

Maximum Likelihood Estimation and Expectation Maximization – P2

Bhiksha Raj

Agenda

- Generative Models
- Fitting models to data
- Where'd the closed forms go?
- Dealing with missing information
- How expectation maximization solves all our problems

What is a generative model

- A model for the probability distribution of a data
 x
 - E.g. a multinomial, Gaussian etc.



 Computational equivalent: a model that can be used to "generate" data with a distribution similar to the given data x

Some "simple" generative models

• The multinomial PMF

 $P(x = v) \equiv P(v)$

- For discrete data
 - v belongs to a discrete set
- Can be expressed as a table of probabilities if the set of possible vs is finite
- Else, requires a parametric form, e.g. Poisson

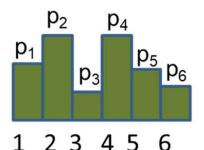
$$P(x=k) = \frac{\lambda^k e^{-\lambda}}{k!} \text{ for } k \ge 0$$

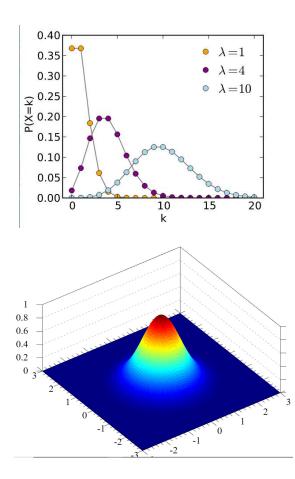
- λ is the Poisson parameter
- The Gaussian PDF

$$P(x = v)$$

$$=\frac{1}{\sqrt{2\pi|\Sigma|}^{D}}\exp\left(-0.5(x-\mu)^{T}\Sigma^{-1}(x-\mu)\right)$$

- For continuous-valued data
- $-\mu$ is the mean of the distribution
- $-\Sigma$ is the Covariance matrix





Learning a generative model for data

- You are given some set of observed data $X = \{x\}$.
- You choose a model $P(x; \theta)$ for the distribution of $x \theta$ are the parameters of the model
- Estimate the theta such that $P(x; \theta)$ best "fits" the observations $X = \{x\}$

- Hoping it will also represent data outside the training set.

Defining "Best Fit": Maximum likelihood

- Assumption: The world is a boring place
 - The data you have observed are very typical of the process
- Consequent assumption: The distribution has a high probability of generating the observed data

Not necessarily true

• Select the distribution that has the *highest* probability of generating the data

Maximum likelihood

- The maximum likelihood principle:
 - $\operatorname{argmax}_{\theta} P(X; \theta) = \operatorname{argmax}_{\theta} \log(P(X; \theta))$
- For the histogram

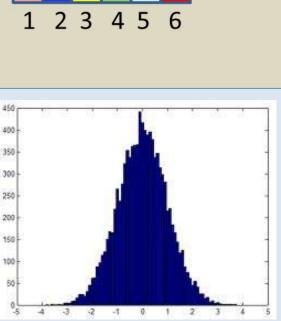
$$- \underset{\{p_1, p_2, p_3, p_4, p_5, p_6\}}{\operatorname{argmax}} \sum_i n_i \log(p_i) \bullet$$

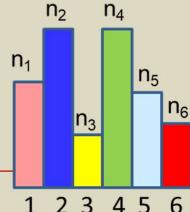


• For the Gaussian

-
$$\underset{\mu,\sigma^2}{\operatorname{argmax}} \sum_{x \in X} \log Gaussian(x; \mu, \sigma^2)$$

$$\Rightarrow \mu = \frac{1}{N} \sum_{x \in X} x; \qquad \sigma^2 = \frac{1}{N} \sum_{x \in X} (x - \mu)^2$$





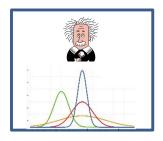
The missing-info challenge

 In some estimation problems there is often some information missing



 If this information were available, estimation would've been trivial



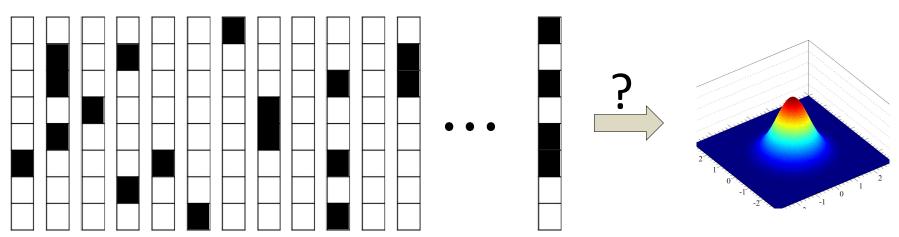


Let's Look at Missing Information

Missing Information about **Underlying Data**

Missing Information about **Underlying Process**

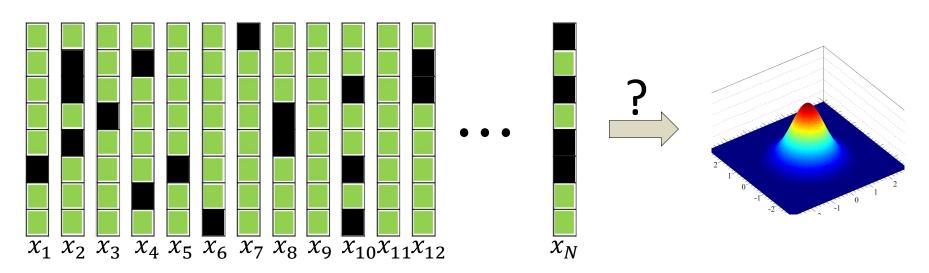
Examples of incomplete data: missing data



Blacked-out components are missing from data

- Objective: Estimate a Gaussian distribution from a collection of vectors
- Problem: Several of the vector components are missing
- Must estimate the mean and covariance of the Gaussian with these incomplete data
 - What would be a good way of doing this?

Maximum likelihood estimation with incomplete data



• Maximum likelihood estimation: Maximize the likelihood of the observed data

$$\underset{\mu,\Sigma}{\operatorname{argmax}} \log(P(O)) = \underset{\mu,\Sigma}{\operatorname{argmax}} \sum_{o \in O} \log \int_{-\infty}^{\infty} P(o,m) dm$$

- This requires the maximization of the log of an integral!
 - No closed form
 - Challenging on a good day, impossible on a bad one

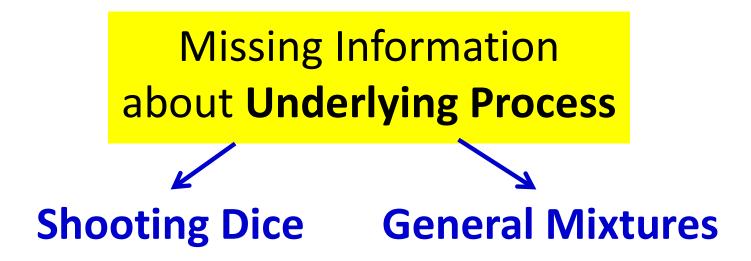
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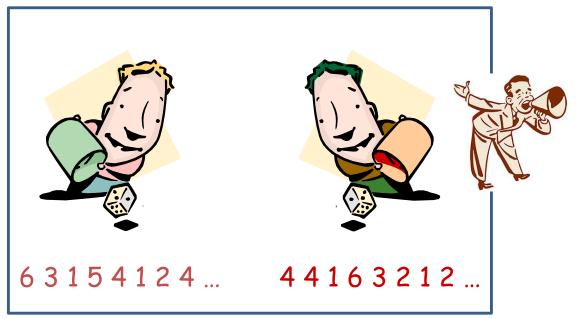
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Let's Look at Missing Information

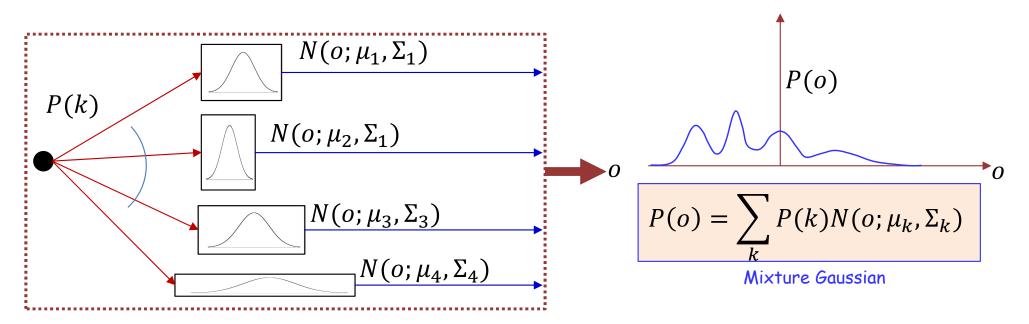
Missing Information about **Underlying Data**





- Two persons shoot loaded dice repeatedly

 The dice are differently loaded for the two of them
- We observe the series of outcomes for both persons
- How to determine the probability distributions of the two dice?



- The generative model randomly selects a Gaussian
- Then it draws an observation from the selected Gaussian
- Given only a collection of observations, how to estimate the parameters of the individual Gaussians, and the probability of selecting Gaussians?

The general form of the problem

- The "presence" of missing data or variables requires them to be marginalized out of your probability
 - By summation or integration
- This results in a maximum likelihood estimate of the form

$$\hat{\theta} = \underset{\theta}{\operatorname{argmax}} \sum_{o} \log \sum_{h} P(h, o; \theta)$$

- The inner summation may also be an integral in some problems
- Explicitly introducing θ in the RHS to show that the probability is computed by a model with parameter θ which must be estimated
- The log of a sum (or integral) makes estimation challenging
 - No closed form solution
 - Need efficient iterative algorithms

Expectation Maximization for Maximum Likelihood Estimation

• Objective: Estimate

$$\theta^* = \operatorname*{argmax}_{\theta} \sum_{o \in O} \log \sum_{h} P(h, o; \theta)$$

• Solution: Iteratively perform the following optimization instead

$$\theta^{k+1} \leftarrow \operatorname*{argmax}_{\theta} \sum_{o \in O} \sum_{h} P(h|o; \theta^{k}) \log P(h, o; \theta)$$

- This maximizes an Empirical Lower Bound (ELBO) and guarantees increasing log likelihood with iterations
 - Giving you a local maximum log likelihood estimate for θ^*

Expectation Maximization for Maximum Likelihood Estimation

• Objective: Estimate

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• Solution: Iteratively perform the following optimization instead

$$\theta^{k+1} \leftarrow \operatorname*{argmax}_{\theta} \sum_{o \in O} \sum_{h} \frac{P(h|o; \theta^k) \log P(h, o; \theta)}{P(h, o; \theta)}$$

- This maximizes an Empirical Lower Bound (ELBO) and guarantees increasing log likelihood with iterations
 - Giving you a local maximum log likelihood estimate for θ^*

Expectation Maximization

- Initialize θ^0
- k = 0
- Iterate (over k) until $\log P(O; \theta)$ converges:
 - Expectation Step

Compute $P(h|o; \theta^k)$ for all $o \in O$ for all h

Maximization step

$$\theta^{k+1} \leftarrow \operatorname{argmax}_{\theta} \sum_{o \in O} \sum_{h} P(h|o; \theta^{k}) \log P(h, o; \theta)$$

Expectation Maximization

• Initialize θ^0

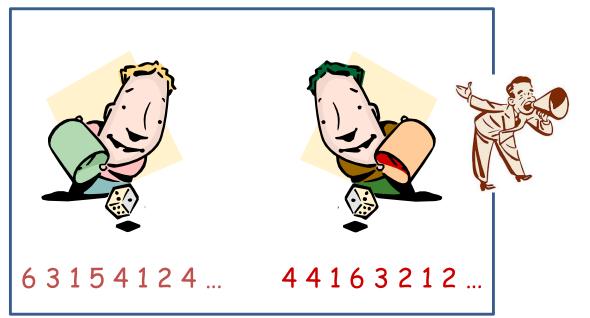
Let's put this to work

- k = 0
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 - Expectation Step

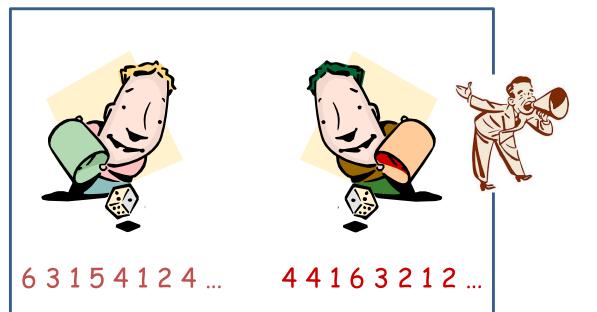
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Maximization step

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$$P(k,o) = P(k)P_k(o) \qquad P(o) = \sum_k P(k)P_k(o)$$



 $P(k,o) = P(k)P_k(o) \qquad P(o) = \sum_k P(k)P_k(o)$

 $P(k|o) = \frac{P(k)P(o|k)}{P(o)} \qquad P(k|o) = \frac{P(k)P_k(o)}{\sum_{k'} P(k')P_{k'}(o)}$

Expectation Maximization

• Initialize θ^0

Let's put this to work

- l = 0
- Iterate (over l) until $\log P(O; \theta)$ converges:
 - Expectation Step

Compute $P(k|o; \theta^l)$ for all $o \in O$ for all k

$$P_{cur}(k|o) = \frac{P(k)P_k(o)}{\sum_{k'} P(k')P_{k'}(o)}$$

Using the current set of estimated parameters

Expectation Maximization

• Initialize θ^0

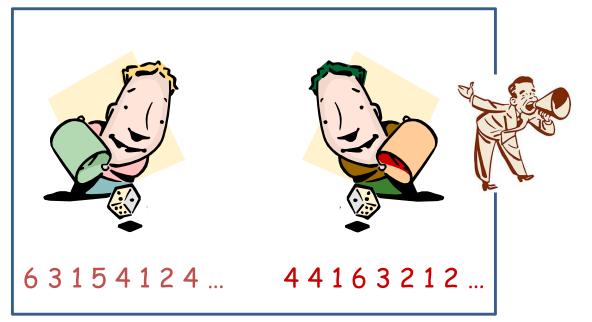
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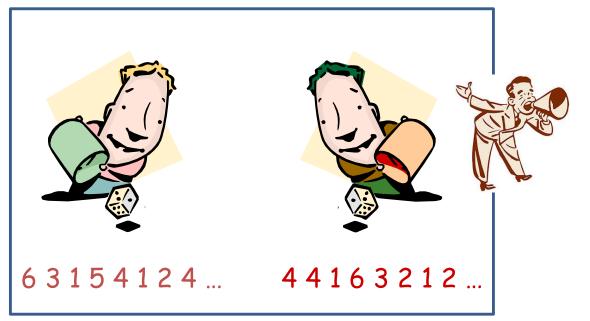
Maximization step

$$\theta^{l+1} \leftarrow \operatorname{argmax}_{\theta} \sum_{o \in O} \sum_{h} P(h|o; \theta^{l}) \log P(h, o; \theta)$$



$$\underset{\theta}{\operatorname{argmax}} \sum_{o \in O} \sum_{h} P(h|o; \theta^{k}) \log P(h, o; \theta)$$

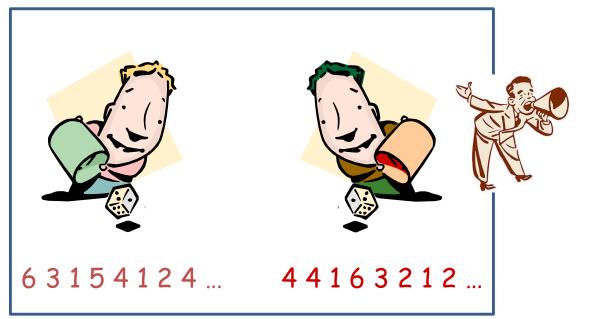
$$\underset{\theta}{\operatorname{argmax}} \sum_{o \in O} \sum_{k} P_{cur}(k|o) \log P(k) P_k(o)$$

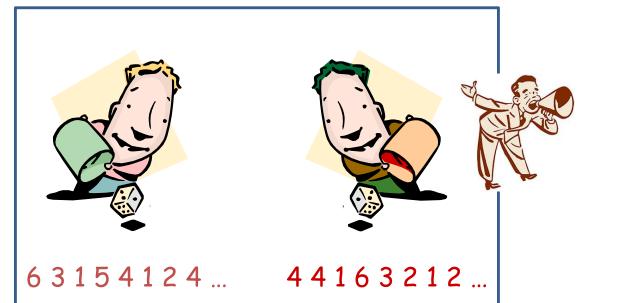


$$\underset{\theta}{\operatorname{argmax}} \sum_{o \in O} \sum_{k} P(h|o; \theta^{k}) \log P(h, o; \theta)$$
$$\underset{\theta}{\operatorname{argmax}} \sum_{o \in O} \sum_{k} P_{cur}(k|o) \log P(k) P_{k}(o) + \lambda \left(\sum_{k} P(k) - 1\right) + \sum_{k} \lambda_{k} \left(\sum_{o} P_{k}(o) - 1\right)$$

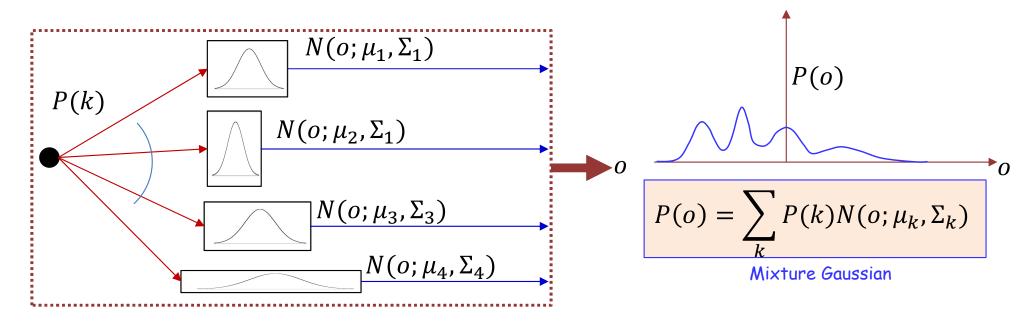
Differentiate and equate to 0

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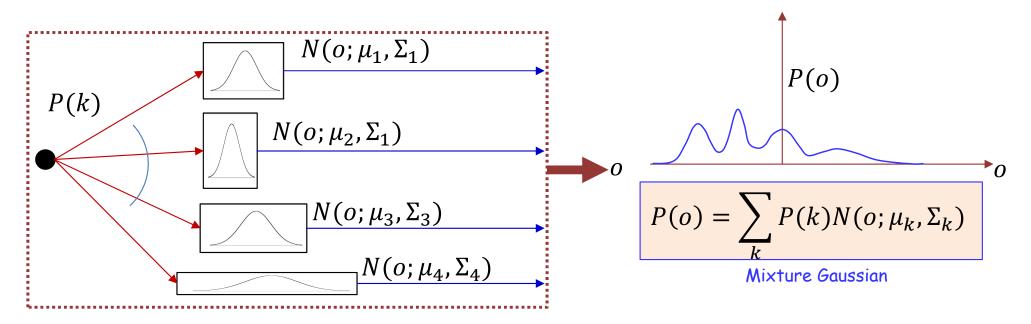




Examples of incomplete data: missing information in Gaussian mixtures



Examples of incomplete data: missing information in Gaussian mixtures



$$P(k,o) = P(k)N(o;\mu_k,\Sigma_k)$$

$$P(k|o) = \frac{P(k)N(o;\mu_k,\Sigma_k)}{\sum_{k'}P(k')N(o;\mu_{k'},\Sigma_{k'})}$$

Expectation Maximization

• Initialize θ^0

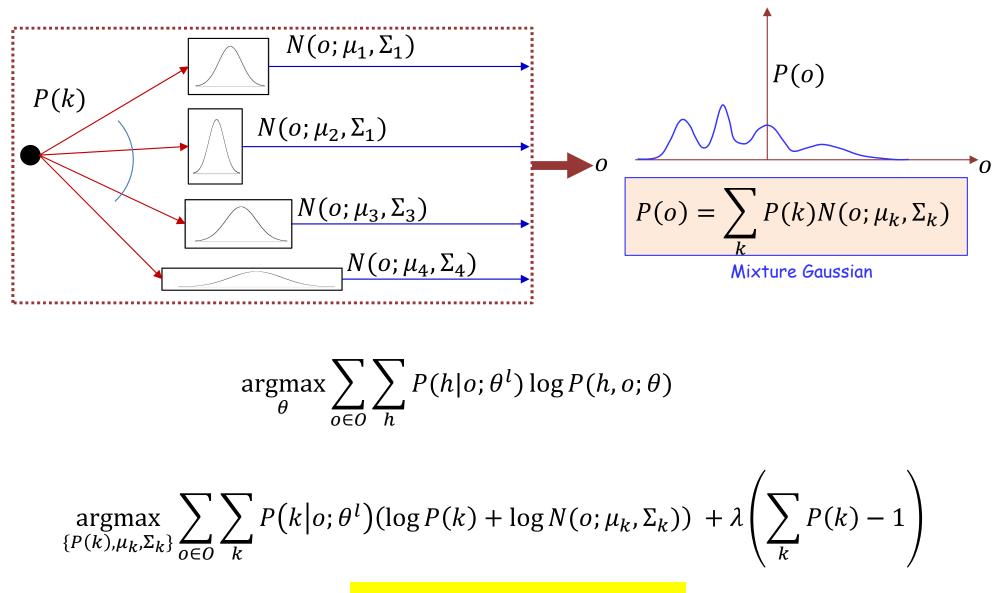
Let's put this to work

- l = 0
- Iterate (over l) until $\log P(0; \theta)$ converges:
 - Expectation Step

Compute $P(k|o; \theta^l)$ for all $o \in O$ for all k

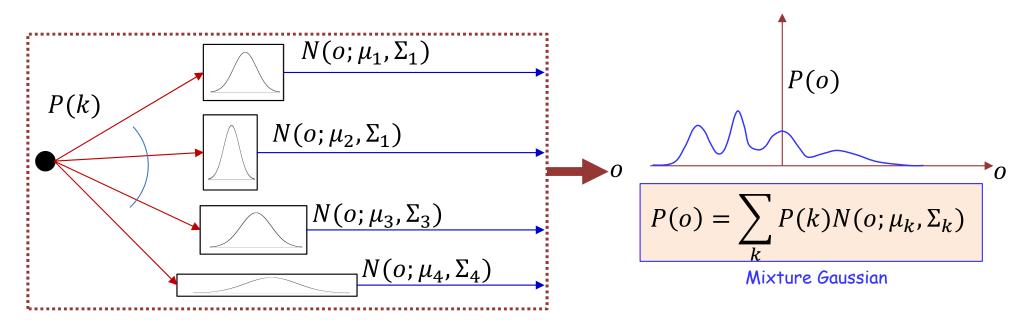
$$P(k|o;\theta^{l}) = \frac{P^{l}(k)N(o;\mu_{k}^{l},\Sigma_{k}^{l})}{\sum_{k'}P^{l}(k')N(o;\mu_{k'}^{l},\Sigma_{k'}^{l})}$$

Using the current set of estimated parameters



Differentiate and equate to 0

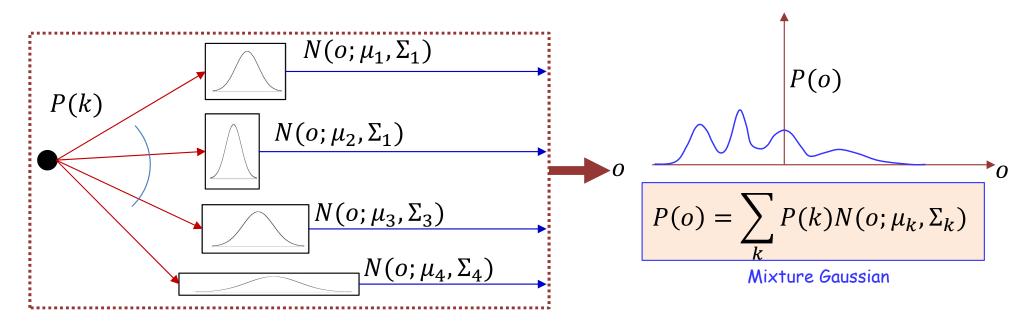
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$$P^{l+1}(k) = \frac{1}{N} \sum_{o} P(k|o; \theta^l)$$

$$\mu_k^{l+1} = \frac{1}{\sum_o P(k|o;\theta^l)} \sum_o P(k|o;\theta^l) o$$

$$\Sigma_k^{l+1} = \frac{1}{\sum_o P(k|o;\theta^l)} \sum_o P(k|o;\theta^l) (o - \mu_k^{l+1}) (o - \mu_k^{l+1})^T$$



$$\kappa | o; \theta^l) = \frac{P^l(k) N(o; \mu^l_k, \Sigma^l_k)}{\sum_{k'} P^l(k') N(o; \mu^l_{k'}, \Sigma^l_{k'})}$$

P(

$$P^{l+1}(k) = \frac{1}{N} \sum_{o} P(k|o; \theta^{l})$$
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$$\Sigma_{k}^{l+1} = \frac{1}{\sum_{o} P(k|o; \theta^{l})} \sum_{o} P(k|o; \theta^{l}) (o - \mu_{k}^{l+1}) (o - \mu_{k}^{l+1})^{T}$$

Ε

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Poll 1: tinyurl.com/mlsp23-20231109-1

- Select all true statements
 - The E step in the EM algorithm computes the a posteriori probability distribution of missing variables
 - The E step in EM maximizes the expectation over missing variables of the log of the probability of the complete data
 - The M step in the EM algorithm computes the a posteriori probability distribution of missing variables
 - The M step in EM maximizes the expectation over missing variables of the log of the probability of the complete data

Poll 1

- Select all true statements
 - The E step in the EM algorithm computes the a posteriori probability distribution of missing variables
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 - The M step in the EM algorithm computes the a posteriori probability distribution of missing variables
 - The M step in EM maximizes the expectation over missing variables of the log of the probability of the complete data

That's so much math, but what does it really do?

- What does EM practically do when we have missing data?
 - What is the intuition behind how it resolves the problem?

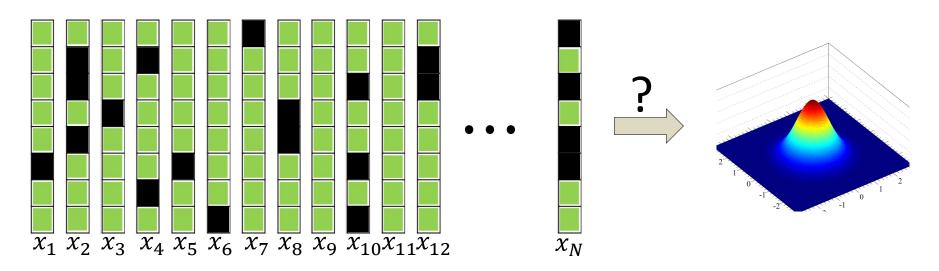
Missing Information about **Underlying Data**

Missing Information about **Underlying Process**

Missing Information about **Underlying Data**

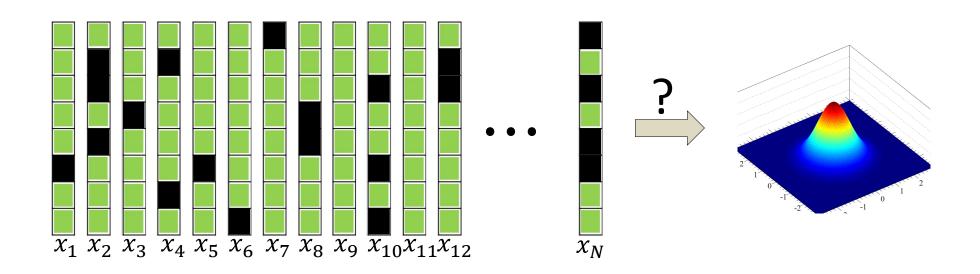
Missing Information about **Underlying Process**

Recall this: Gaussian estimation with incomplete vectors

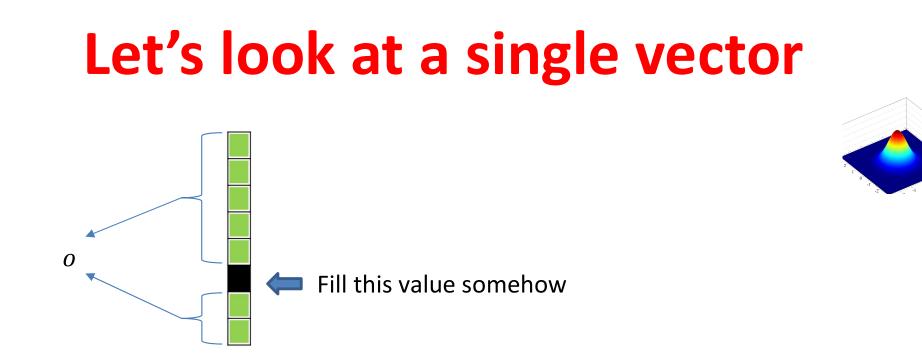


- These are the actual data we have: A set $O = \{o_1, ..., o_N\}$ of *incomplete* vectors
 - Comprising only the observed components of the data
- We are *missing* the data $M = \{m_1, \dots, m_N\}$
 - Comprising the missing components of the data
- The *complete* data includes both the observed and missing components
 X = {x₁, ..., x_N}, x_i = (o_i, m_i)
 – Keep in mind that at the complete data are *not* available (the missing components are missing)

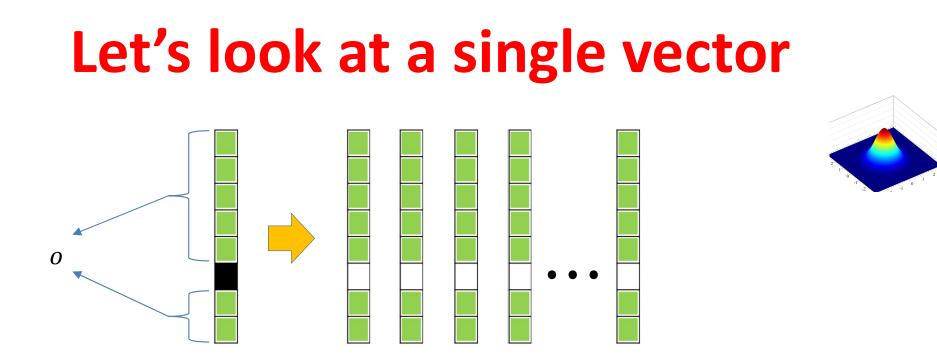
Let's look at a single vector



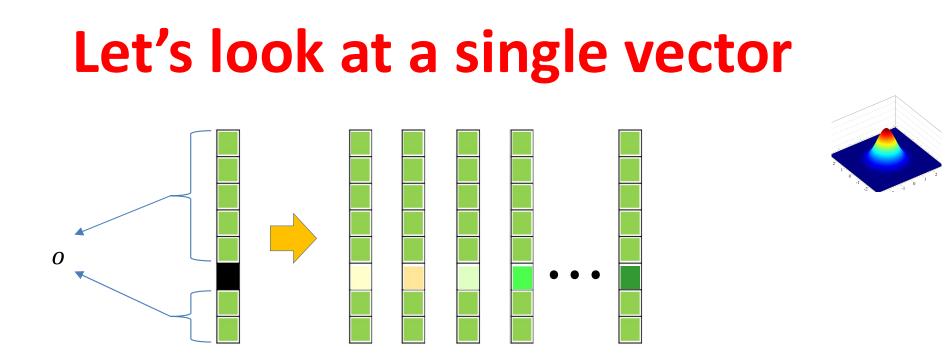
- These are the actual data we have: A set $O = \{o_1, \dots, o_N\}$ of *incomplete* vectors
 - Comprising only the *observed* components of the data
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- The *complete* data includes both the observed and missing components
 X = {x₁, ..., x_N}, x_i = (o_i, m_i)
 – Keep in mind that at the complete data are *not* available (the missing components are missing)



- We will try to complete the vector by filling in the missing value with *plausible* values that match the observed components
- Plausible: Values that "go with" the observed values, according to the distribution of the data

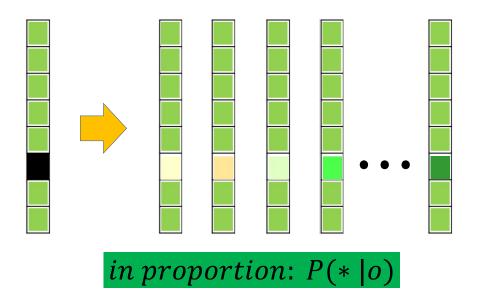


 Question: If we have a very large number of vectors from the Gaussian, all with the same observed components o, what would their missing components be?



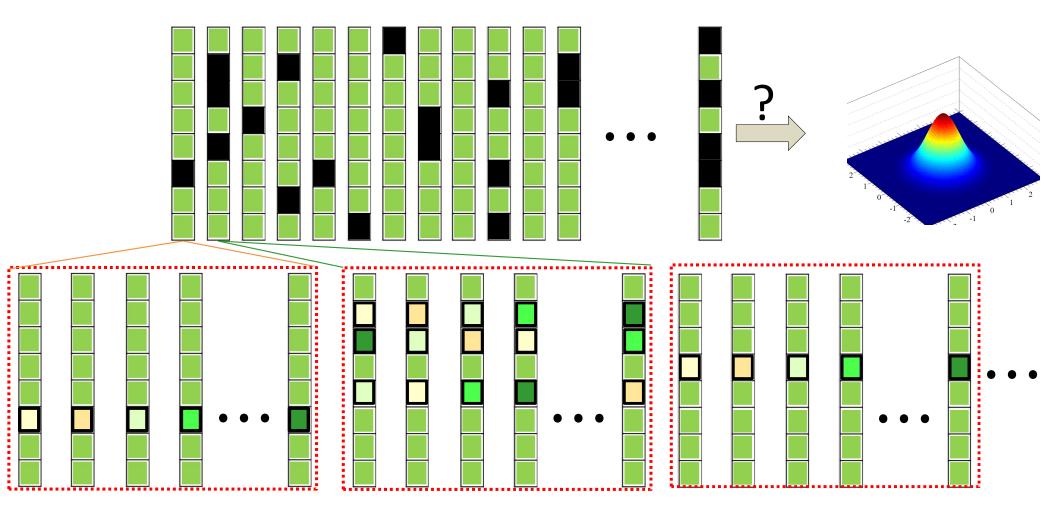
- Question: If we have a very large number of vectors from the Gaussian, all with the same observed components o, what would their missing components be?
- We would see every possible value, but in proportion to their probability: P(m|o) (conditioned on the observations)

Completing incomplete vectors



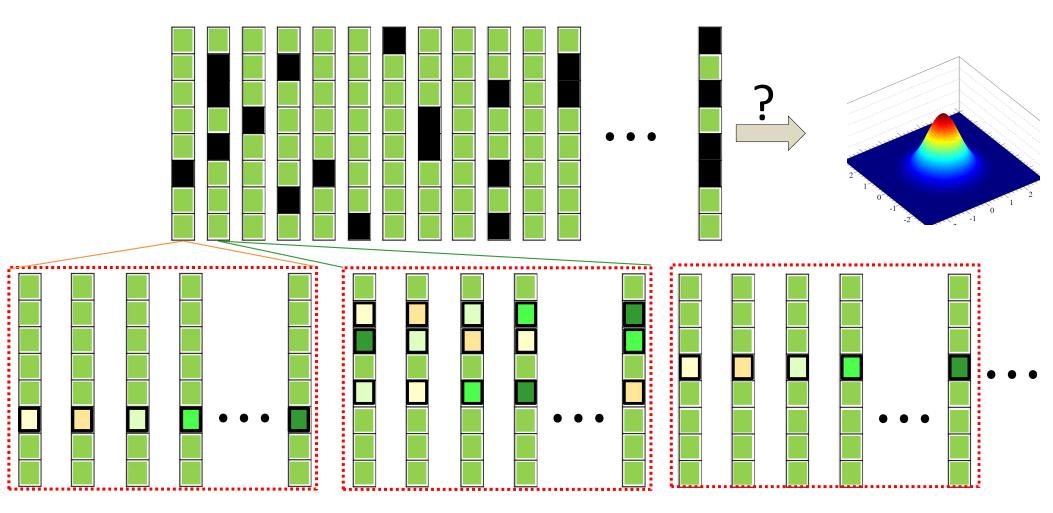
- Complete vector by filling up the missing components with *every possible value*
 - I.e. make many complete "clones" of the incomplete vector
- But assign a *proportion* to each value
 - Proportion is P(m|o)
 - Which can be computed if we know P(x) = P(o, m)

Gaussian estimation with incomplete vectors



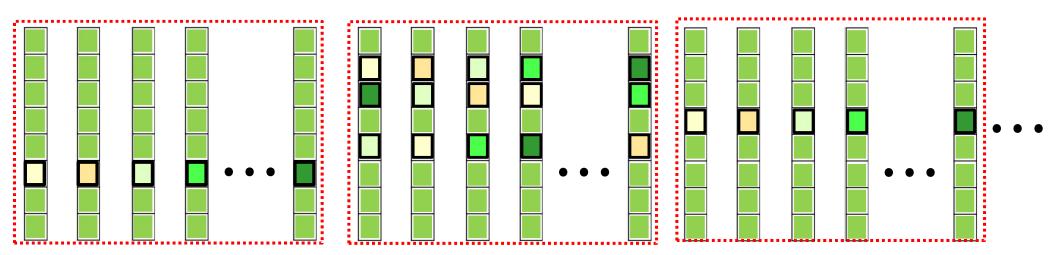
- "Expand" every incomplete vector out into all possibilities
 - In appropriate proportions P(m|o)
 - For already complete observations, there is no expansion
- Estimate the statistics from the expanded data

Gaussian estimation with incomplete vectors



- " "Expand" every incomplete vector out into all possibilities
 - In appropriate proportions P(m|o) From a previous estimate of the model
 - For already complete observations, there is no expansion
- Estimate the statistics from the expanded data

Estimating the Gaussian Parameters



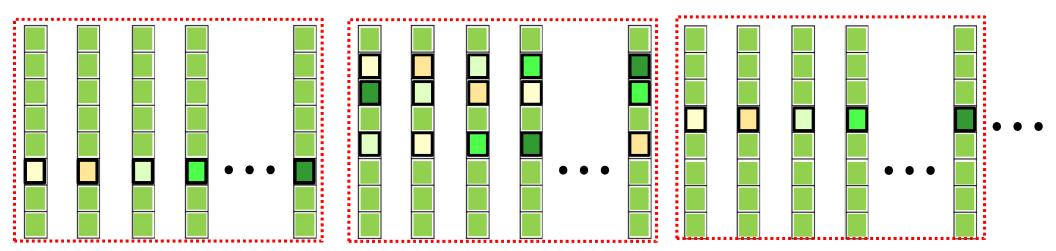
- Compute the statistics from the (proportionately) expanded set
- Let $x_i(m)$ be the "completed" version of the observation o_i , when the missing components are filled with value m

$$x_i(m) = (m, o_i)$$

- There will be one such vector for every value of m
- Estimate the statistics from the expanded data

$$\mu^{k+1} = \frac{1}{N} \sum_{o \in O} \int_{-\infty}^{\infty} P(m|o; \theta^k) x_i(m) dm$$
$$\Sigma^{k+1} = \frac{1}{N} \sum_{o \in O} \int_{-\infty}^{\infty} P(m|o; \theta^k) (x_i(m) - \mu^{k+1}) (x_i(m) - \mu^{k+1})^T dm$$

EM for computing the Gaussian Parameters



- Initial $\theta^0 = (\mu^0, \Sigma^0)$
- Until $P(0; \theta)$ converges:

$$\mu^{k+1} = \frac{1}{N} \sum_{o \in O} \int_{-\infty}^{\infty} P(m|o; \theta^k) x_i(m) dm$$

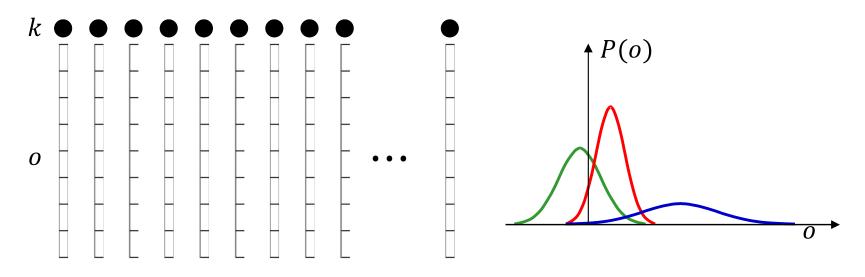
$$\Sigma^{k+1} = \frac{1}{N} \sum_{o \in O} \int_{-\infty}^{\infty} P(m|o; \theta^k) (x_i(m) - \mu^{k+1}) (x_i(m) - \mu^{k+1})^T dm$$

Where $x_i(m) = (m, o_i)$ and the parameters of $P(m|o; \theta^k)$ are derived from the $P(x; \theta^k) = Gaussian(x; \mu^k, \Sigma^k)$

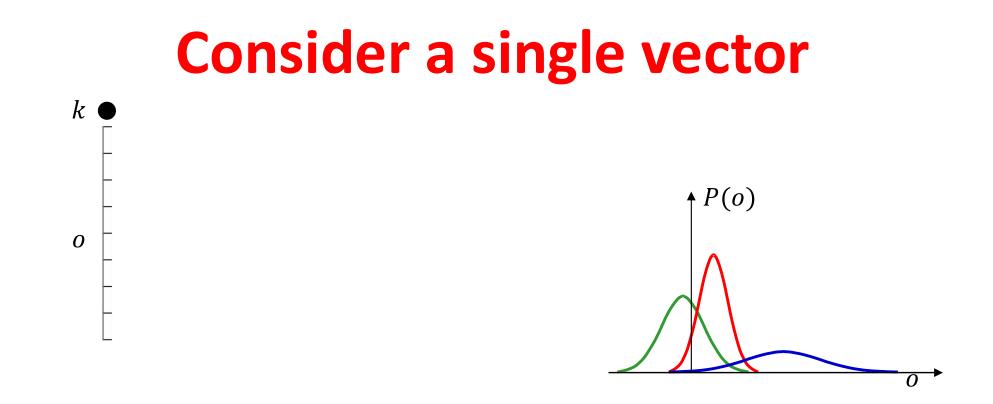
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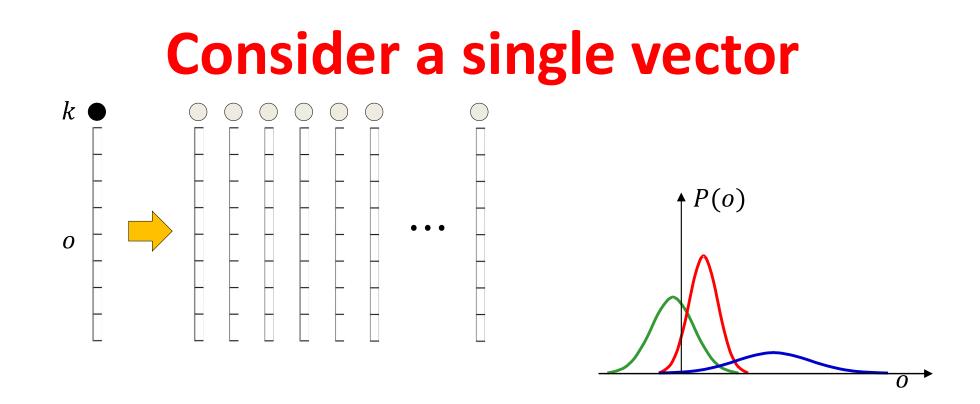
The GMM problem of incomplete data: missing information



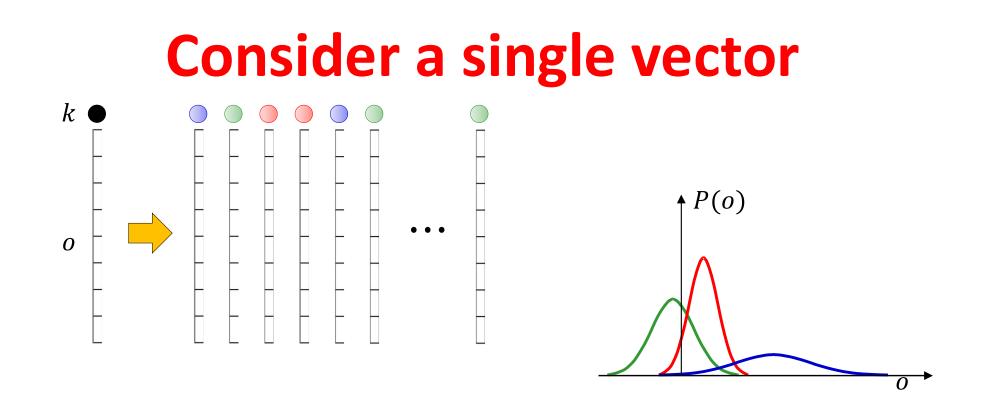
- Problem : We are not given the actual Gaussian for each observation
 - Our data are incomplete
- What we want : $(o_1, k_1), (o_2, k_2), (o_3, k_3) \dots$
- What we have: $o_1, o_2, o_3 \dots$



- Every Gaussian is capable of generating this vector
 - With different probabilities

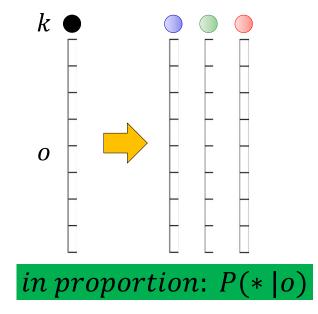


- Every Gaussian is capable of generating this vector
 With different probabilities
- If we saw a large number of these vectors, how many of these would have come from each Gaussian?



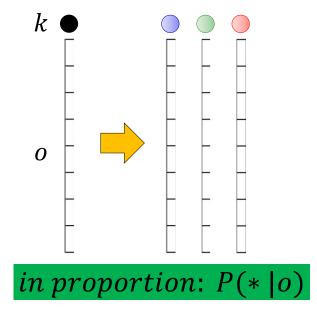
- Every Gaussian is capable of generating this vector
 - With different probabilities
- If we saw a large number of these vectors, how many of these would have come from each Gaussian
- All of them, but in proportion to P(k|o)

Completing incomplete vectors



- Complete the data by attributing to every Gaussian
 - I.e. make many complete "clones" of the data
- But assign a *proportion* to each completed vector
 - Proportion is P(k|o)
 - Which can be computed if we know P(k) and P(o|k)
- Then estimate the parameters using the complete data

Completing incomplete vectors

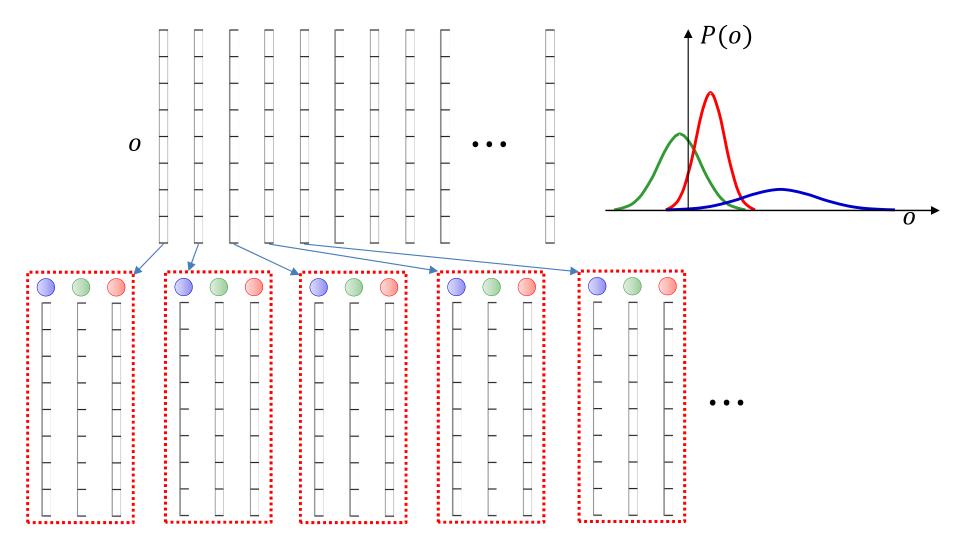


- Complete the data by attributing to every Gaussian
 - I.e. make many complete "clones" of the data

From previous estimate of model

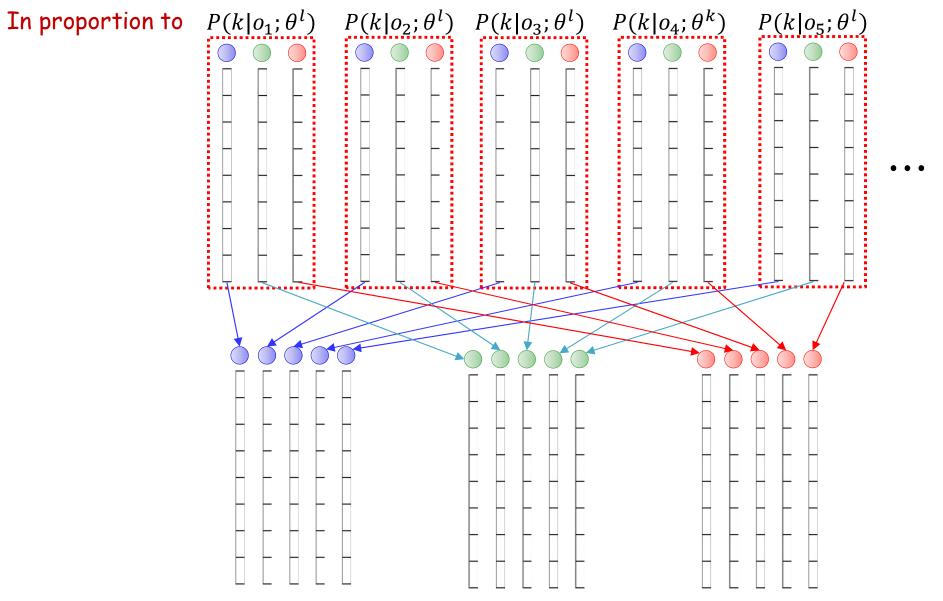
- But assign a proportion to each completed vector
 - Proportion is P(k|o)
 - Which can be computed if we know P(k) and P(o|k)
- Then estimate the parameters using the complete data

EM for GMMs



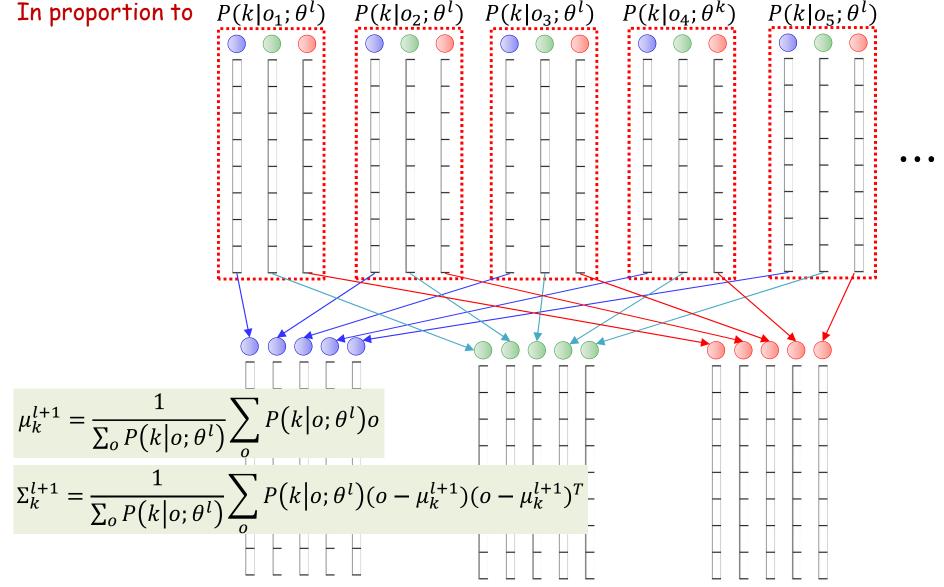
- "Complete" each vector in every possible way:
 - assign each vector to every Gaussian
 - In proportion $P(k|o; \theta^l)$ (computed from current model estimate)
- Compute statistics from "completed" data

EM for GMMs



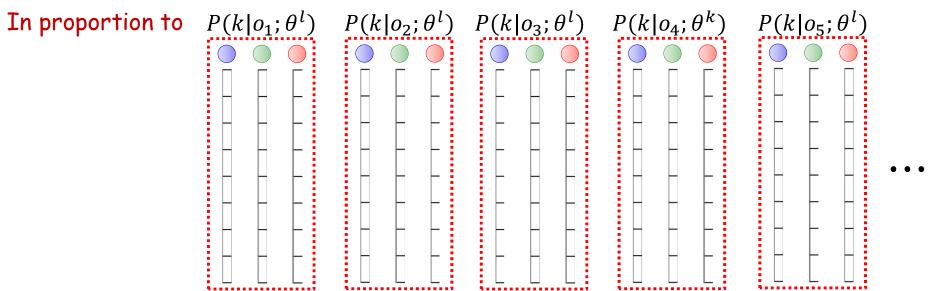
- Now you can segregate the vectors by Gaussian
 - The number of segregated complete vectors from each observation will be in proportion to $P(k|o; \theta^l)$ 59

ENT FOR GMMS The $P(k|o_1; \theta^l) P(k|o_2; \theta^l) P(k|o_3; \theta^l) P(k|o_4; \theta^k) P(k|o_4; \theta^k)$



- *Now* you can segregate the vectors by Gaussian
 - The number of segregated complete vectors from each observation will be in proportion to $P(k|o; \theta^l)$ 60

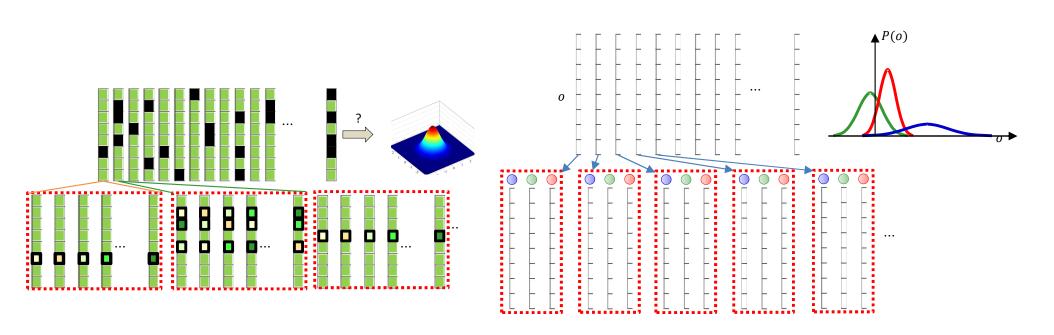
EM for GMMs



- Initialize μ_k^0 and Σ_k^0 for all k
- Iterate (over *l*):
 - Compute $P(k|o; \theta^l)$ for all o
 - Compute the proportions by which *o* is assigned to all Gaussians
 - Update:

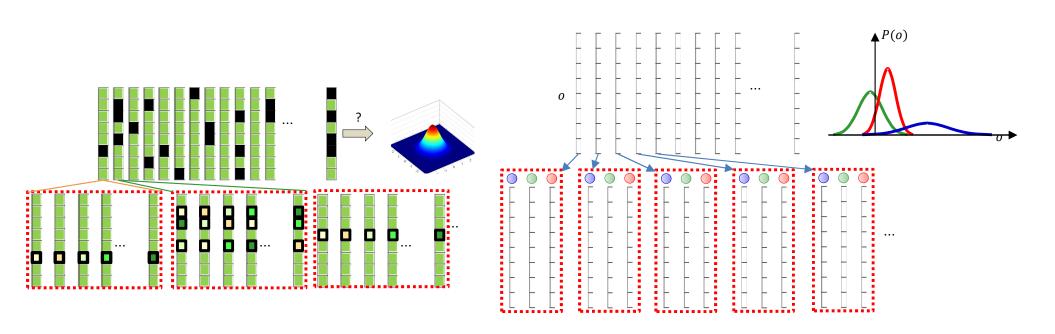
$$- \mu_{k}^{l+1} = \frac{1}{\sum_{o} P(k|o;\theta^{l})} \sum_{o} P(k|o;\theta^{l}) o$$
$$- \Sigma_{k}^{l+1} = \frac{1}{\sum_{o} P(k|o;\theta^{l})} \sum_{o} P(k|o;\theta^{l}) (o - \mu_{k}^{l+1}) (o - \mu_{k}^{l+1})^{T}$$

General EM principle



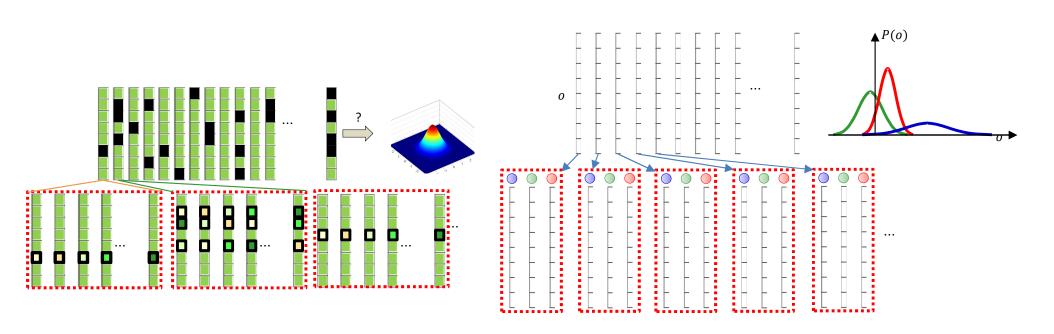
- "Complete" the data by considering *every* possible value for missing data/variables
 - In proportion to their posterior probability, given the observation, P(m|o) (or P(k|o))
- Reestimate parameters from the "completed" data

General EM principle



- "Complete" the data by considering every possible value for missing data/variables
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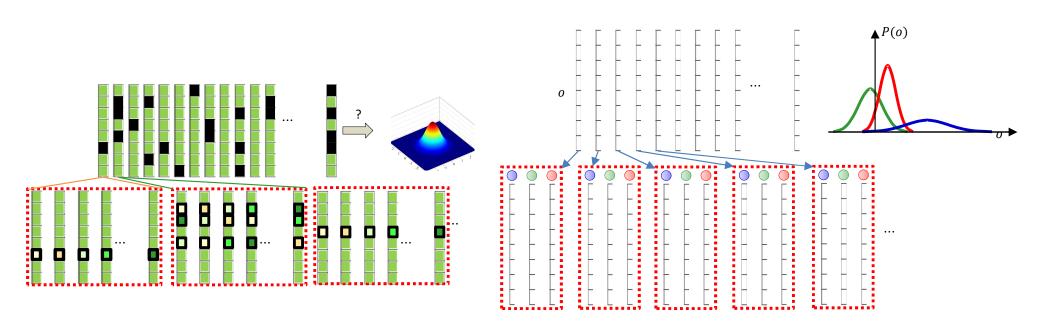
General EM principle



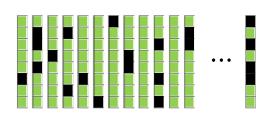
- "Complete" the data by considering *every* possible value for missing data/variables
 - In proportion to their posterior probability, given the observation, P(m|o) (or P(k|o))

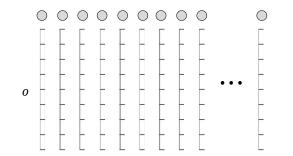
Sufficient to "complete" the data by sampling missing values from the posterior P(m|o) (or P(k|o)) instead

Alternate EM principle

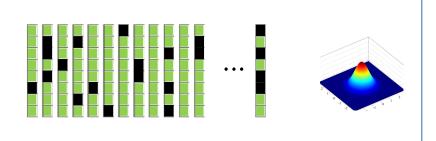


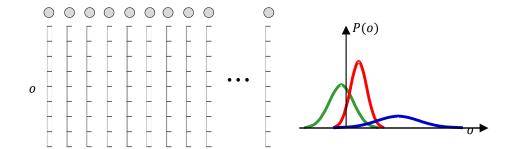
- "Complete" the data by sampling possible value for missing data/variables from P(m|o) (or P(k|o))
- Reestimate parameters from the "completed" data



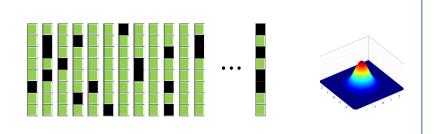


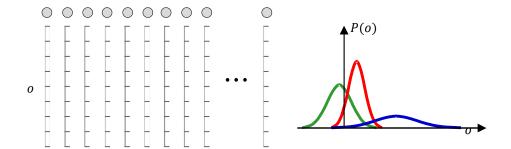
• Initially, some data/information are missing



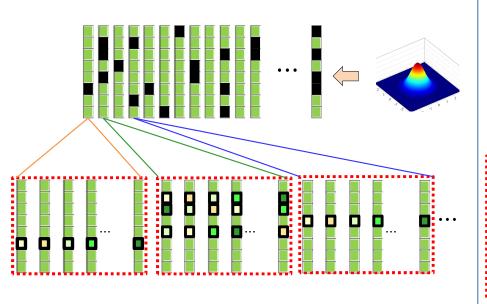


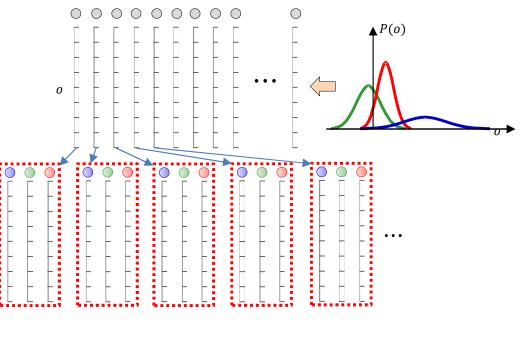
- Initially, some data/information are missing
- Initialize model parameters



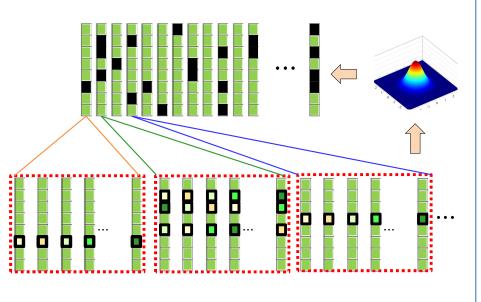


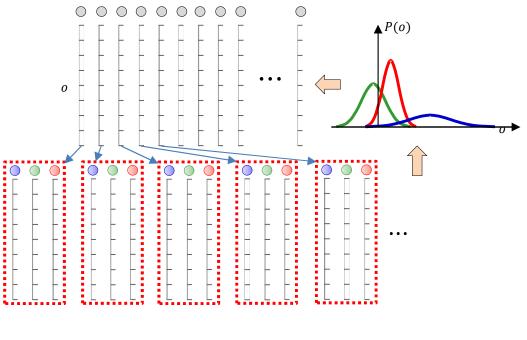
- Initially, some data/information are missing
- Initialize model parameters
- Iterate:



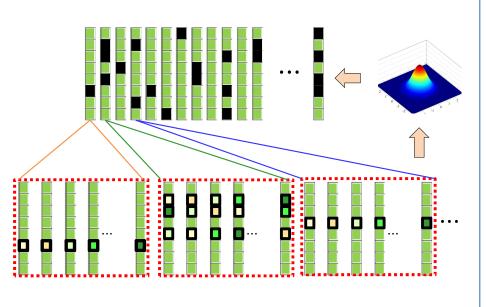


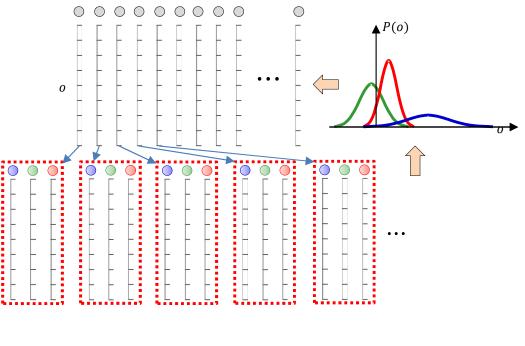
- Initially, some data/information are missing
- Initialize model parameters
- Iterate
 - Complete the data according to the posterior probabilities P(m|o) computed by the current model
 - By explicitly considering every possible value, with its posterior-based proportionality
 - Or by sampling the posterior probability distribution P(m|o)





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 - Reestimate the model





- Initially, some data/information are missing
- Initialize model parameters
- <mark>Iterate</mark>
 - Complete the data according to the posterior probabilities P(m|o) computed by the current model
 - By explicitly considering every possible value, with its posterior-based proportionality
 - Or by sampling the posterior probability distribution P(m|o)
 - Reestimate the model

Poll 2: tinyurl.com/<u>mlsp23-20231109</u>-2

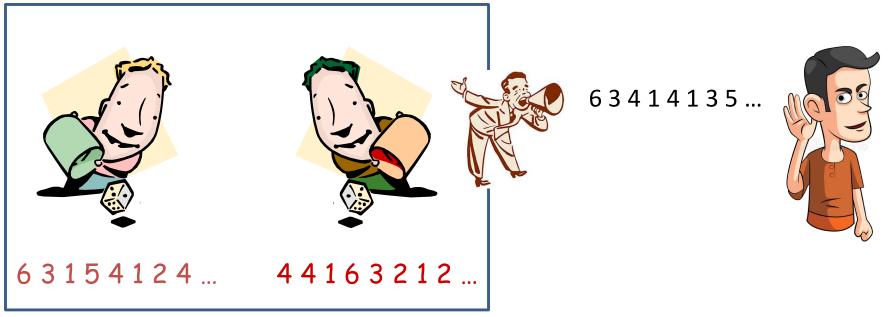
- EM attempts to "complete" the data, and estimate the model parameters with the now completed data
 - True
 - False
- It completes the data by drawing missing values in proportion to P(m|o), where o are the observed data
 - True
 - False
- Instead of attempting to complete the data with every possible value of the missing variables, we can complete them by sampling P(m|o) and reestimate the parameters with the completed data
 - True
 - False

Poll 2

- EM attempts to "complete" the data, and estimate the model parameters with the now completed data
 - True
 - False
- It completes the data by drawing missing values in proportion to P(m|o), where o are the observed data
 - True
 - False
- Instead of attempting to complete the data with every possible value of the missing variables, we can complete them by sampling P(m|o) and reestimate the parameters with the completed data
 - True
 - False

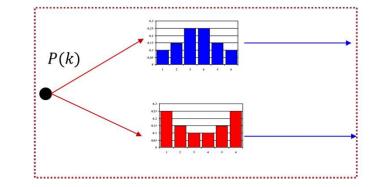
Lets try it out...

Your friendly neighborhood gamblers

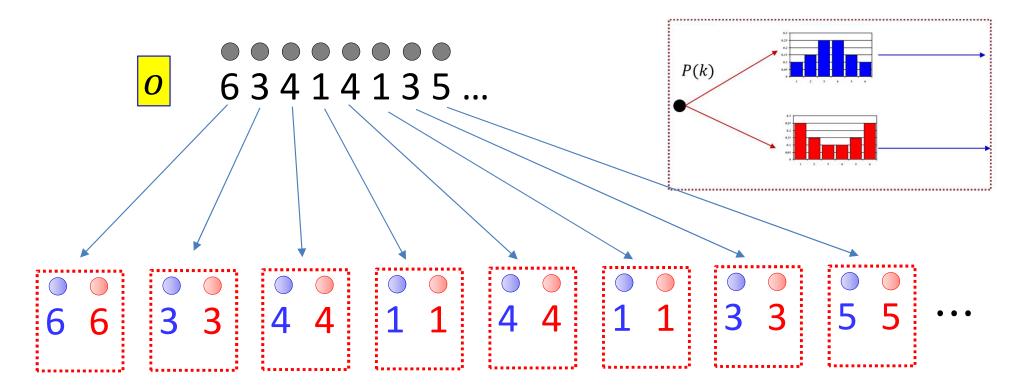


- Two gamblers shoot dice in a closed room
 - The dice are differently loaded for the two of them
- A crazy crier randomly select one of the them and calls out his number
 - But doesn't mention whose number he chose
- You only see the numbers
 - But do not know which of them rolled the number
- How to determine the probability distributions of the two dice?

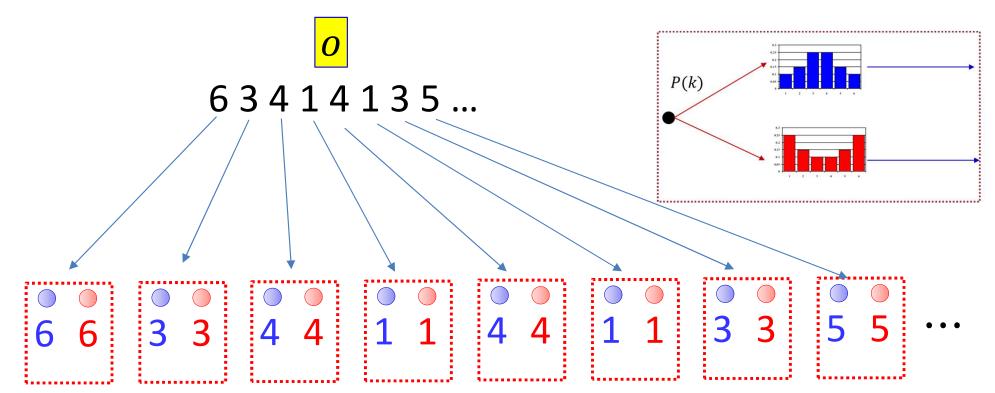




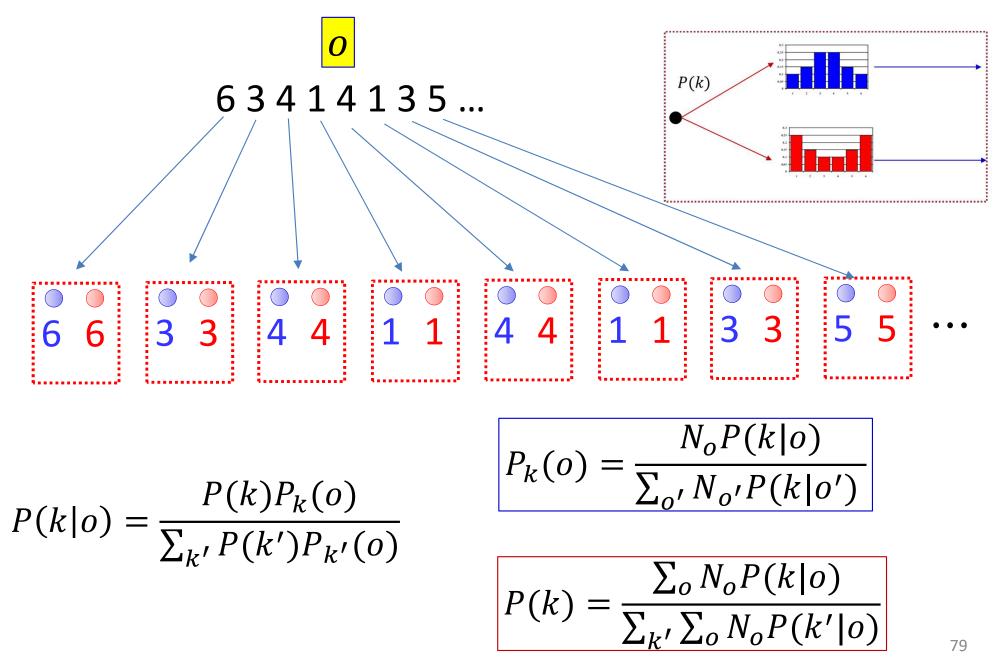
• The "color" of the dice (multinomial) is missing



- The "color" of the dice (multinomial) is missing
- "Complete" each observation in every possible way:
 - assign each vector to every multinomial
 - In proportion $P(k|o; \theta^l)$ (computed from current model estimate)
- Compute statistics from "completed" data



$$P(k|o) = \frac{P(k)P_k(o)}{\sum_{k'} P(k')P_{k'}(o)}$$



But now for something somewhat different

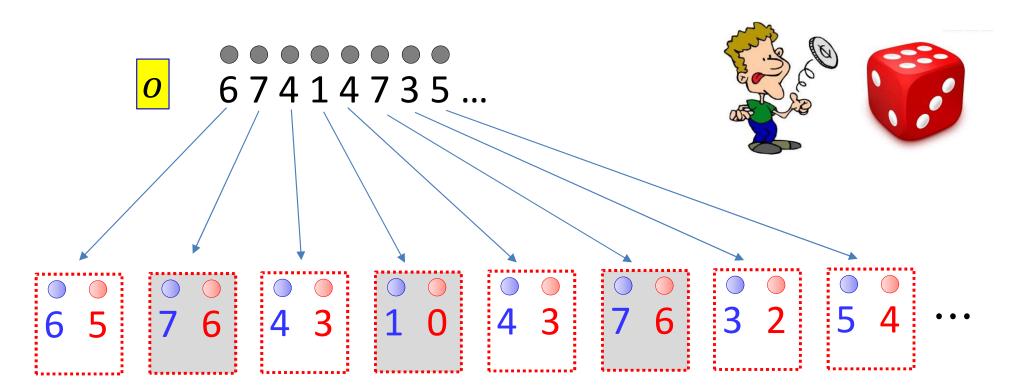


- Caller rolls a dice and flips a coin
- He calls out the number rolled if the coin shows head
- Otherwise he calls the number+1
- Can we estimate p(heads) and p(number) for the dice from a collection of outputs

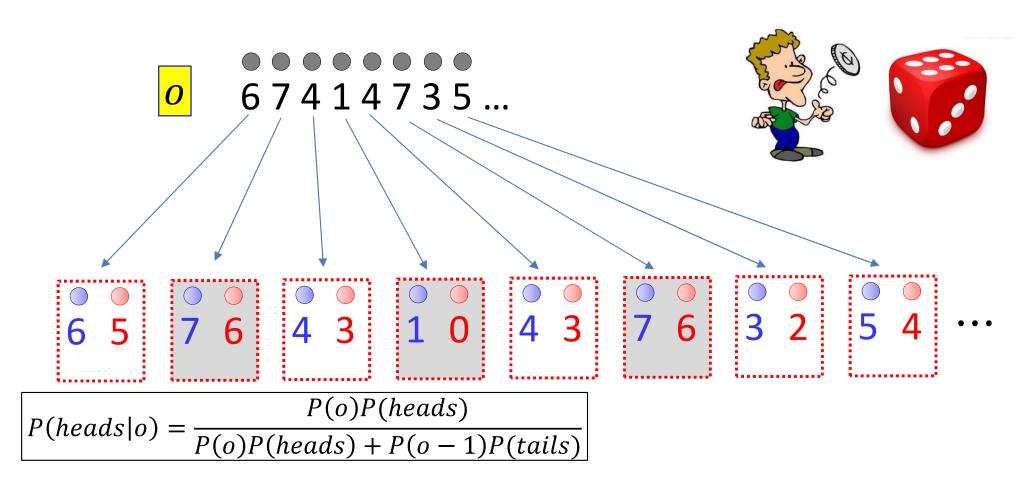


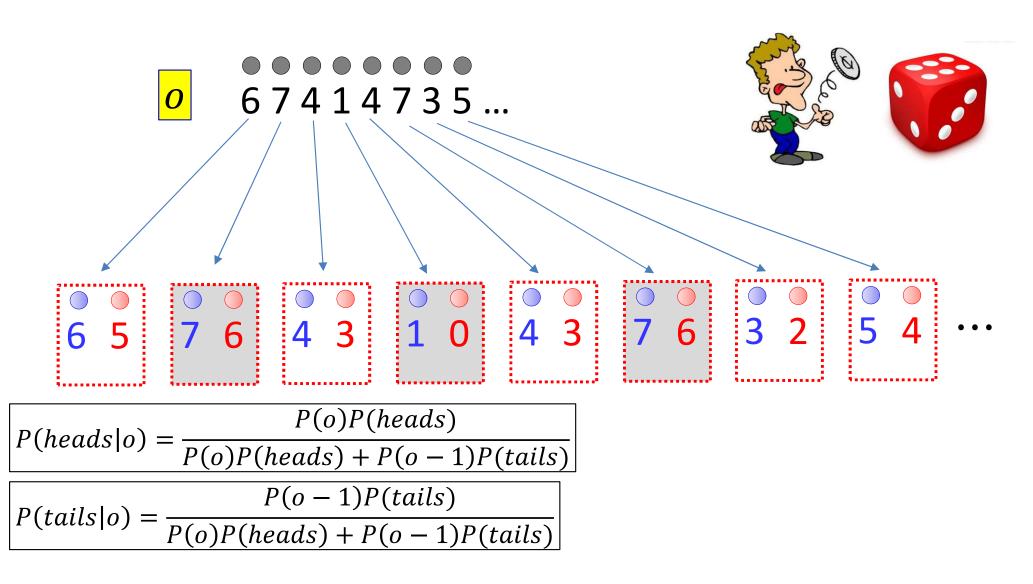


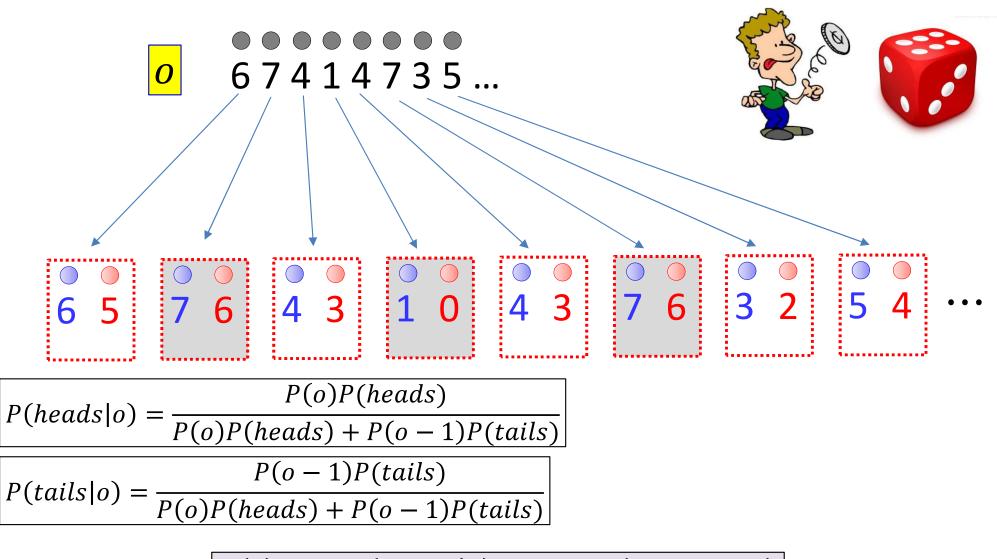
• The "face" of the coin is missing



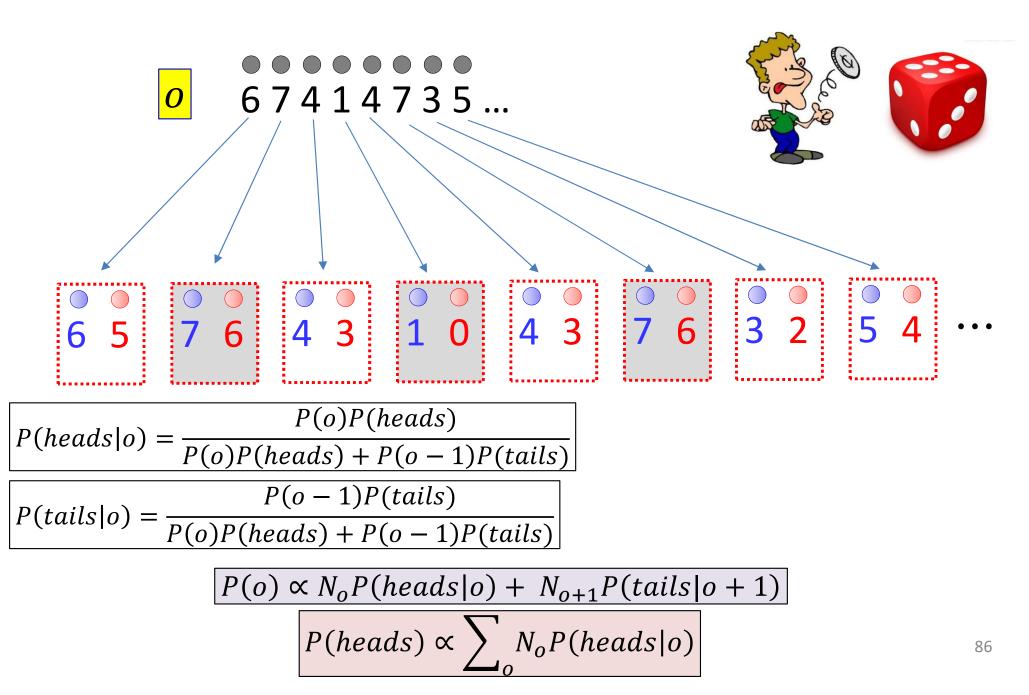
- The "face" of the coin is missing
- "Complete" each observation in every possible way:
 - assign each vector to every face
 - In proportion $P(f|o; \theta^l)$ (computed from current model estimate)
- Compute statistics from "completed" data







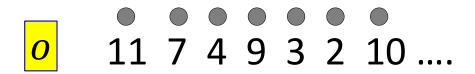
 $P(o) \propto N_o P(heads|o) + N_{o+1} P(tails|o+1)$



But now for something somewhat different

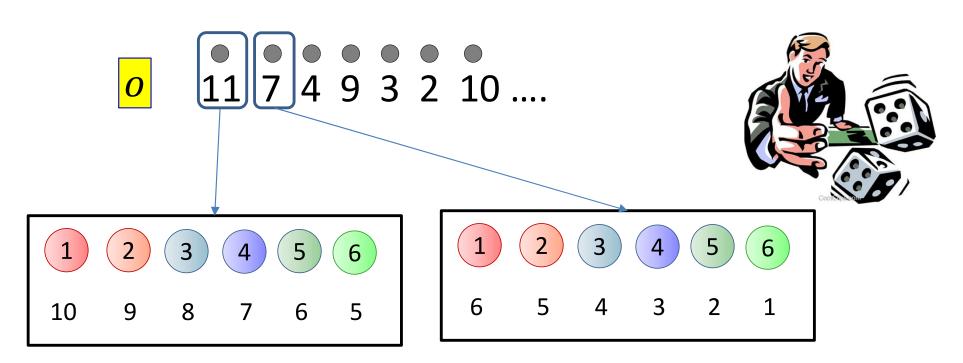


- Roller rolls two dice
- He calls out the sum
- Determine P(dice) from a collection of outputs



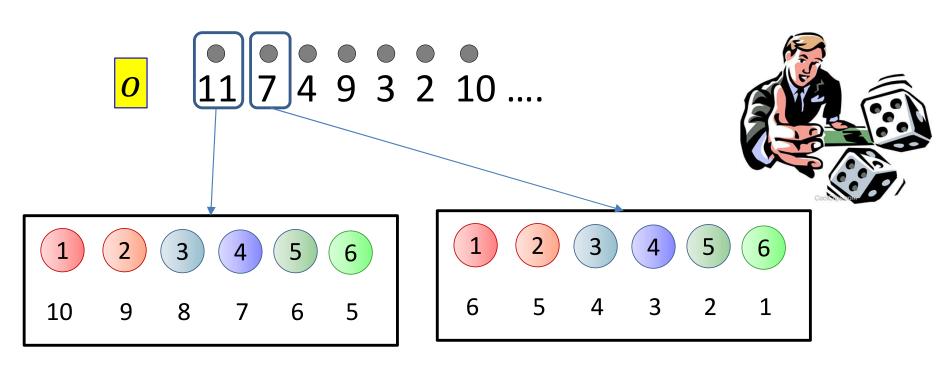


• The "first" dice info is missing

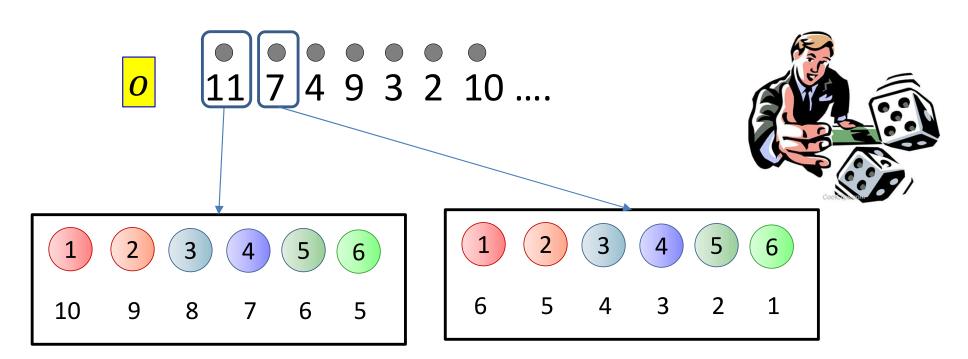


- The "first" dice info is missing
- Assign it to every value for the first dice

But note what happens to the second



$$P(n|o) = P(n, o - n|o) = \frac{P_1(n)P_2(o - n)}{\sum_{m=1}^6 P_1(m)P_2(o - m)}$$



$$P(n, o - n|o) = \frac{P_1(n)P_2(o - n)}{\sum_{m=1}^6 P_1(m)P_2(o - m)}$$

$$P_1(n) \propto \sum_{o=2}^{12} N_k P(n, o - n|o)$$

Poll 3: tinyurl.com/<u>mlsp23-20231109</u>-3

- The EM algorithm can be applied in any problem with missing data
 - True
 - False
- EM can also be applied when the observed data are drawn from the distribution obtained through the convolution of two component distributions which must be estimated
 - True
 - False

Poll 3

- The EM algorithm can be applied in any problem with missing data
 - True
 - False
- EM can also be applied when the observed data are drawn from the distribution obtained through the convolution of two component distributions which must be estimated
 - True
 - False

In closing

 Have seen a method for learning the parameters of generative models when some components of the data (or the underlying drawing process) are not observed

- The technique operates by "completing" incomplete data by filling in missing values in proportion to their posterior probabilities
- Coming up : apply this concept to various problems