INT104 ARTIFICIAL INTELLIGENCE

L10- Unsupervised Learning II
Gaussian mixture model (GMM)

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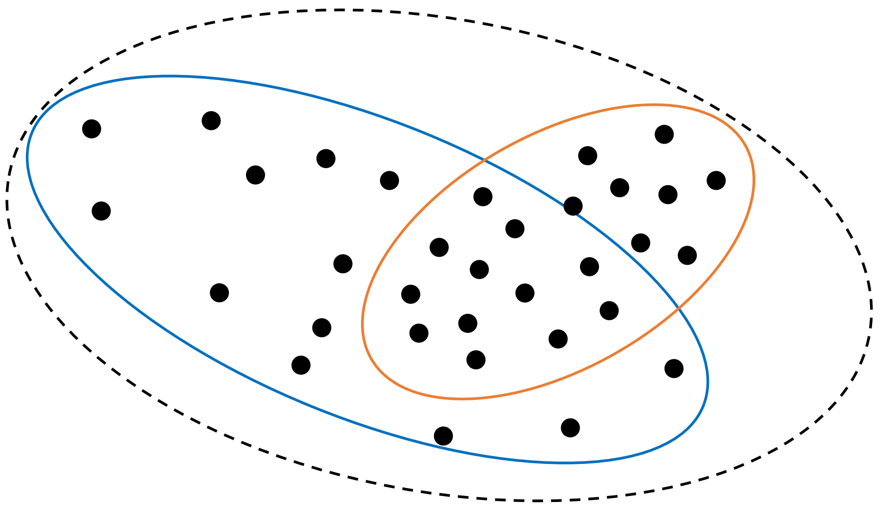
CONTENT

- Mixture Gaussian Model and EM method
  - Gaussian distribution
  - Mixture of gaussians
  - EM (Expectation-Maximization) method

Motivation

K-means make ***hard*** assignments to data points: $x^{(i)}$ must belong to one of the clusters $1,2,\cdots,K$

Sometimes, one data point can belong to multiple clusters

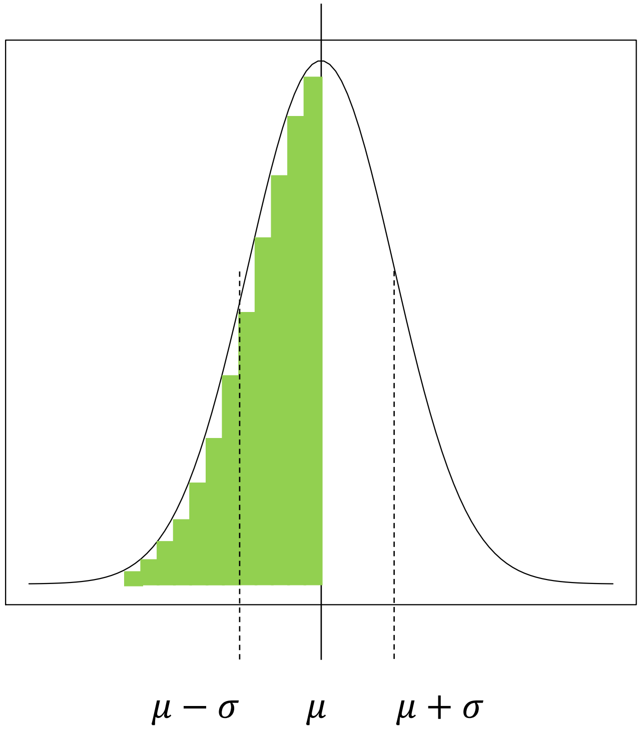


- Clusters may overlap
- Hard assignment may be simplistic
- Need a *soft* assignment:
  data points belong to clusters with different ***probabilities***

Gaussian (Normal) distribution

1-D (univariate) Gaussian $\mathcal{N}(\mu, \sigma)$

Probability density function (PDF): $p(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$ μ: mean σ: standard deviation



$$P(x < \mu) = \int_{-\infty}^{\mu} p(x)dx = 0.5 = P(x > \mu)$$

$$P(x < \mu - \sigma) = \int_{-\infty}^{\mu} p(x)dx \approx 0.157 = P(x > \mu + \sigma)$$

Gaussian is ubiquitous

In biology, the *logarithm* of various variables

- Measures of size: length, height, weight, …
- Blood pressure of adult humans

In finance, the logarithm of change rates

- Price indices
- Stock market indices

In linguistics, the logarithm of

- Word frequency
- Sentence length

Many scores

- Z-scores, t-scores
- Bell curve grading

Tend to have a Gaussian distribution

Gaussian model

μ and σ fully define a gaussian distribution

Use them as parameter $\theta = (\mu, \sigma)$ to define the model:

suppose each data point is randomly *drawn* from the distribution

μ, σ are **unknown**, but they can be learned (estimated) from **data**

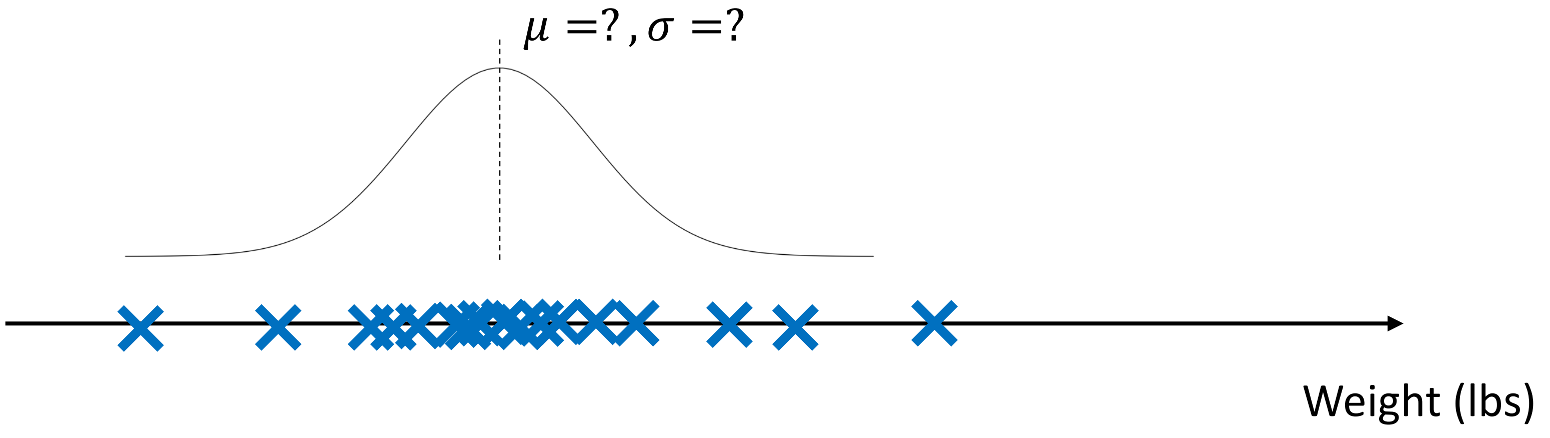
Job: find the parameters that best fit the data

What is “best fit”? → **Maximum Likelihood Estimation** (**MLE**)

Gaussian model example

Data: weight of Salmon fish. Assumption: The weight is from a Gaussian distribution

Task: to estimate the μ, σ of Salman



Maximum Likelihood Estimation (MLE)

Given m data points $X = \{x^{(1)}, \cdots, x^{(m)}\}$ Fit a Gaussian model $\mathcal{N}(\mu, \sigma)$, $\theta = (\mu, \sigma)$

PDF at $x^{(i)}$: $p\left(x^{(i)}|\theta\right) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x^{(i)}-\mu)^2}{2\sigma^2}}$ $\Rightarrow$ How likely it is to observe $x^{(i)}$ given θ

Assuming all data points are independent, then the likelihood of observing the whole dataset:

$$p(X|\theta) = \prod_{i=1}^{m} p\left(x^{(i)}|\theta\right) = \prod_{i=1}^{m} \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x^{(i)}-\mu)^2}{2\sigma^2}}$$

A good estimation of θ needs to maximize $p(X|\theta)$, the **likelihood** of data given the parameters

Maximum Likelihood Estimation (MLE) (cont.)

Likelihood function: $$\mathcal{L}(\theta) = p(X|\theta) = \prod_{i=1}^{m} \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x^{(i)}-\mu)^2}{2\sigma^2}}$$

It is easier to work with **log-likelihood**:

$$\mathcal{LL}(\theta) = \log\big(\mathcal{L}(\theta)\big) = -\frac{m\log(2\pi)}{2} - m\log(\sigma) - \sum_{i=1}^{m} \frac{(x^{(i)}-\mu)^2}{2\sigma^2}$$

Goal: find the $\theta = (\mu, \sigma)$ that maximizes $\mathcal{LL}(\theta)$

Maximum Likelihood Estimation (MLE) (cont.)

$$\mathcal{LL}(\theta) = \log(\mathcal{L}(\theta)) = -\frac{m\log(2\pi)}{2} - m\log(\sigma) - \sum_{i=1}^{m}\frac{(x^{(i)}-\mu)^2}{2\sigma^2}$$

Take the derivative of $\mathcal{LL}(\theta)$ w.r.t μ and σ

$$\frac{\partial\mathcal{LL}(\theta)}{\partial\mu} = -\frac{1}{\sigma^2}\sum_{i=1}^{m}(x^{(i)}-\mu) = -\frac{1}{\sigma^2}\left[\sum_{i=1}^{m}x^{(i)} - m\mu\right]$$

$$\frac{\partial\mathcal{LL}(\theta)}{\partial\sigma} = -\frac{m}{\sigma} + \frac{1}{\sigma^3}\sum_{i=1}^{m}(x^{(i)}-\mu)^2$$

$\mathcal{LL}(\theta)$ has extreme values when $\frac{\partial\mathcal{LL}(\theta)}{\partial\mu} = 0$ and $\frac{\partial\mathcal{LL}(\theta)}{\partial\sigma} = 0$

$$\Rightarrow \quad \mu = \frac{1}{m}\sum_{i=1}^{m}x^{(i)} = \bar{X} \qquad \sigma = \sqrt{\frac{1}{m}\sum_{i=1}^{m}(x^{(i)}-\mu)^2}$$

Mean of data
(sample mean)

Variance of data
(sample variance)

When μ is estimated by $\bar{X}$,
$\sigma = \sqrt{\frac{1}{m-1}\sum_{i=1}^{m}(x^{(i)}-\bar{X})^2} = \sqrt{Var(X)}$
in order to get an unbiased estimate

These are the reasonable estimates of μ and σ from the data

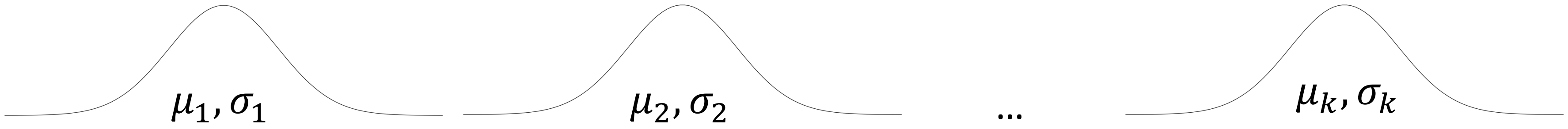
Mixture of Gaussians

Previous example has the assumption that data are drawn from ***one*** Gaussian distribution $\mathcal{N}(\mu, \sigma)$

What if there are ***multiple*** Gaussian distributions: $\mathcal{N}(\mu_1, \sigma_1)$, $\mathcal{N}(\mu_2, \sigma_2)$, …, $\mathcal{N}(\mu_k, \sigma_k)$

How do we generate the data?

Step 1: Draw from k distributions with probabilities $Q_1, Q_2, \cdots, Q_k$

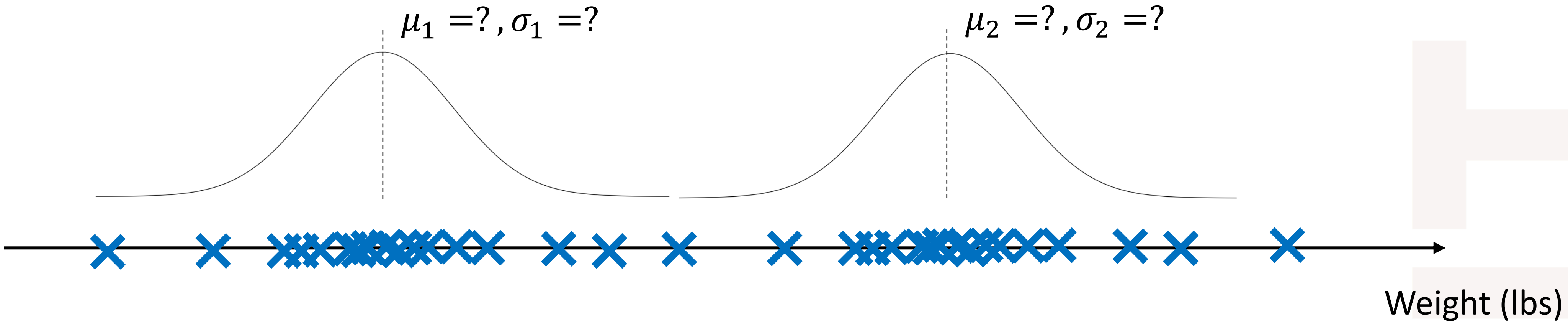


Step 2: Suppose distribution j is chosen, draw a data point from $\mathcal{N}(\mu_j, \sigma_j)$

$$p\left(x^{(i)} \middle| \mu_j, \sigma_j\right) = \frac{1}{\sqrt{2\pi}\sigma_j} e^{-\frac{(x^{(i)}-\mu_j)^2}{2\sigma_j{}^2}}$$

Example of 2 Gaussians

Weights of two kinds of fish: Salmon & Tuna fish



How a data point is generated

A data point $x^{(i)}$ is generated according to the following process:

First, select the fish <u>*kind*</u> with

- Probability ϕ_S of being Salmon
- Probability ϕ_T of being Tuna
- $\phi_S + \phi_T = 1$

Given the fish <u>*kind*</u>, generate the data point from the corresponding Gaussian distribution

- $p\left(x^{(i)} \middle| S\right) \sim \mathcal{N}(\mu_S, \sigma_S)$ for Salmon
- $p\left(x^{(i)} \middle| T\right) \sim \mathcal{N}(\mu_T, \sigma_T)$ for Tuna

Introduce latent (unobserved) variable

Model parameters: $\Theta = (\phi_S, \phi_T, \mu_S, \mu_T, \sigma_S, \sigma_T)$

Parameters for mixture probabilities

Parameters for each Gaussian distribution

For each data point $x^{(i)}$, we don't know if it is a Salmon or Tuna

Let $z^{(i)}$ be the latent random variable indicating which Gaussian distribution $x^{(i)}$ is from

$z^{(i)} = 1$ for Salmon, $z^{(i)} = 2$ for Tuna

Then the likelihood of $x^{(i)}$ is:

$$p(x^{(i)}|\Theta) = \sum_{z^{(i)}} p(x^{(i)}, z^{(i)}|\Theta)$$

Let Q_i be the distribution of $z^{(i)}$
s.t. $\sum_{z^{(i)}} Q_i(z^{(i)}) = 1$
$Q_i(z^{(i)} = j)$ is the probability of $z^{(i)} = j$

Rewrite the likelihood

$$p(x^{(i)}|\Theta) = \sum_{z^{(i)}} Q_i(z^{(i)}) \frac{p(x^{(i)}, z^{(i)}|\Theta)}{Q_i(z^{(i)})}$$

Log likelihood of data

The likelihood of the whole data: $\mathcal{L}(\theta) = p(X|\Theta) = \prod_{i=1}^{m} p\left(x^{(i)}, z^{(i)}|\Theta\right) = \prod_{i=1}^{m} \sum_{z^{(i)}} Q_i(z^{(i)}) \frac{p(x^{(i)}, z^{(i)}|\Theta)}{Q_i(z^{(i)})}$

Log likelihood: $\mathcal{LL}(\theta) = \sum_{i=1}^{m} \log\left(\sum_{z^{(i)}} Q_i(z^{(i)}) \frac{p(x^{(i)}, z^{(i)}|\Theta)}{Q_i(z^{(i)})}\right) = \sum_{i=1}^{m} \log\left(Q_i\left(z^{(i)} = 1\right) \frac{p\left(x^{(i)}, z^{(i)}|\Theta\right)}{Q_i(z^{(i)} = 1)} + Q_i\left(z^{(i)} = 2\right) \frac{p\left(x^{(i)}, z^{(i)}|\Theta\right)}{Q_i(z^{(i)} = 2)}\right)$

It is difficult to take the derivative of $\mathcal{LL}(\theta)$ w.r.t. $\phi_S, \phi_T, \mu_S, \mu_T, \sigma_S, \sigma_T$, and solve them analytically

Solution: Instead of maximizing $\mathcal{LL}(\theta)$, we can maximize the lower bound of $\mathcal{LL}(\theta)$

Idea: Find some expression E, s.t. $\mathcal{LL}(\theta) \geq E$. When we maximize E, $\mathcal{LL}(\theta)$ is also maximized.

E should have a form that is easier to calculate derivatives

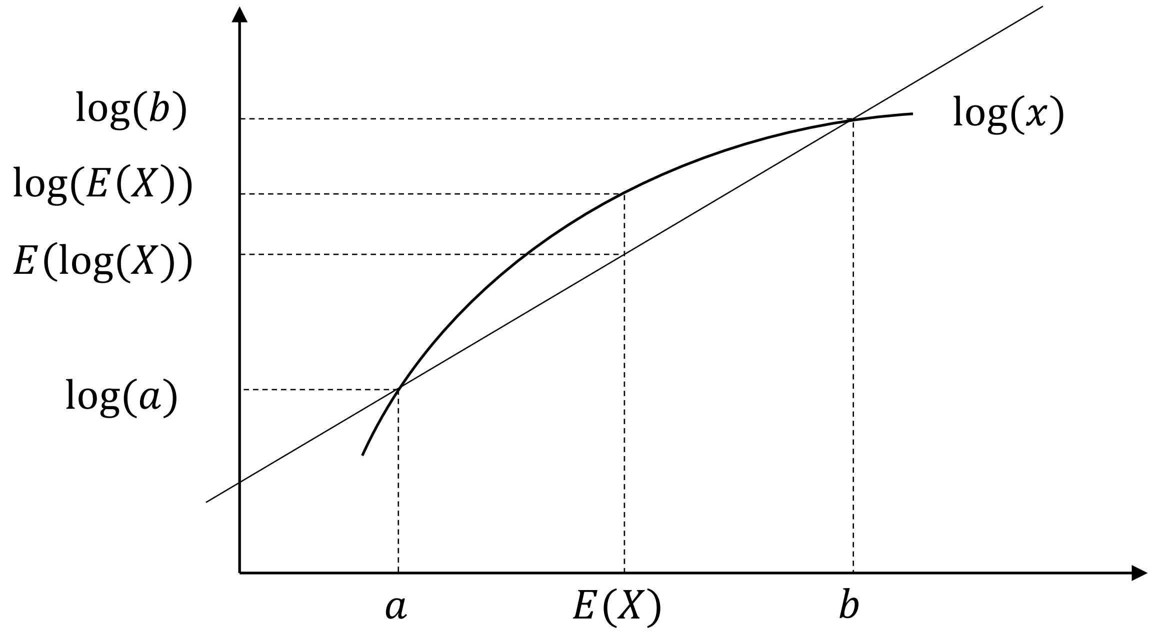
Find the lower bound of $\mathcal{LL}(\theta)$ (optional)

$$\mathcal{LL}(\theta) = \sum_{i=1}^{m} \log\left(\underbrace{Q_i\left(z^{(i)}=1\right)}_{\text{Probability}} \boxed{a} + \underbrace{Q_i\left(z^{(i)}=2\right)}_{\text{Probability}} \boxed{b}\right)$$

Let a, b be two values of a random variable X

Then $Q_i\left(z^{(i)}=1\right)a + Q_i\left(z^{(i)}=2\right)b$ is the expectation of $E(X)$

Because log(x) is convex $\log\left(E(X)\right) \geq E(\log(X))$



$$\mathcal{LL}(\theta) \geq \sum_{i=1}^{m} Q_i\left(z^{(i)}=1\right)\log(a) + Q_i\left(z^{(i)}=2\right)\log(b)$$

$$= \sum_{i=1}^{m} \sum_{z^{(i)}} Q_i\left(z^{(i)}\right)\log\left(\frac{p(x^{(i)}, z^{(i)}|\Theta)}{\underline{Q_i(z^{(i)})}}\right)$$

We need to replace $Q_i\left(z^{(i)}\right)$ with something we know

Jensen's inequality: $f(E(X)) \geq E(f(X))$, when f is convex

How to estimate Q_i (optional)

$$\mathcal{LL}(\theta) \geq \sum_{i=1}^{m} \sum_{z^{(i)}} \underline{Q_i(z^{(i)})} \log\left(\frac{p(x^{(i)}, z^{(i)}|\Theta)}{\underline{Q_i(z^{(i)})}}\right)$$

$Q_i(z^{(i)})$ is unknown, but we can guess it after observing $x^{(i)}$

I.e., after observing a data point $x^{(i)}$, we can "guess" which distribution it is from

A **reasonable** way to guess:

$$\frac{1}{\sqrt{2\pi}\sigma_S} e^{-\frac{(x^{(i)}-\mu_S)^2}{2\sigma_S{}^2}}$$

If $x^{(i)}$ is drawn from Salmon, then the likelihood of $x^{(i)}$ is $\quad p(x^{(i)}|S)p(S) = \underline{p(x^{(i)}|\mu_S, \sigma_S)}\phi_S$

If $x^{(i)}$ is drawn from Tuna, then the likelihood of $x^{(i)}$ is $\quad p(x^{(i)}|T)p(T) = p(x^{(i)}|\mu_T, \sigma_T)\phi_T$

Then the chance of $x^{(i)}$ being Salmon is:

$$p(S|x^{(i)}) = \underbrace{\frac{p(x^{(i)}|S)p(S)}{p(x^{(i)}|S)p(S) + p(x^{(i)}|T)p(T)}}_{\text{Posterior, } w_S^{(i)}}$$

The chance of $x^{(i)}$ being Tuna is:

$$p(T|x^{(i)}) = \underbrace{\frac{p(x^{(i)}|T)p(T)}{p(x^{(i)}|S)p(S) + p(x^{(i)}|T)p(T)}}_{\text{Posterior, } w_T^{(i)}}$$

New form of Log-likelihood function (optional)

$$\mathcal{LL}(\theta) \geq \sum_{i=1}^{m} \sum_{z^{(i)}} Q_i(z^{(i)}) \log\left(\frac{p(x^{(i)}, z^{(i)}|\Theta)}{Q_i(z^{(i)})}\right) = \sum_{i=1}^{m} w_S^{(i)} \log\left(\frac{p(x^{(i)}, z^{(i)} = 1|\Theta)}{w_S^{(i)}}\right) + w_T^{(i)} \log\left(\frac{p(x^{(i)}, z^{(i)} = 2|\Theta)}{w_T^{(i)}}\right) = \mathcal{LL}'(\theta)$$

$$p(x^{(i)}, z^{(i)} = 1|\Theta) = p(x^{(i)}|\mu_S, \sigma_S)\phi_S = \boxed{\frac{\phi_S}{\sqrt{2\pi}\sigma_S} e^{-\frac{(x^{(i)}-\mu_S)^2}{2\sigma_S^2}}}$$

$$p(x^{(i)}, z^{(i)} = 2|\Theta) = p(x^{(i)}|\mu_T, \sigma_T)\phi_T = \boxed{\frac{\phi_T}{\sqrt{2\pi}\sigma_T} e^{-\frac{(x^{(i)}-\mu_T)^2}{2\sigma_T^2}}}$$

Treating w_S and w_T as known, the derivatives of $\mathcal{LL}'(\theta)$ is much easier to calculate

$$\lfloor \mathcal{LL}(\theta) \rfloor = \mathcal{LL}'^{(\theta)} = \sum_{i=1}^{m} w_S^{(i)} \log\left(\frac{\phi_S}{w_S^{(i)}\sqrt{2\pi}\sigma_S} e^{-\frac{(x^{(i)}-\mu_S)^2}{2\sigma_S^2}}\right) + w_T^{(i)} \log\left(\frac{\phi_T}{w_T^{(i)}\sqrt{2\pi}\sigma_T} e^{-\frac{(x^{(i)}-\mu_T)^2}{2\sigma_T^2}}\right)$$

Maximizing $\mathcal{LL}'(\theta)$ (optional)

$$\lfloor \mathcal{LL}(\theta) \rfloor = \mathcal{LL}'^{(\theta)} = \sum_{i=1}^{m} w_S^{(i)} \log\left(\frac{\phi_S}{w_S^{(i)}\sqrt{2\pi}\sigma_S} e^{-\frac{(x^{(i)}-\mu_S)^2}{2\sigma_S^2}}\right) + w_T^{(i)} \log\left(\frac{\phi_T}{w_T^{(i)}\sqrt{2\pi}\sigma_T} e^{-\frac{(x^{(i)}-\mu_T)^2}{2\sigma_T^2}}\right)$$

$$\frac{\partial \mathcal{LL}'(\theta)}{\partial \mu_S} = \sum_{i=1}^{m} \frac{\partial}{\partial \mu_S}\left[w_S^{(i)} \log\left(\frac{\phi_S}{\sqrt{2\pi}\sigma_S} e^{-\frac{(x^{(i)}-\mu_S)^2}{2\sigma_S^2}}\right)\right] = \sum_{i=1}^{m} w_S^{(i)}(x^{(i)} - \mu_S) = 0 \Longrightarrow \mu_S = \frac{\sum_{i=1}^{m} w_S^{(i)} x^{(i)}}{\sum_{i=1}^{m} w_S^{(i)}}$$

$$\frac{\partial \mathcal{LL}'(\theta)}{\partial \sigma_S} = \sum_{i=1}^{m} \frac{\partial}{\partial \sigma_S}\left[w_S^{(i)} \log\left(\frac{\phi_S}{\sqrt{2\pi}\sigma_S} e^{-\frac{(x^{(i)}-\mu_S)^2}{2\sigma_S^2}}\right)\right] = \sum_{i=1}^{m} w_S^{(i)}\left[\left(x^{(i)} - \mu_S\right)^2 - \sigma_S^2\right] = 0 \Longrightarrow \sigma_S^2 = \frac{\sum_{i=1}^{m} w_S^{(i)}\left(x^{(i)} - \mu_S\right)^2}{\sum_{i=1}^{m} w_S^{(i)}}$$

Find the terms that only depends on ϕ_S and ϕ_T $\longrightarrow$ ϕ_S and ϕ_T cannot take any value Under constraint: $\phi_S + \phi_T = 1$

$$\mathcal{LL}'(\theta) = \sum_{i=1}^{m} w_S^{(i)} \log(\phi_S) + w_T^{(i)} \log(\phi_T) \longrightarrow$$

Construct a Lagrangian: $\mathcal{L}(\phi_S) = \left(\sum_{i=1}^{m} w_S^{(i)} \log(\phi_S) + w_T^{(i)} \log(\phi_T)\right) + \beta(\phi_S + \phi_T - 1)$

$$\frac{\partial \mathcal{L}(\phi_S)}{\partial \phi_S} = \frac{\sum_{i=1}^{m} w_S^{(i)}}{\phi_S} + \beta = 0 \Longrightarrow \phi_S = \frac{\sum_{i=1}^{m} w_S^{(i)}}{-\beta} \quad \phi_T = \frac{\sum_{i=1}^{m} w_T^{(i)}}{-\beta} \Longrightarrow -\beta = \sum_{i=1}^{m}\left(w_S^{(i)} + w_T^{(i)}\right) = m$$

Solutions of maximizing $\mathcal{L}\mathcal{L}'(\theta)$ (optional)

$$\begin{cases} \mu_S = \dfrac{\sum_{i=1}^m w_S^{(i)} x^{(i)}}{\sum_{i=1}^m w_S^{(i)}} \\[2ex] \sigma_S^2 = \dfrac{\sum_{i=1}^m w_S^{(i)} \left(x^{(i)} - \mu_S\right)^2}{\sum_{i=1}^m w_S^{(i)}} \\[2ex] \phi_S = \dfrac{\sum_{i=1}^m w_S^{(i)}}{m} \end{cases}$$

$$\begin{cases} \mu_T = \dfrac{\sum_{i=1}^m w_T^{(i)} x^{(i)}}{\sum_{i=1}^m w_T^{(i)}} \\[2ex] \sigma_T^2 = \dfrac{\sum_{i=1}^m w_T^{(i)} \left(x^{(i)} - \mu_T\right)^2}{\sum_{i=1}^m w_T^{(i)}} \\[2ex] \phi_T = \dfrac{\sum_{i=1}^m w_T^{(i)}}{m} \end{cases}$$

Repeatedly update all parameters, $\phi_S, \phi_T, \mu_S, \mu_T, \sigma_S, \sigma_T$ until convergence

In which,

$$w_S^{(i)} = p\left(S|x^{(i)}\right) = \frac{p\left(x^{(i)}|S\right)\phi_S}{p\left(x^{(i)}|S\right)\phi_S + p\left(x^{(i)}|T\right)\phi_T}$$

$$w_T^{(i)} = p\left(T|x^{(i)}\right) = \frac{p\left(x^{(i)}|S\right)\phi_S}{p\left(x^{(i)}|S\right)\phi_S + p\left(x^{(i)}|T\right)\phi_T}$$

E-M (Expectation-Maximization) Algorithm (1-D Gaussian)

Assume the data $\{x^{(i)}\}$ are drawn from *k* Gaussian distributions with probabilities $\phi_1, \phi_2, \cdots, \phi_k$
Each distribution has parameters μ_j, σ_j $(j = 1,2,\cdots,k)$

Randomly initialize all parameters $\phi_1, \phi_2, \cdots, \phi_k$ and μ_j, σ_j $(j = 1,2,\cdots,k)$

Repeat until convergence {

E-step: For each $x^{(i)}$, compute the expectation of which distribution it is from

$$w_j^{(i)} \coloneqq p\left(z^{(i)} = j \middle| x^{(i)}\right) = \frac{p(x^{(i)}|\mu_j, \sigma_j)\phi_j}{\sum_j p(x^{(i)}|\mu_j, \sigma_j)\phi_j} \qquad \text{For } j = 1,2,\cdots,k$$

M-step: Update the parameters (as if $w_j^{(i)}$ is correct) by maximizing the likelihood:

$$\underbrace{\mu_j \coloneqq \frac{\sum_{i=1}^m w_j^{(i)} x^{(i)}}{\sum_{i=1}^m w_j^{(i)}}}_{\text{Weighted average}} \qquad \sigma_j^2 \coloneqq \frac{\sum_{i=1}^m w_j^{(i)} \left(x^{(i)} - \mu_j\right)^2}{\sum_{i=1}^m w_j^{(i)}} \qquad \phi_j \coloneqq \frac{\sum_{i=1}^m w_j^{(i)}}{m} \qquad \text{For } j = 1,2,\cdots,k$$

}

Compare with K-means

Randomly initialize all k centroids $\mu_1, \mu_2, \cdots, \mu_k$

Repeat until convergence {

E-step: For each $x^{(i)}$, assign it to the closest centroid

$$c^{(i)} \coloneqq \arg\min_j \left\| x^{(i)} - \mu_j \right\|^2$$

M-step: Update the positions of centroids

$$\mu_j \coloneqq \frac{\sum_{i=1}^{m} 1\{c^{(i)} = j\} x^{(i)}}{\sum_{i=1}^{m} 1\{c^{(i)} = j\}}$$

}

Demonstration with k = 2, 1-D Gaussian

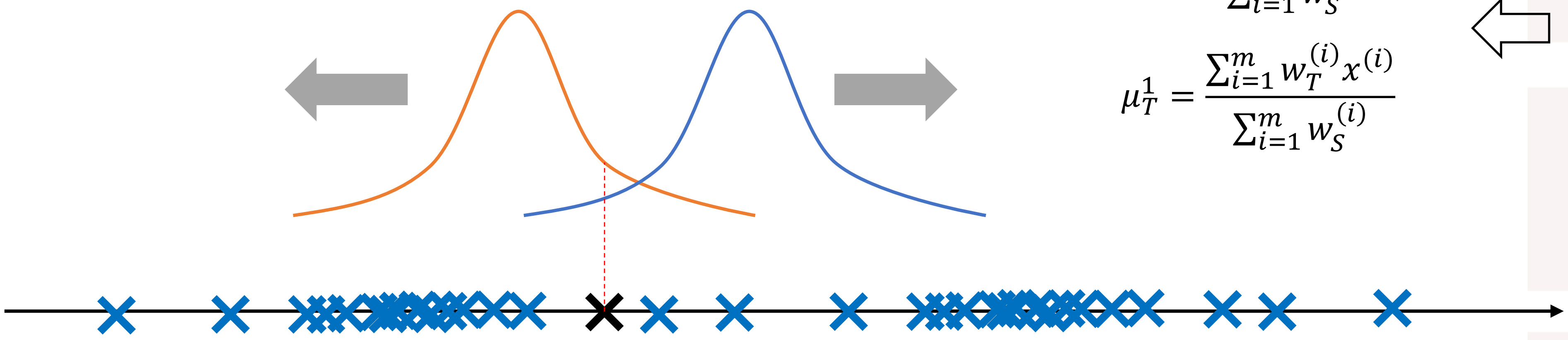
Random initialization

Salmon: $\phi_S^0, \mu_S^0, \sigma_S^0$ Tuna: $\phi_T^0, \mu_T^0, \sigma_T^0$

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

$$\mu_T^1 = \frac{\sum_{i=1}^m w_T^{(i)} x^{(i)}}{\sum_{i=1}^m w_S^{(i)}}$$

M-step



Weight (lbs)

These points tend to have larger $w_S^{(i)}$

$w_S^{(i)} = 0.6$

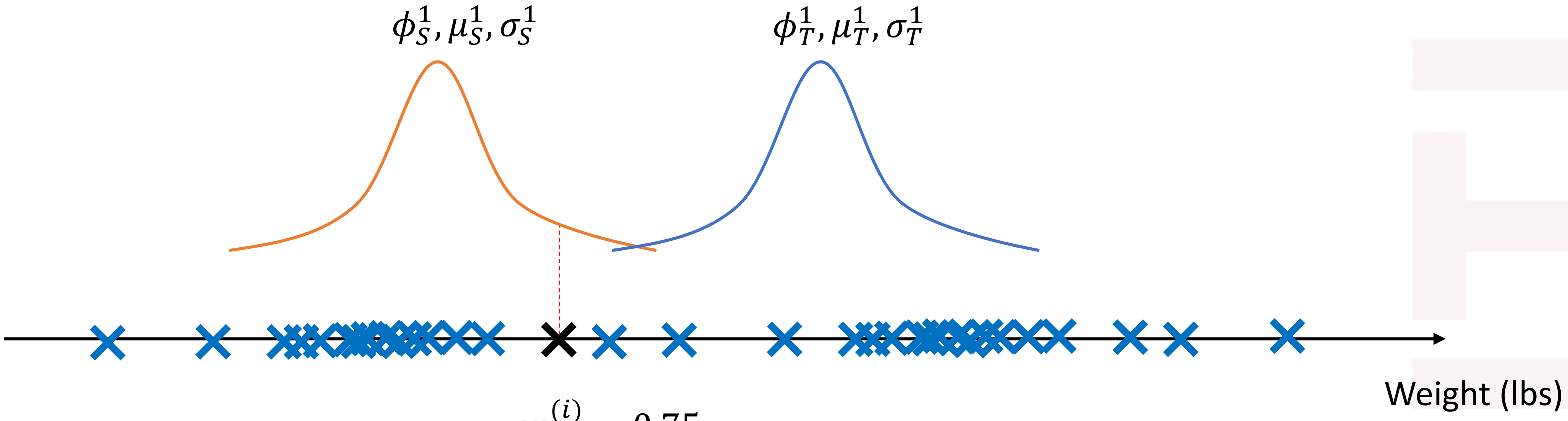
$w_T^{(i)} = 0.4$

These points tend to have larger $w_T^{(i)}$

E-step

Demonstration with k = 2, 1-D Gaussian

After 1 iteration

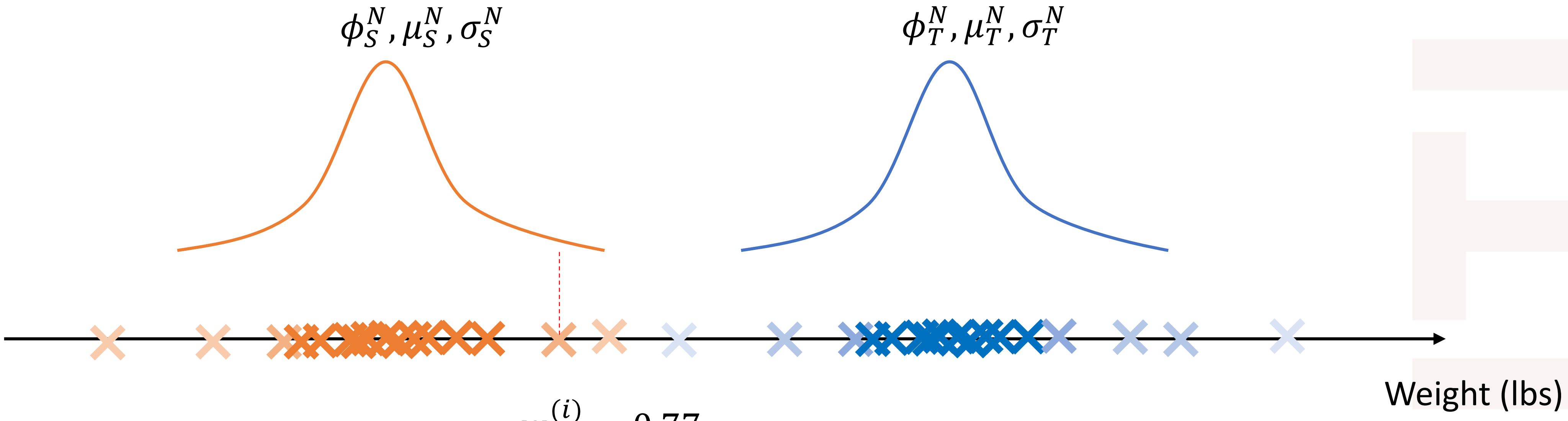


$w_S^{(i)} = 0.75$

$w_T^{(i)} = 0.25$

Demonstration with k = 2, 1-D Gaussian

After N iterations, all parameters converge



$$\underbrace{\begin{matrix} w_S^{(i)} = 0.77 \\ w_T^{(i)} = 0.23 \end{matrix}}$$

This data point is 0.77 chance a Salmon, and 0.23 chance a Tuna

No hard assignment!

What about multivariate Gaussians?

A random vector $X = \begin{pmatrix} X_1 \\ \vdots \\ X_n \end{pmatrix}$ is said to have a multivariate Gaussian distribution

If its probability density function is: $$p(x) = \frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu)\right)$$

Mean: $\mu \in \mathbb{R}^n$ Covariance matrix: Σ

Property: $$\frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} \exp\left(-\frac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu)\right) dx_1 dx_2 \cdots dx_n = 1.$$

Covariance matrix

If X_i, Y_j are a pair of 1-D random variables

Then the covariance is defined as: $Cov[X_i, Y_j] = E\left[(X - E(X_i))\left(Y - E(Y_j)\right)\right] = E[X_i Y_j] - E(X_i)E(Y_j)$

If $X = \begin{pmatrix} X_1 \\ \vdots \\ X_n \end{pmatrix}, Y = \begin{pmatrix} Y_1 \\ \vdots \\ Y_n \end{pmatrix}$ are a pair of n-D random variables

Then the covariance matrix Σ is a $n \times n$ symmetric matrix

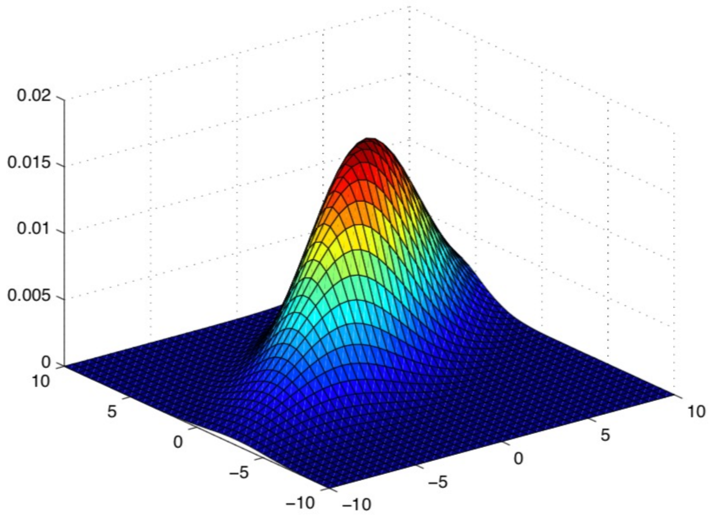
whose (i, j) th entry is $Cov[X_i, Y_j]$

$$\Sigma = \begin{bmatrix} Cov[X_1, Y_1] & Cov[X_1, Y_2] & & Cov[X_1, Y_n] \\ Cov[X_2, Y_1] & Cov[X_2, Y_2] & \cdots & Cov[X_2, Y_n] \\ \vdots & \vdots & & \vdots \\ Cov[X_n, Y_1] & Cov[X_n, Y_2] & & Cov[X_n, Y_n] \end{bmatrix}$$

When n=2, 2-D Gaussian distribution

$$x = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \qquad \mu = \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix} \qquad \Sigma = \begin{bmatrix} \sigma_1^2 & \sigma_1\sigma_2 \\ \sigma_1\sigma_2 & \sigma_2^2 \end{bmatrix}$$

$$p(x) = \frac{1}{2\pi \begin{vmatrix} \sigma_1^2 & \sigma_1\sigma_2 \\ \sigma_1\sigma_2 & \sigma_2^2 \end{vmatrix}^{1/2}} \exp\left(-\frac{1}{2} \begin{pmatrix} x_1 - \mu_1 \\ x_2 - \mu_2 \end{pmatrix}^T \begin{bmatrix} \sigma_1^2 & \sigma_1\sigma_2 \\ \sigma_1\sigma_2 & \sigma_2^2 \end{bmatrix}^{-1} \begin{pmatrix} x_1 - \mu_1 \\ x_2 - \mu_2 \end{pmatrix} \right)$$



Special case: covariance matrix is diagonal

$$\Sigma = \begin{bmatrix} \sigma_1^2 & 0 \\ 0 & \sigma_2^2 \end{bmatrix} \qquad p(x) = \frac{1}{2\pi \begin{vmatrix} \sigma_1^2 & 0 \\ 0 & \sigma_2^2 \end{vmatrix}^{1/2}} \exp\left(-\frac{1}{2} \begin{pmatrix} x_1 - \mu_1 \\ x_2 - \mu_2 \end{pmatrix}^T \begin{bmatrix} \sigma_1^2 & 0 \\ 0 & \sigma_2^2 \end{bmatrix}^{-1} \begin{pmatrix} x_1 - \mu_1 \\ x_2 - \mu_2 \end{pmatrix} \right)$$

$$= \frac{1}{2\pi\sqrt{\sigma_1^2\sigma_2^2}} \exp\left(-\frac{1}{2} \begin{pmatrix} x_1 - \mu_1 \\ x_2 - \mu_2 \end{pmatrix}^T \begin{bmatrix} {}^{1}/{\sigma_1^2} & 0 \\ 0 & {}^{1}/{\sigma_2^2} \end{bmatrix}^{-1} \begin{pmatrix} x_1 - \mu_1 \\ x_2 - \mu_2 \end{pmatrix} \right)$$

$$= \frac{1}{2\pi\sigma_1\sigma_2} \exp\left(-\frac{1}{2\sigma_1^2}(x_1 - \mu_1)^2 - \frac{1}{2\sigma_2^2}(x_2 - \mu_2)^2 \right)$$

$$= \underbrace{\frac{1}{2\pi\sigma_1} \exp\left(-\frac{1}{2\sigma_1^2}(x_1 - \mu_1)^2 \right)}_{\text{PDF for } x_1} \cdot \underbrace{\frac{1}{2\pi\sigma_2} \exp\left(-\frac{1}{2\sigma_2^2}(x_2 - \mu_2)^2 \right)}_{\text{PDF for } x_2} \Rightarrow$$

Product of two independent 1-D Gaussian distribution

Contours of 2-D Gaussians

$$x = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$

$$\mu = \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix}$$

$$\Sigma = \begin{bmatrix} \sigma_1^2 & 0 \\ 0 & \sigma_2^2 \end{bmatrix}$$

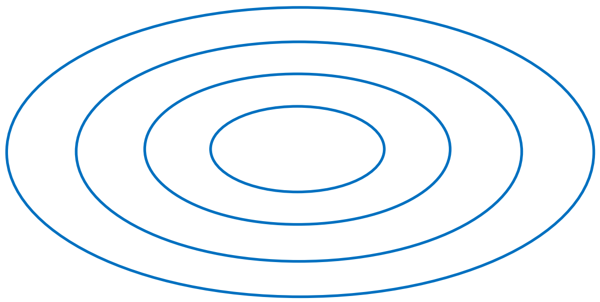
$$p(x) = \frac{1}{2\pi\sigma_1\sigma_2} \exp\left(-\frac{1}{2\sigma_1^2}(x_1 - \mu_1)^2 - \frac{1}{2\sigma_2^2}(x_2 - \mu_2)^2 \right)$$

To draw contours, let $p(x)$ be a constant

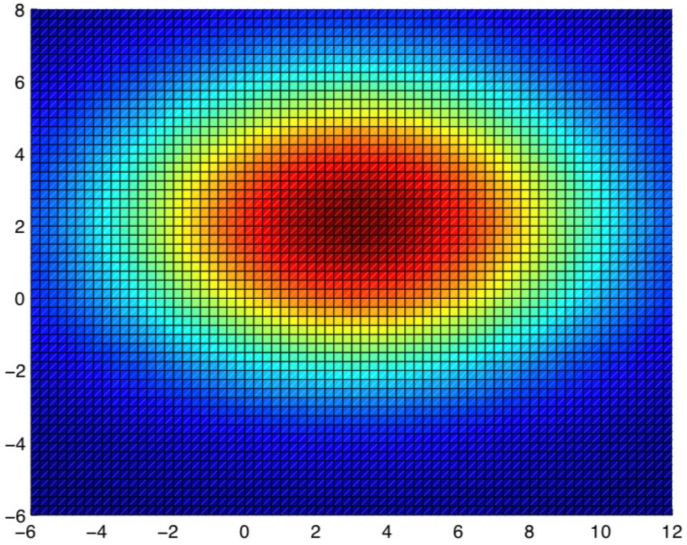
$$p(x) = c \quad \Rightarrow \quad 1 = \frac{(x_1 - \mu_1)^2}{2\sigma_1^2 \log\left(\frac{1}{2\pi c \sigma_1 \sigma_2}\right)} + \frac{(x_2 - \mu_2)^2}{2\sigma_2^2 \log\left(\frac{1}{2\pi c \sigma_1 \sigma_2}\right)}$$

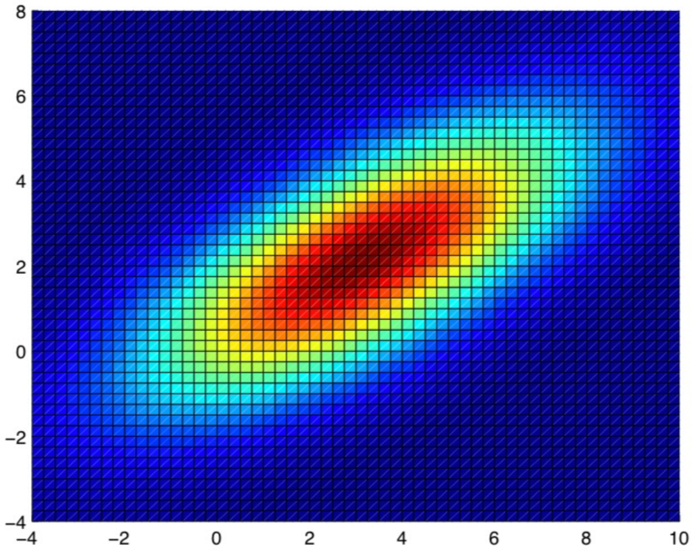
$$1 = \frac{(x_1 - \mu_1)^2}{r_1^2} + \frac{(x_2 - \mu_2)^2}{r_2^2}$$

An ellipse!



Covariance matrix decides the shape of ellipse





$\mu = \begin{pmatrix} 3 \\ 2 \end{pmatrix}$ $\Sigma = \begin{bmatrix} 25 & 0 \\ 0 & 9 \end{bmatrix}$

$\mu = \begin{pmatrix} 3 \\ 2 \end{pmatrix}$ $\Sigma = \begin{bmatrix} 10 & 5 \\ 5 & 5 \end{bmatrix}$

E-M algorithm for mixture of multivariate gaussians

Assume the data $\{x^{(i)}\}$ are drawn from *k n*-D Gaussian distributions with probabilities $\phi_1, \phi_2, \cdots, \phi_k$
Each distribution has parameters μ_j, Σ_j $(j = 1,2,\cdots,k)$

Randomly initialize all parameters $\phi_1, \phi_2, \cdots, \phi_k$ and μ_j, Σ_j $(j = 1,2,\cdots,k)$

Repeat until convergence {

E-step: For each $x^{(i)}$, compute the expectation of which distribution it is from

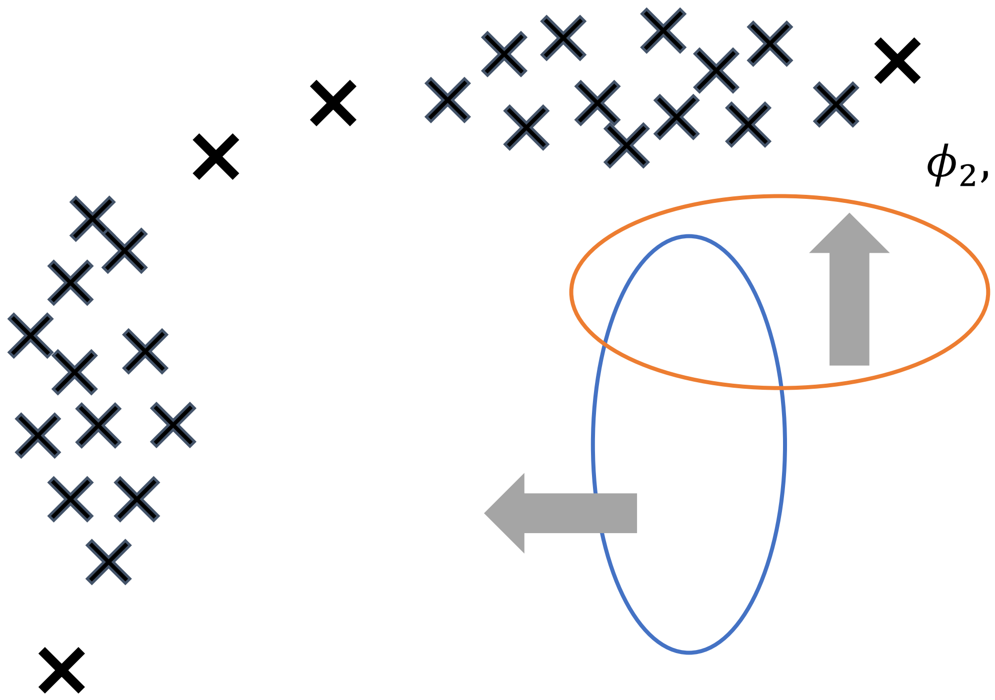
$$w_j^{(i)} \coloneqq p\left(z^{(i)} = j \middle| x^{(i)}\right) = \frac{p(x^{(i)}|\mu_j, \Sigma_j)\phi_j}{\sum_j p(x^{(i)}|\mu_j, \Sigma_j)\phi_j} \qquad \text{For } j = 1,2,\cdots,k$$

M-step: Update the parameters (as if $w_j^{(i)}$ is correct) by maximizing the likelihood:

$$\mu_j \coloneqq \frac{\sum_{i=1}^m w_j^{(i)} x^{(i)}}{\sum_{i=1}^m w_j^{(i)}} \qquad \Sigma_j \coloneqq \frac{\sum_{i=1}^m w_j^{(i)}\left(x^{(i)} - \mu_j\right)\left(x^{(i)} - \mu_j\right)^T}{\sum_{i=1}^m w_j^{(i)}} \qquad \phi_j \coloneqq \frac{\sum_{i=1}^m w_j^{(i)}}{m} \qquad \text{For } j = 1,2,\cdots,k$$

}

Demo of learning a mixture of 2-D Gaussians



Random initialization

For each $x^{(i)}$, compute

$$w_1^{(i)} := \frac{p(x^{(i)}|\mu_1, \Sigma_1)\phi_1}{p(x^{(i)}|\mu_1, \Sigma_1)\phi_1 + p(x^{(i)}|\mu_2, \Sigma_2)\phi_2}$$

$$w_2^{(i)} := \frac{p(x^{(i)}|\mu_2, \Sigma_2)\phi_2}{p(x^{(i)}|\mu_1, \Sigma_1)\phi_1 + p(x^{(i)}|\mu_2, \Sigma_2)\phi_2}$$

Update:

$$\mu_1 := \frac{\sum_{i=1}^m w_1^{(i)} x^{(i)}}{\sum_{i=1}^m w_1^{(i)}} \qquad \mu_2 := \frac{\sum_{i=1}^m w_2^{(i)} x^{(i)}}{\sum_{i=1}^m w_2^{(i)}}$$

Demo of learning a mixture of 2-D Gaussians (cont.)