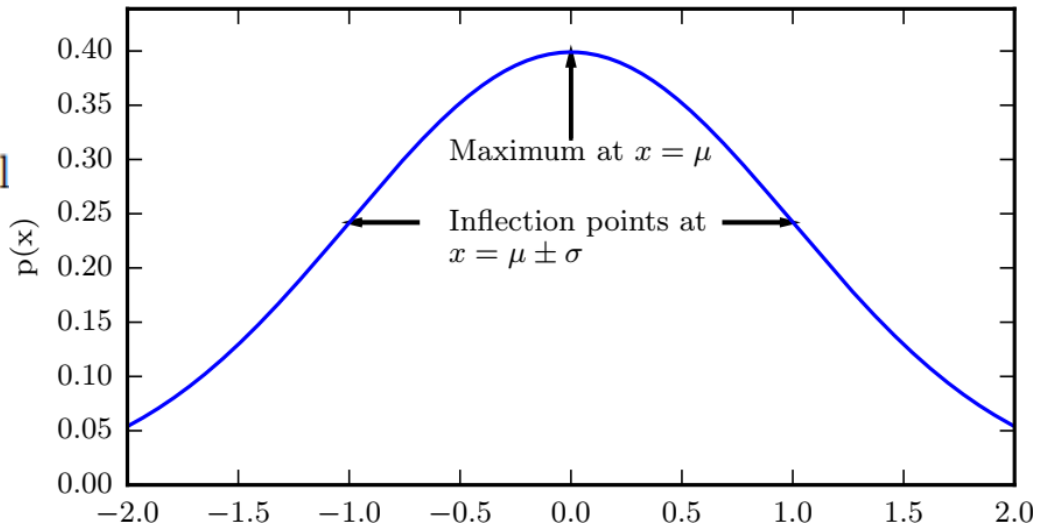
$$f(\vec{X}) = (2\pi)^{-p/2}|\Sigma|^{-1/2}\exp\left(-\frac{1}{2}(\vec{X}-\vec{\mu})^T\Sigma^{-1}(\vec{X}-\vec{\mu})\right),$$

where $\vec{\mu}$ is a constant vector of dimension p and Σ is a $p \times p$ positive semi-definite which is invertible (called, in this case, *positive definite*). Then, $E\vec{X} = \vec{\mu}$ and $\mathrm{Cov}(\vec{X}) = \Sigma$.

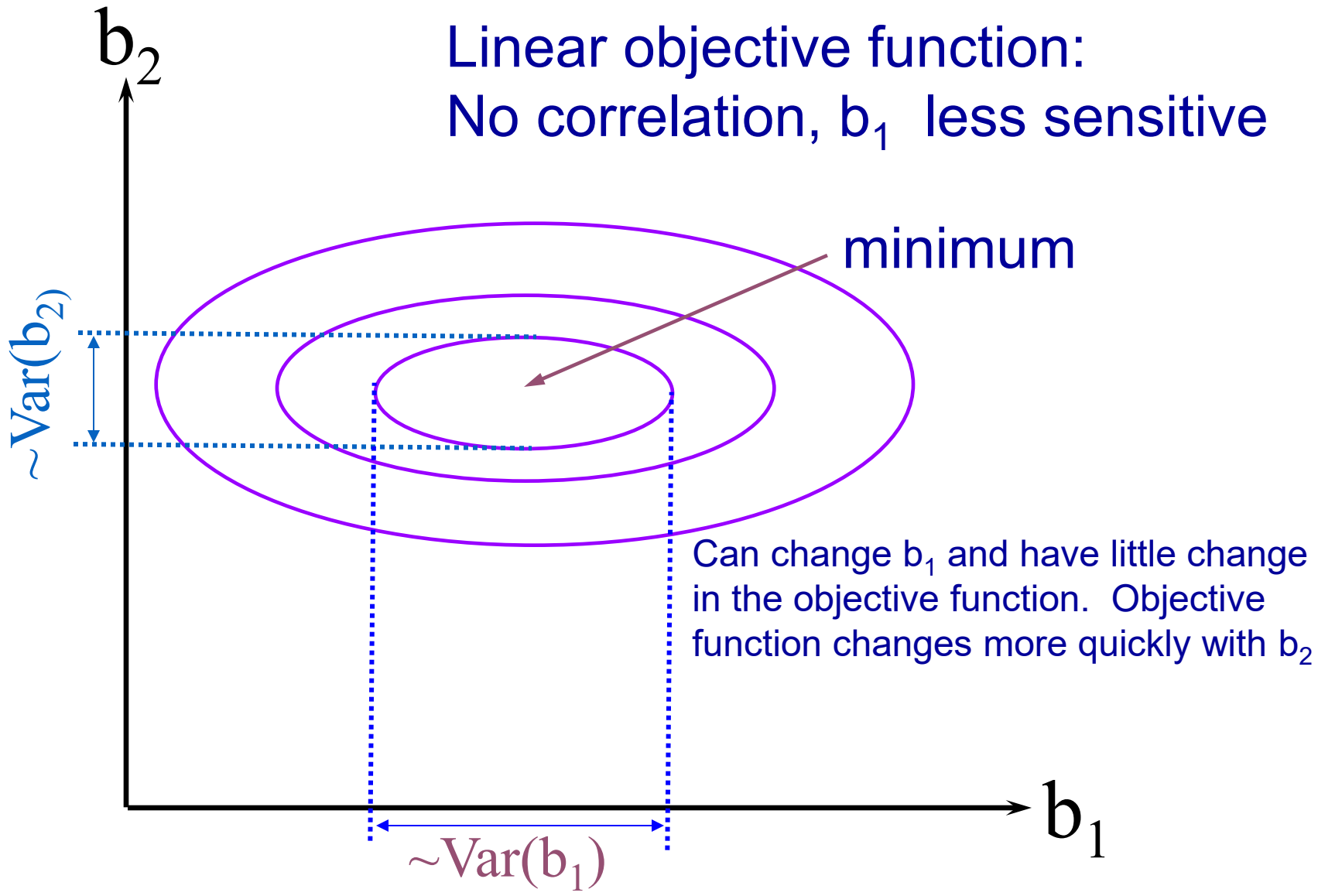
The *standard multivariate normal distribution* is obtained when $\vec{\mu} = 0$ and $\Sigma = I_p$, the $p \times p$ identity matrix:

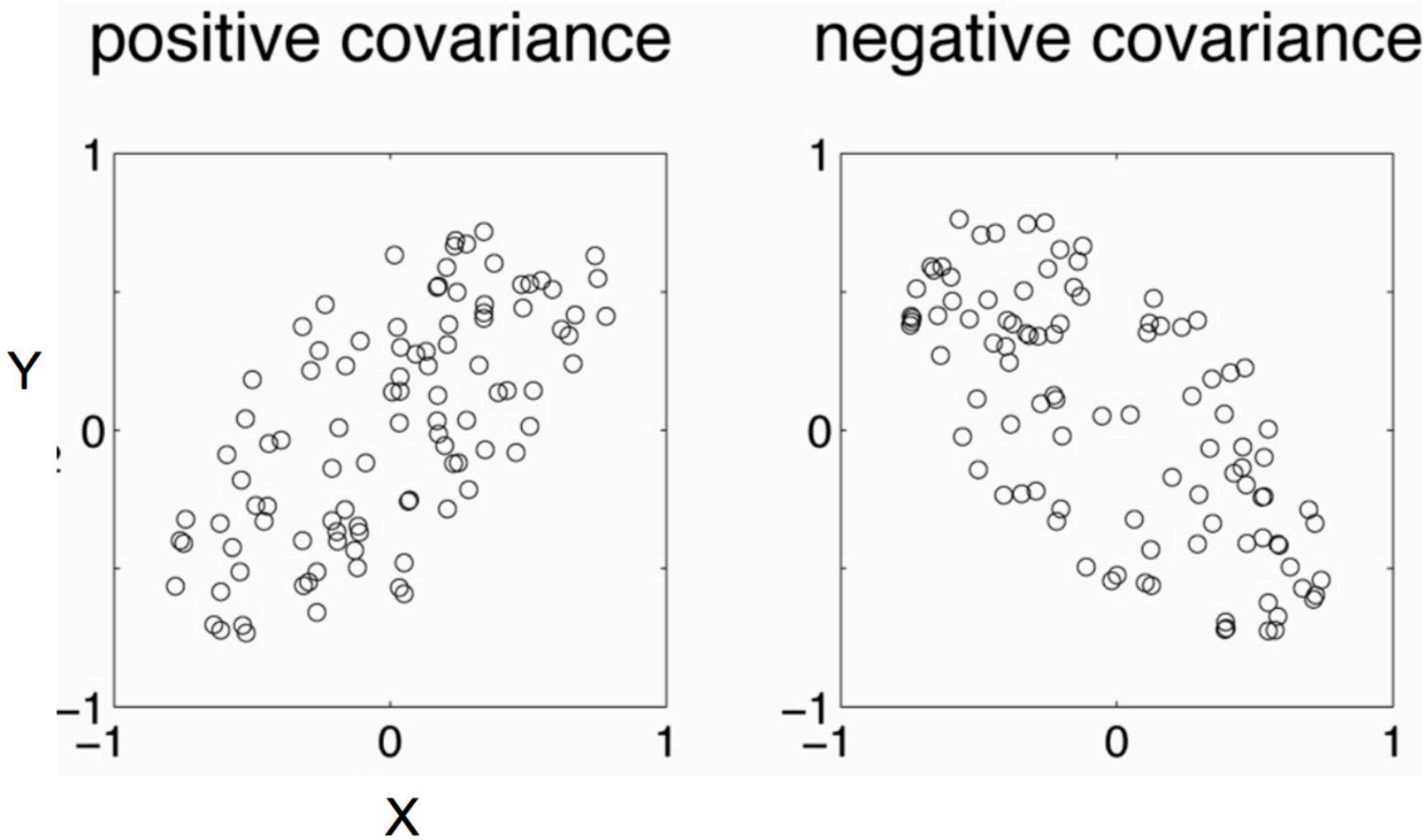
$$f(\vec{X}) = (2\pi)^{-p/2}\exp\left(-\frac{1}{2}\vec{X}^T\vec{X}\right).$$

This corresponds to the case where $X_1, \ldots, X_p$ are i.i.d. standard normal



Example: Parameter Variance & Covariance





Positive: Both dimensions increase or decrease together

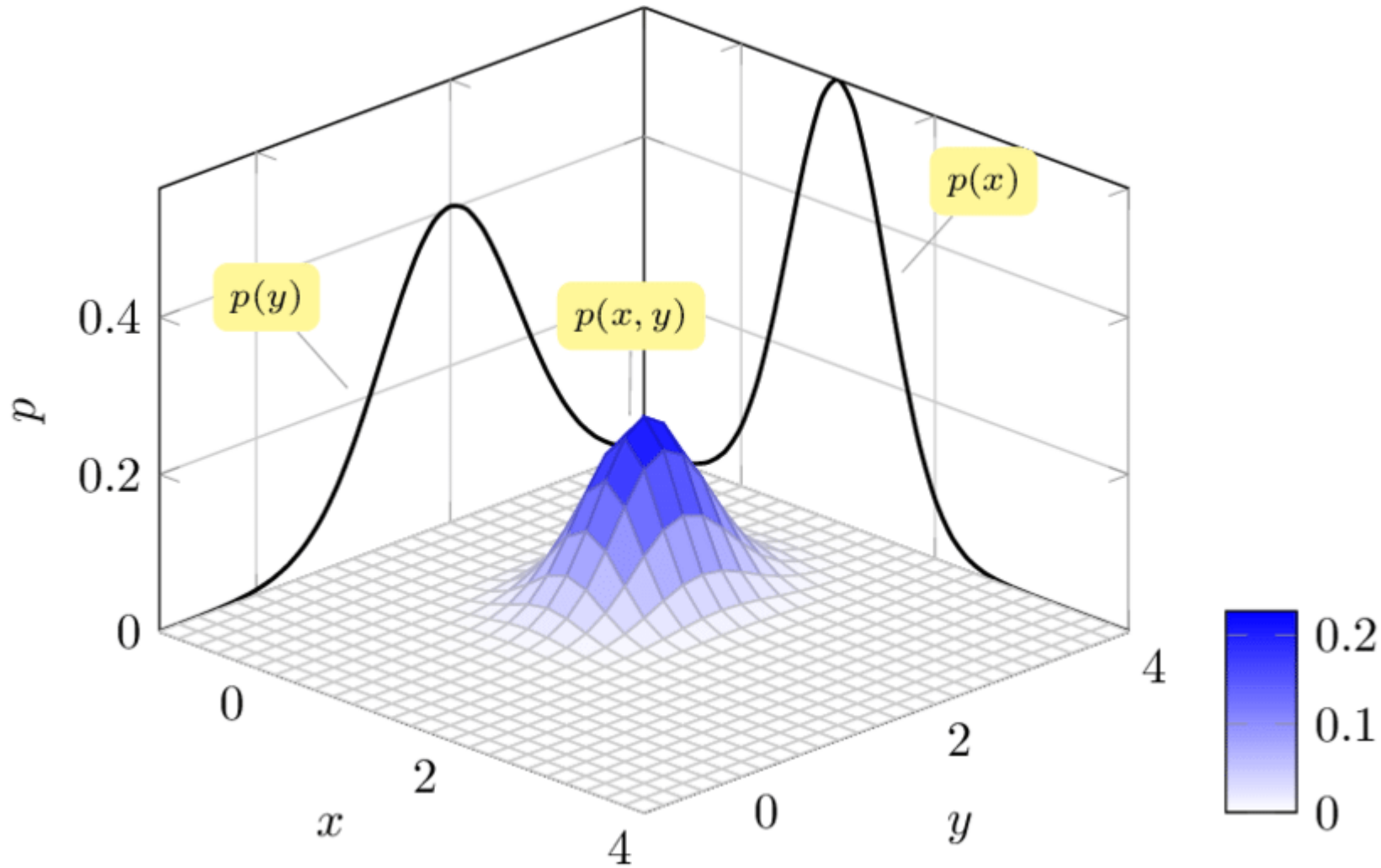
Negative: While one increases the other decreases

Covariance

- Used to find relationships between dimensions in high dimensional data sets

$$q_{jk} = \frac{1}{N} \sum_{i=1}^{N} (X_{ij} - E(X_j))(X_{ik} - E(X_k))$$

The sample mean

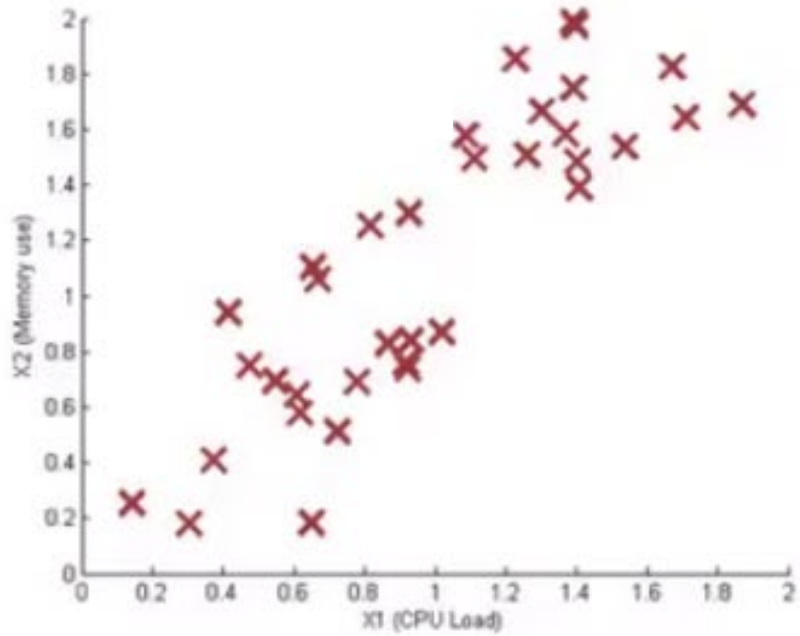

$p(y)$
$p(x, y)$
$p(x)$
p
0.4
0.2
0
0
2
4
x
0
2
4
y
0.2
0.1
0

Anomaly detection with the multivariate Gaussian

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

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

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



2. Given a new example x, compute

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

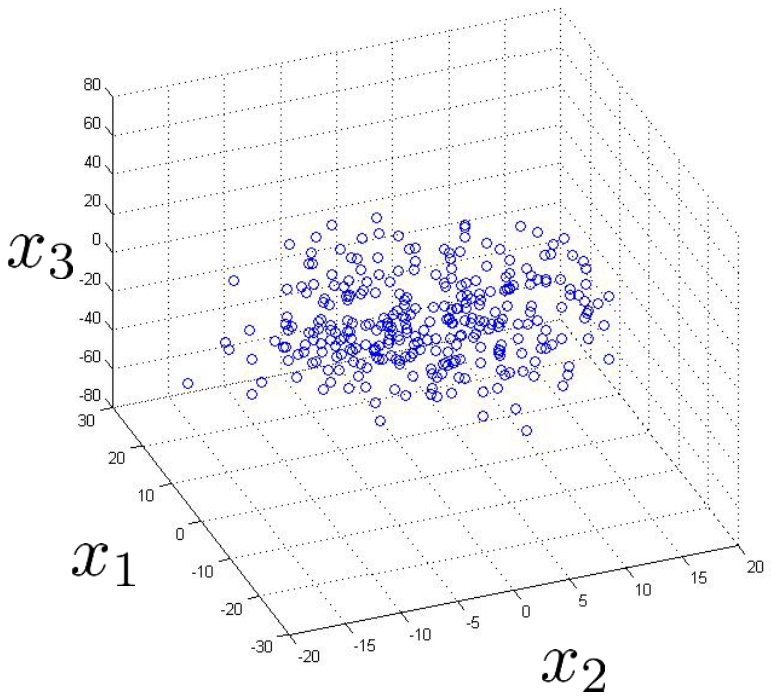
Flag an anomaly if $p(x) < \varepsilon$

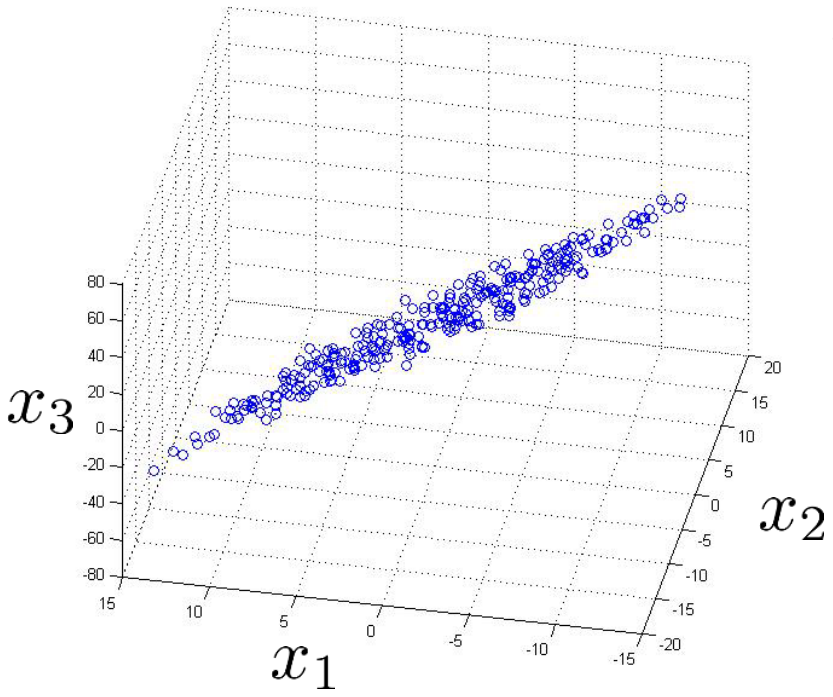
Why? Well, Dimensionality Reduction…

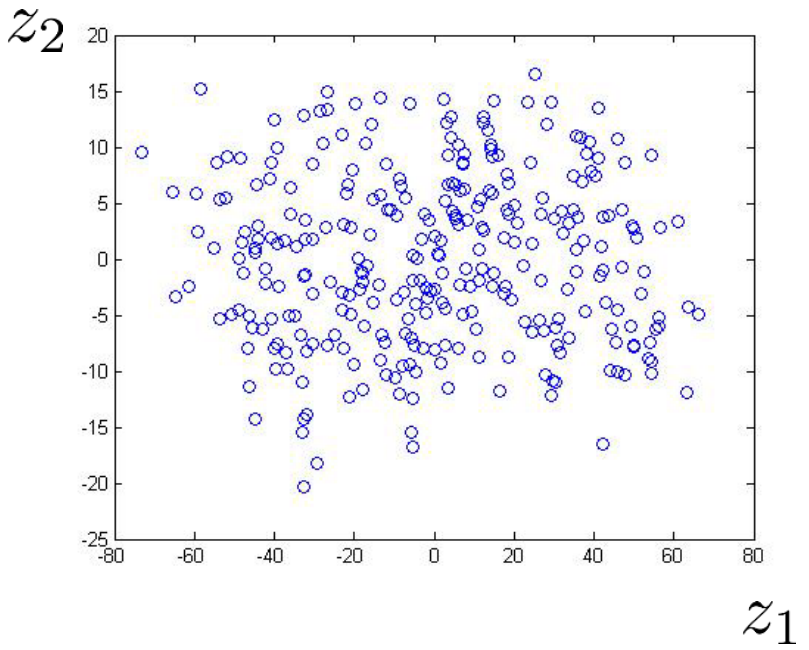
- PCA (Principal Component Analysis):
  - Find projection that maximize the variance (based on Gaussian assumptions)
- ICA (Independent Component Analysis):
  - Similar to PCA except assumes non-Gaussian features
- Multidimensional Scaling:
  - Find projection that best preserves inter-point distances
- LDA(Linear Discriminant Analysis):
  - Maximizing the component axes for class-separation
- …

Data Compression

Reduce data from 3D to 2D



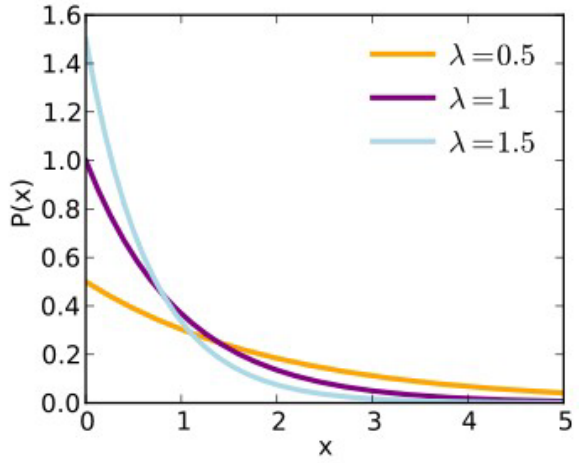




More Distributions

Exponential:

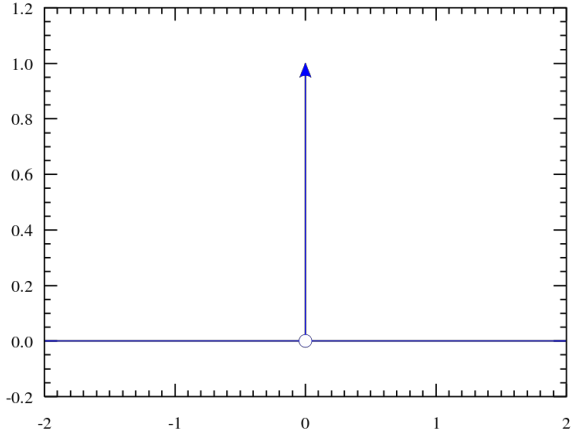
$$p(x;\lambda) = \lambda \mathbf{1}_{x\geq 0} \exp\left(-\lambda x\right).$$



Used to predict the waiting time until the next event occurs, such as a success, failure, or arrival

Dirac

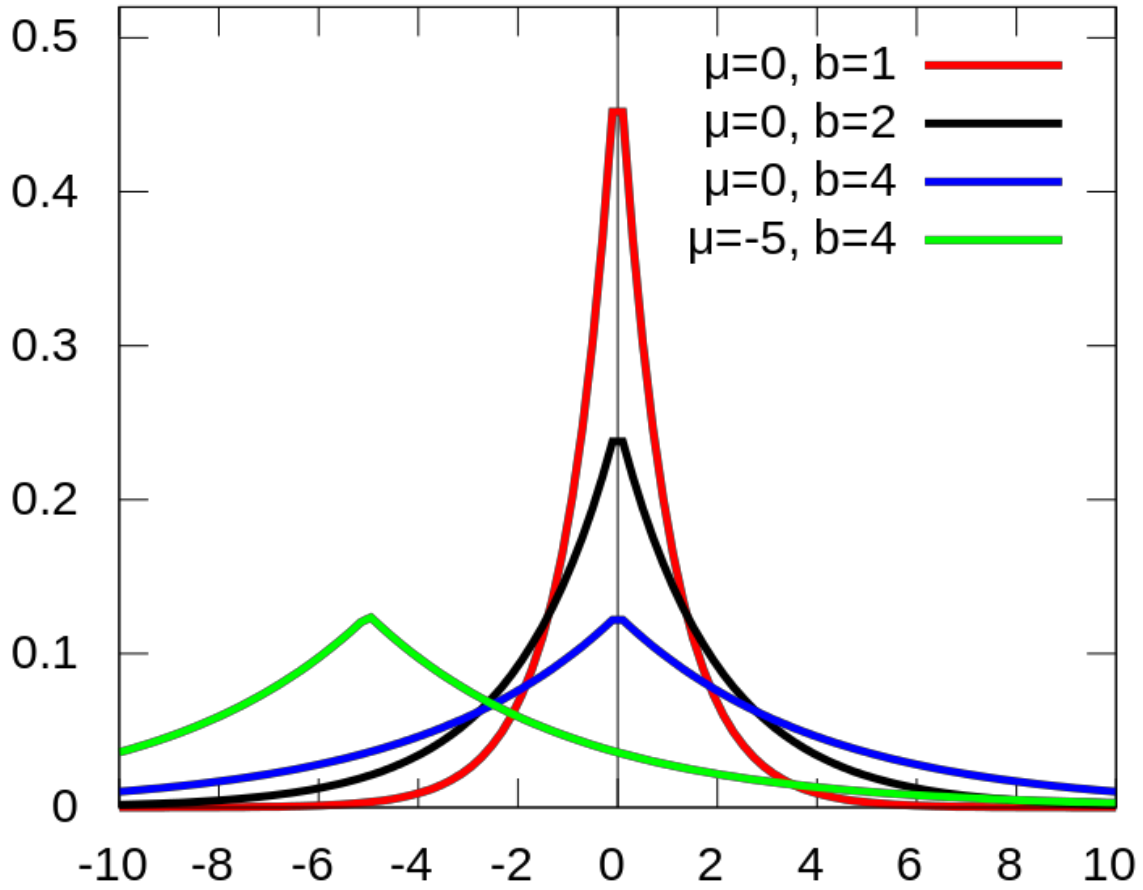
$$p(x) = \delta(x-\mu)$$



"Dirac density" of an idealized point mass or point charge -- a function that is equal to zero everywhere except for zero (integral over the entire real line is equal to one)

Laplace Distribution

$$\text{Laplace}(x;\mu,\gamma) = \frac{1}{2\gamma}\exp\left(-\frac{|x-\mu|}{\gamma}\right)$$



Bernoulli Distribution

The Bernoulli distribution is the "coin flip" distribution.

X is Bernoulli if its probability function is:

$$X = \begin{cases} 1 & w.p. \quad p \\ 0 & w.p. \quad 1-p \end{cases}$$

X=1 is usually interpreted as a "success." E.g.:

- X=1 for heads in coin toss
- X=1 for male in survey
- X=1 for defective in a test of product
- X=1 for "made the sale" tracking performance

Bernoulli Distribution

$$P(\mathrm{x} = 1) = \phi$$

$$P(\mathrm{x} = 0) = 1 - \phi$$

$$P(\mathrm{x} = x) = \phi^{x}(1 - \phi)^{1-x}$$

$$\mathbb{E}_{\mathrm{x}}[\mathrm{x}] = \phi$$

$$\mathrm{Var}_{\mathrm{x}}(\mathrm{x}) = \phi(1 - \phi)$$

Can prove/derive each of these properties!

p is ϕ in these formulas!

Empirical Distribution

$$\delta(x) = \begin{cases} 0, & x \neq 0 \\ \infty, & x = 0 \end{cases}$$

such that:

$$\int_{-\infty}^{\infty} \delta(x)dx = 1$$

Dirac delta function

$$\hat{p}(\boldsymbol{x}) = \frac{1}{m}\sum_{i=1}^{m} \delta(\boldsymbol{x} - \boldsymbol{x}^{(i)})$$

An **empirical (Dirac) distribution function** is distribution function associated with empirical measure of a sample
(the data “is” the distribution)

Mixture Distributions

$$P(\mathrm{x}) = \sum_i P(\mathrm{c} = i) P(\mathrm{x} \mid \mathrm{c} = i)$$

Gaussian mixture with
three components

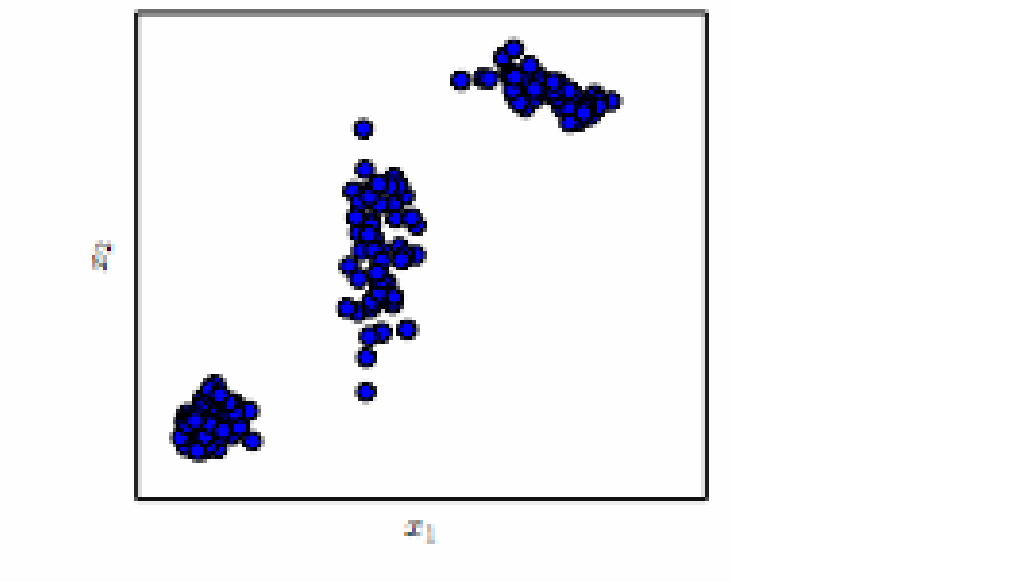


Figure 3.2

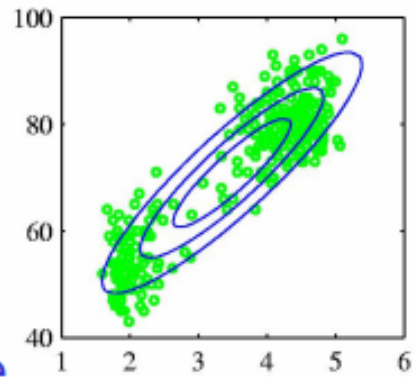
Mixtures of Gaussians

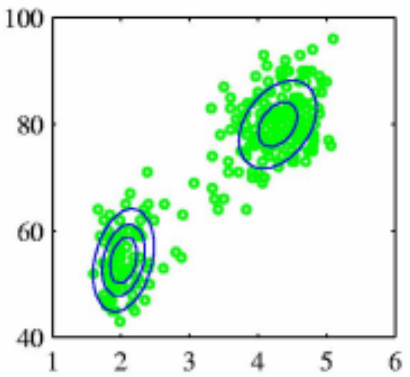
- Gaussian has limitations in modeling real data sets
- Old Faithful (Hydrothermal Geyser in Yellowstone)
  - 272 observations
  - Duration (mins, horiz axis) *vs* Time to next eruption (vertical axis)
  - Simple Gaussian unable to capture structure
  - Linear superposition of two Gaussians is better
- Linear combinations of Gaussians can give very complex densities

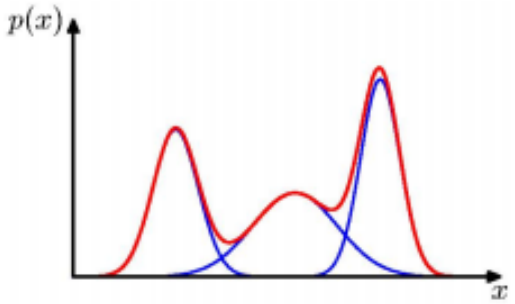
$$p(\mathrm{x}) = \sum_{k=1}^{K} \pi_k N(x \mid \mu_k, \Sigma_k)$$

π_k are mixing coefficients that sum to one

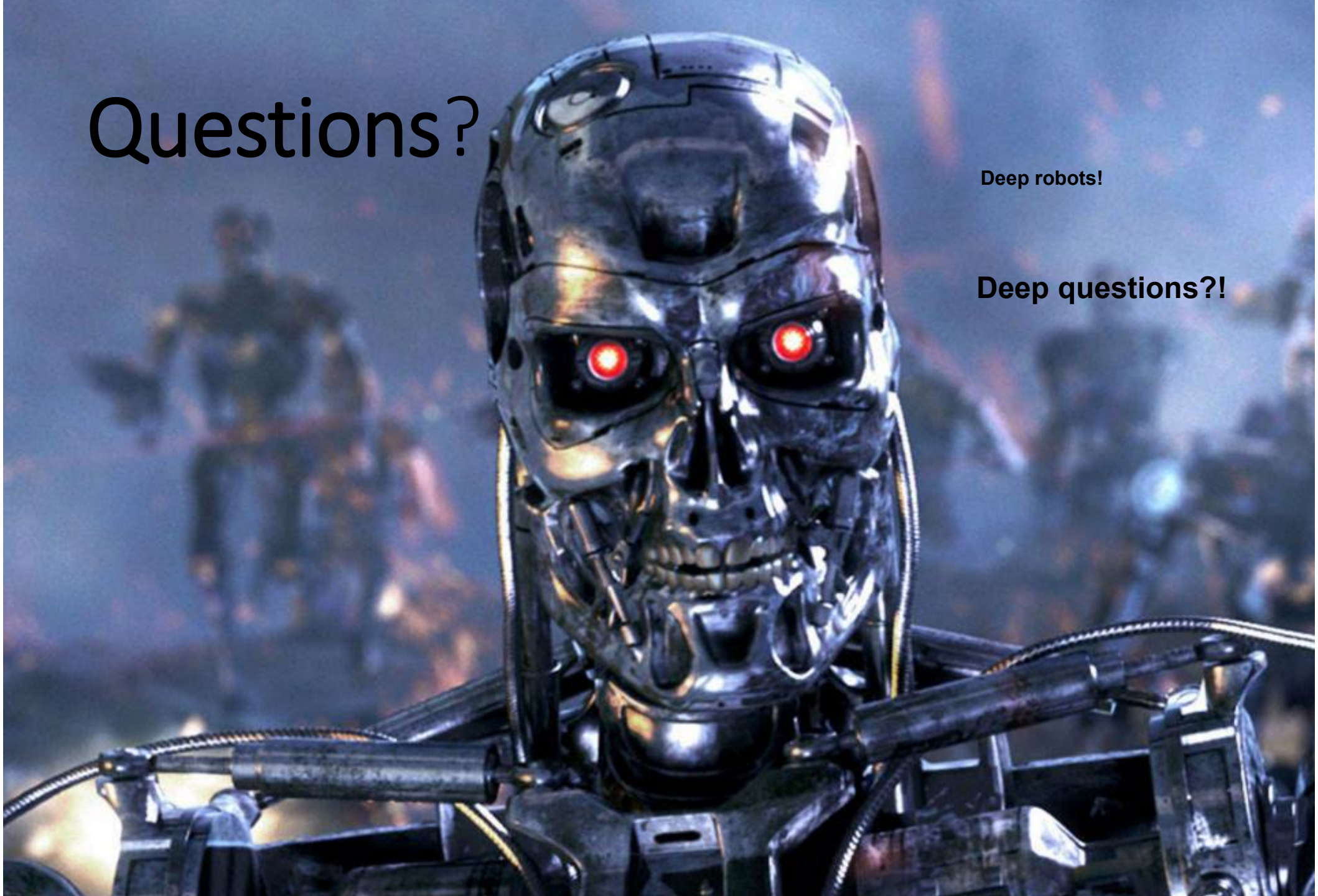
- One –dimension
  - Three Gaussians in blue
  - Sum in red







We will build this model later in this class!


Questions?
Deep robots!
Deep questions?!