

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

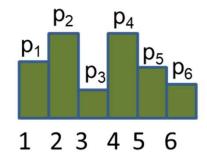
$$P(x = k) = \frac{\lambda^k e^{-\lambda}}{k!} \text{ for } k \ge 0$$

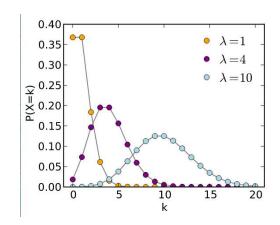
- λ is the Poisson parameter
- The Gaussian PDF

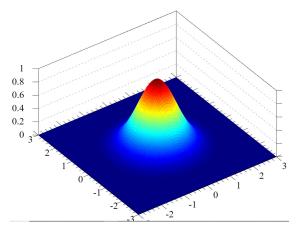
$$P(x = v)$$

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

- For continuous-valued data
- $-\mu$ is the mean of the distribution
- Σ 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

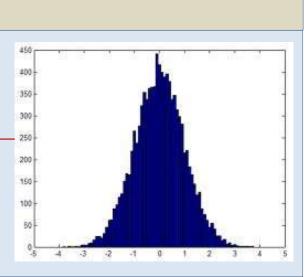
- The maximum likelihood principle:
 - $\operatorname{argmax}_{\theta} P(X; \theta) = \operatorname{argmax}_{\theta} \log(P(X; \theta))$
- For the histogram
 - $\underset{\{p_1,p_2,p_3,p_4,p_5,p_6\}}{\operatorname{argmax}} \sum_{i} n_i \log(p_i) \leftarrow$
 - $\Rightarrow p_i = \frac{n_i}{N}$ (N is the total number of observations)



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

$$\Rightarrow \mu = \frac{1}{N} \sum_{x \in X} x$$
;

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



 n_4

 n_3

1 2 3 4 5 6

 n_5

The missing-info challenge

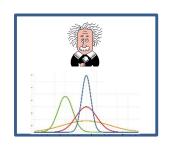
 In some estimation problems there is often some information missing





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





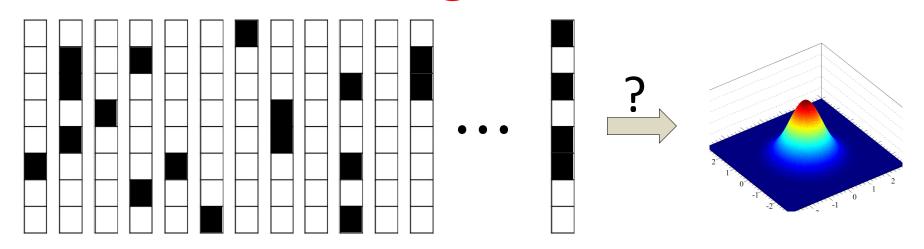
Let's Look at Missing Information

Missing Information about **Underlying Data**

Missing Information about **Underlying Process**

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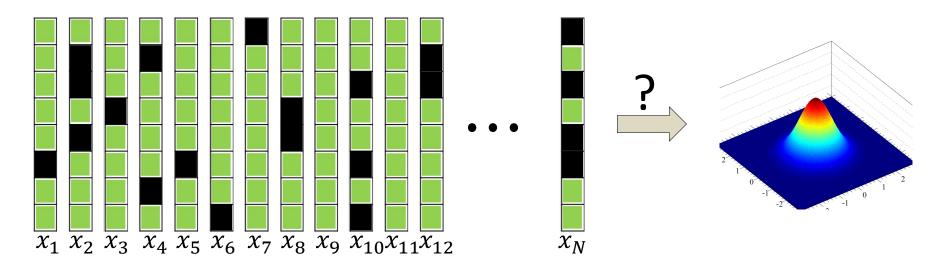
Examples of incomplete data:missing data



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

Let's Look at Missing Information

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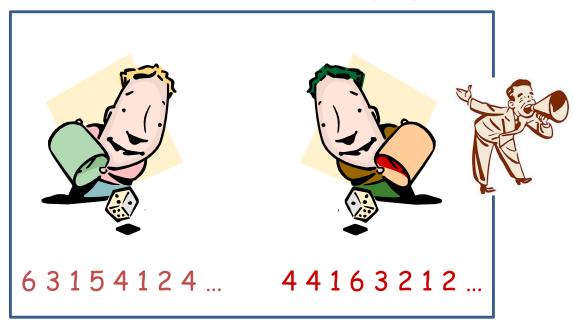
Let's Look at Missing Information

Missing Information about **Underlying Data**

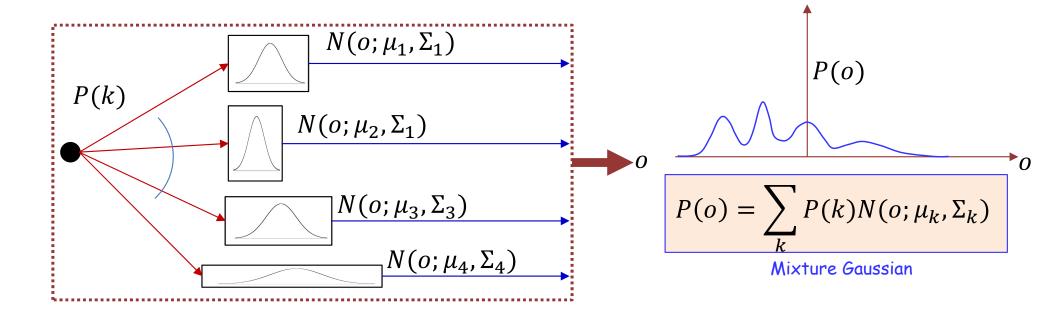
Missing Information about **Underlying Process**

Shooting Dice

General Mixtures



- 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

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

Solution: Iteratively perform the following optimization instead

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

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

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Expectation Maximization

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

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

Maximization step

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

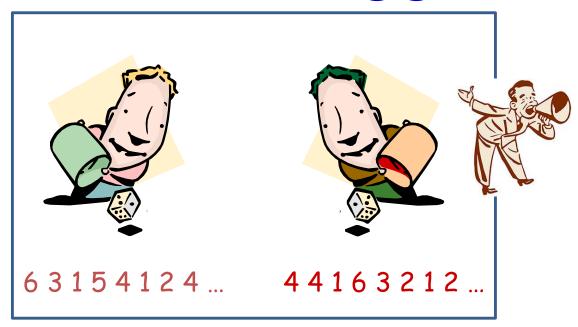
Expectation Maximization

• Initialize θ^0

Let's put this to work

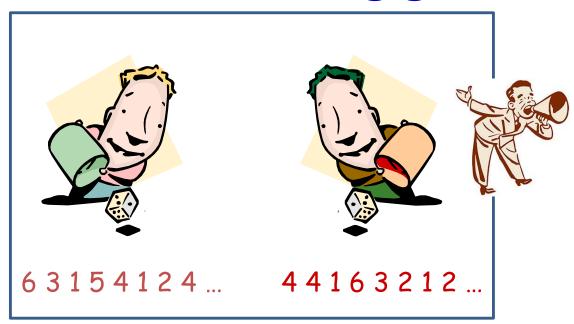
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 - Maximization step

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



$$P(k,o) = P(k)P_k(o)$$

$$P(o) = \sum_{k} P(k)P_k(o)$$



$$P(k,o) = P(k)P_k(o)$$

$$P(o) = \sum_{k} P(k)P_k(o)$$

$$P(k|o) = \frac{P(k)P(o|k)}{P(o)}$$

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

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

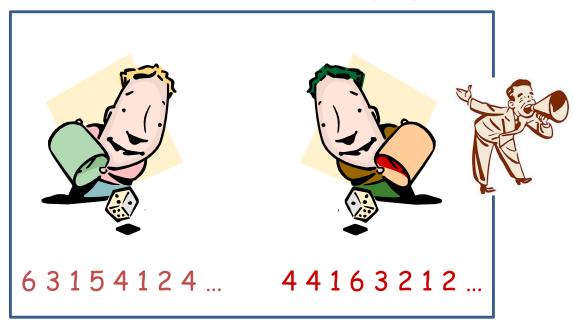
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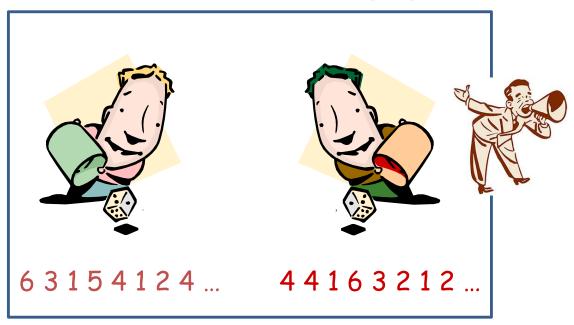
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 - Maximization step

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



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

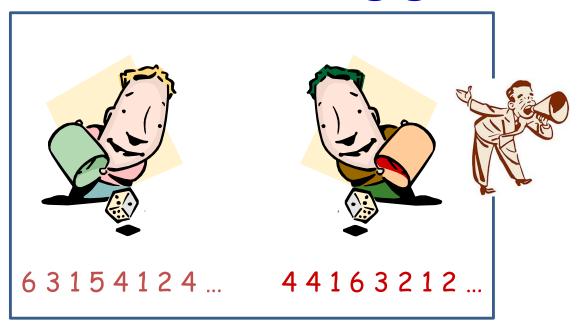
$$\underset{\theta}{\operatorname{argmax}} \sum_{o \in O} \sum_{k} P_{cur}(k|o) \log P(k) P_{k}(o)$$



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

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

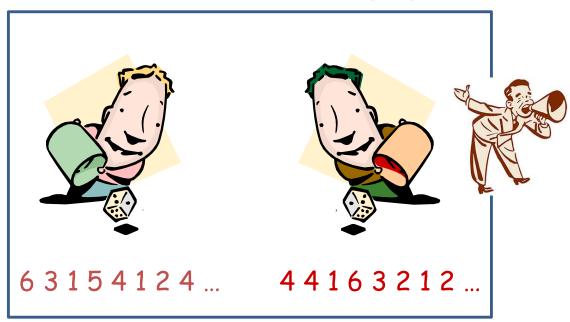
Differentiate and equate to 0



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

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

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



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



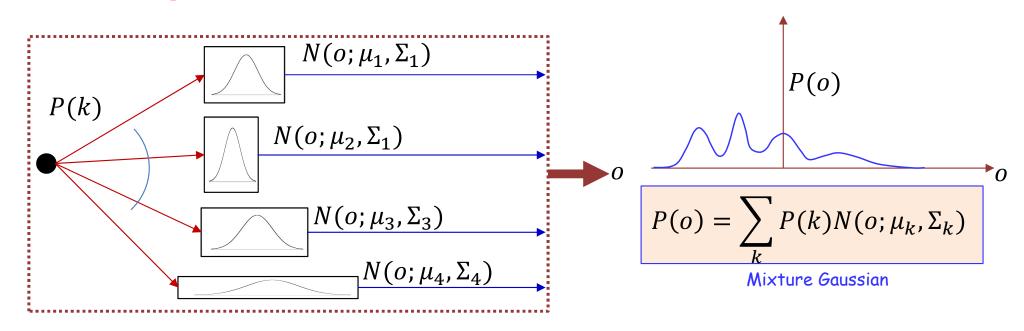
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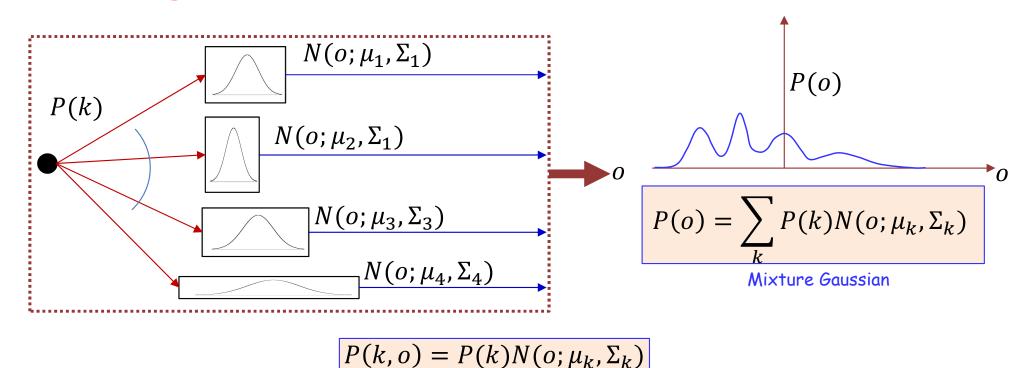
E

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Examples of incomplete data: missing information in Gaussian mixtures



Examples of incomplete data: missing information in Gaussian mixtures



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

Expectation Maximization

• Initialize θ^0

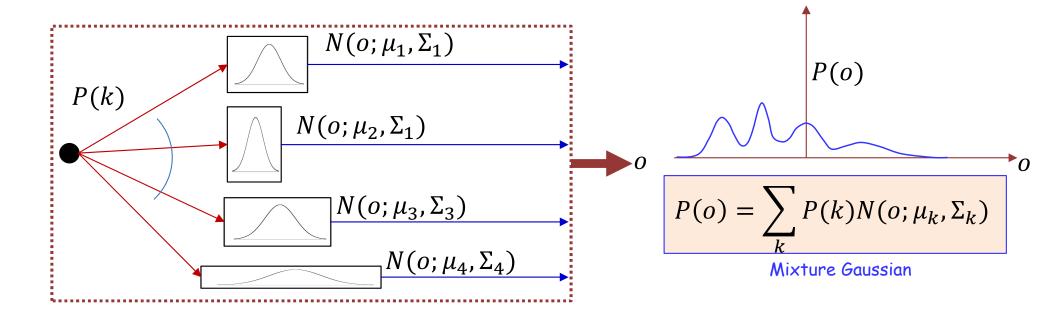
Let's put this to work

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



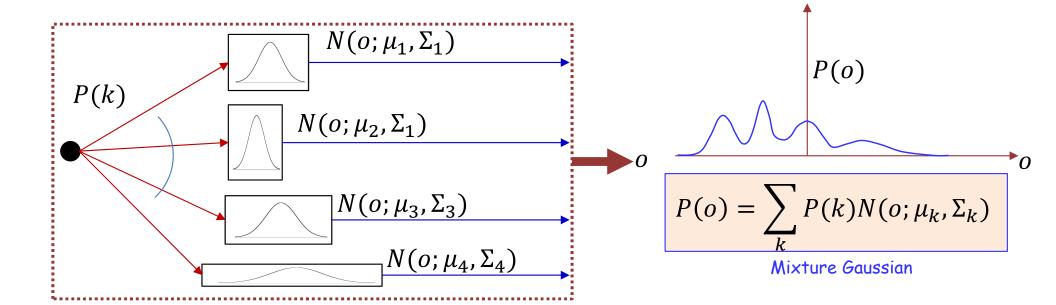
$$\underset{\theta}{\operatorname{argmax}} \sum_{o \in O} \sum_{h} P(h|o; \theta^{l}) \log P(h, o; \theta)$$

$$\underset{\{P(k),\mu_k,\Sigma_k\}}{\operatorname{argmax}} \sum_{o \in O} \sum_k P(k \mid o; \theta^l) (\log P(k) + \log N(o; \mu_k, \Sigma_k)) + \lambda \left(\sum_k P(k) - 1\right)$$

Differentiate and equate to 0

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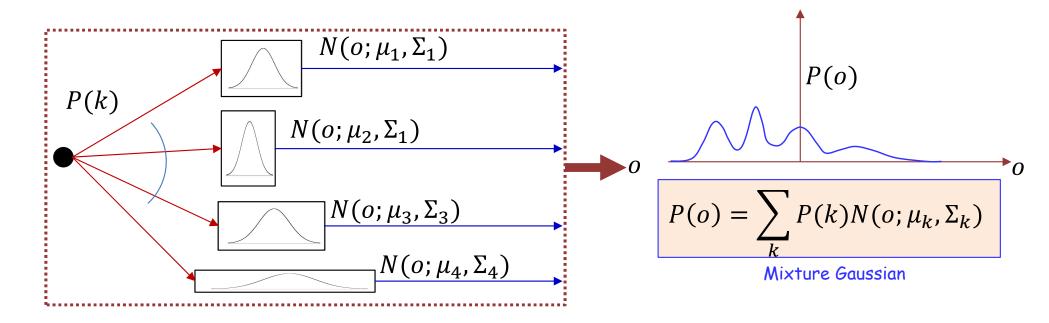
32



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

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

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



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

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E

M

Poll 1: tinyurl.com/mlsp22-20221110-1

- 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

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 - 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?

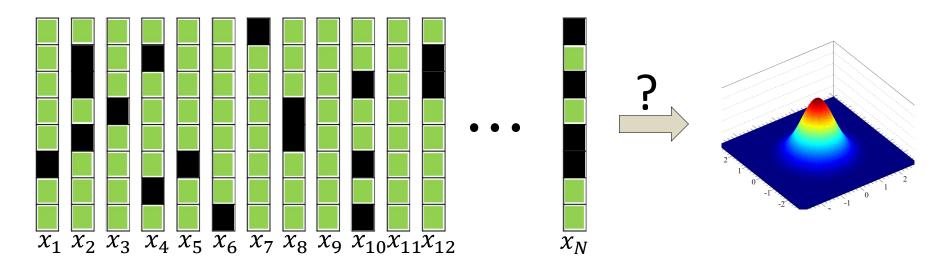
Missing Information about **Underlying Data**

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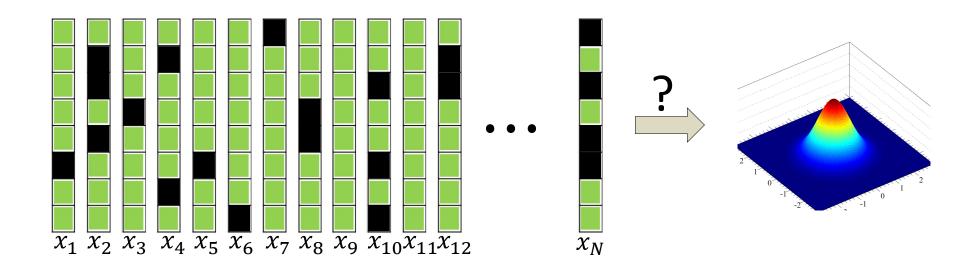
Recall this: Gaussian estimation with incomplete vectors



- 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 $M = \{m_1, ..., m_N\}$
 - Comprising the missing components of the data
- The complete data includes both the observed and missing components

$$X = \{x_1, \dots, x_N\}, \qquad x_i = (o_i, m_i)$$

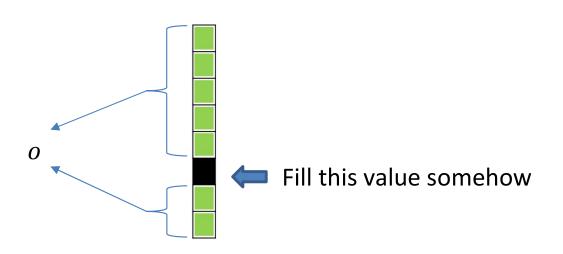
Keep in mind that at the complete data are not available (the missing components are missing)

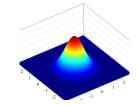


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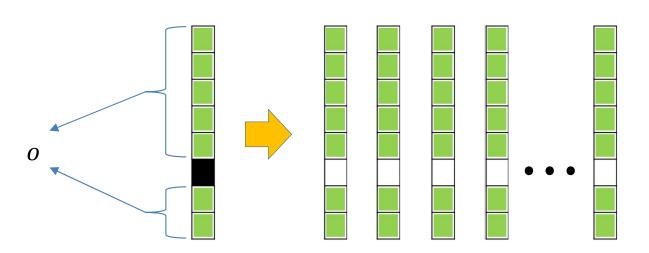
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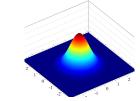
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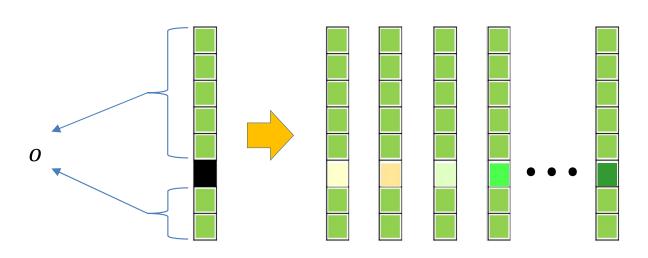


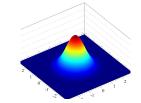
- We will try to complete the vector by filling in the missing value with plausible values that match the observed components
- Plausible: Values that "go with" the observed values, according to the distribution of the data





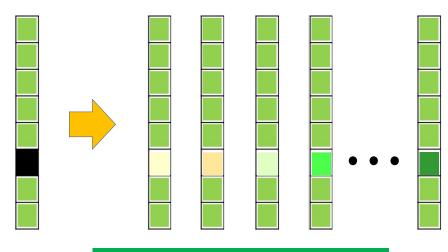
 Question: If we have a very large number of vectors from the Gaussian, all with the same observed components o, what would their missing components be?





- 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)

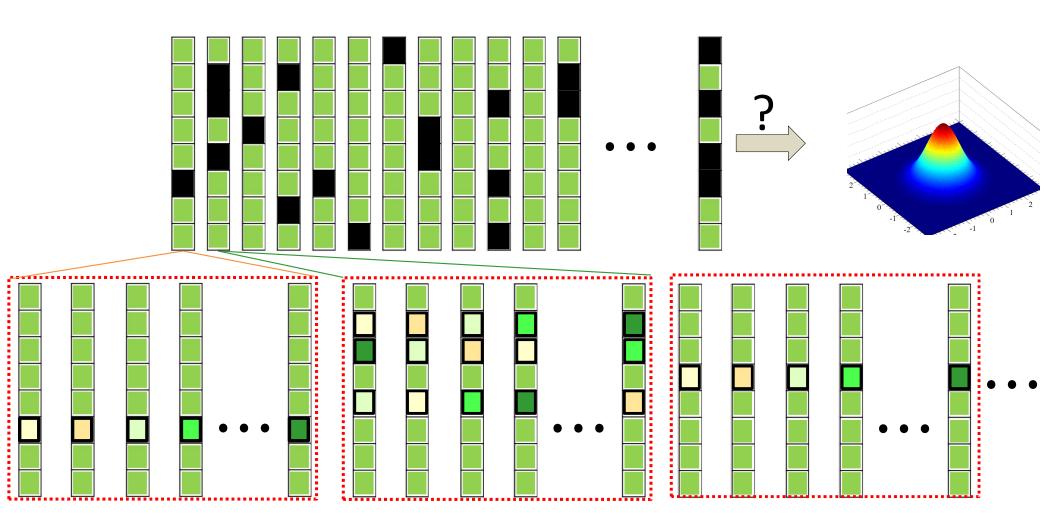
Completing incomplete vectors



in proportion: P(* | o)

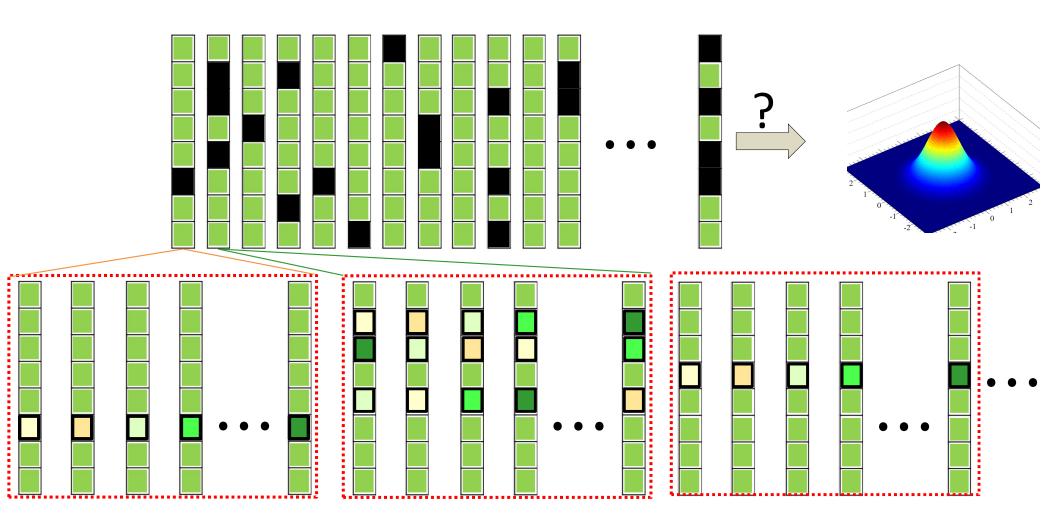
- Complete vector by filling up the missing components with every possible value
 - I.e. make many complete "clones" of the incomplete vector
- But assign a proportion to each value
 - Proportion is P(m|o)
 - Which can be computed if we know P(x) = P(o, m)

Gaussian estimation with incomplete vectors



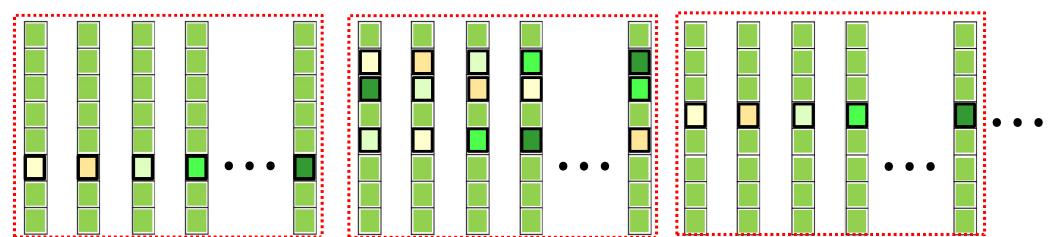
- "Expand" every incomplete vector out into all possibilities
 - In appropriate proportions P(m|o)
 - For already complete observations, there is no expansion
- Estimate the statistics from the expanded data

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

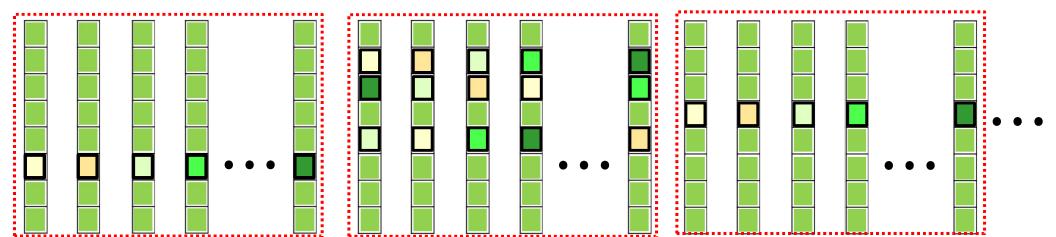
$$x_i(m) = (m, o_i)$$

- $-\hspace{0.5cm}$ 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:

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

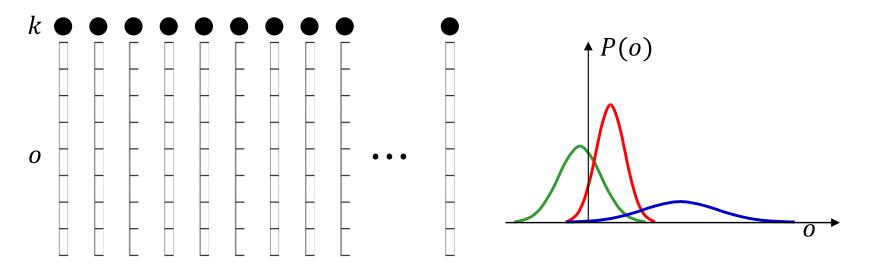
$$\Sigma^{k+1} = \frac{1}{N} \sum_{o \in O} \int_{-\infty}^{\infty} P(m|o; \theta^k) (x_i(m) - \mu^{k+1}) (x_i(m) - \mu^{k+1})^T dm$$

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

Missing Information about **Underlying Data**

Missing Information about **Underlying Process**

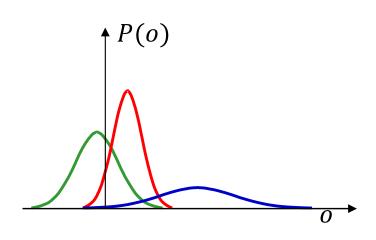
The GMM problem of incomplete data: missing information



- 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 ...

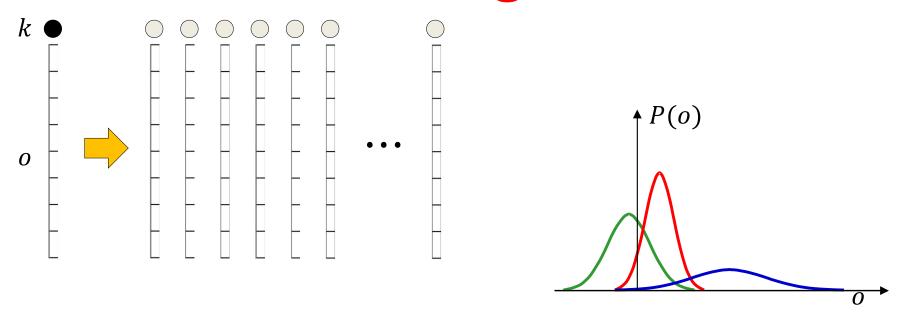
Consider a single vector





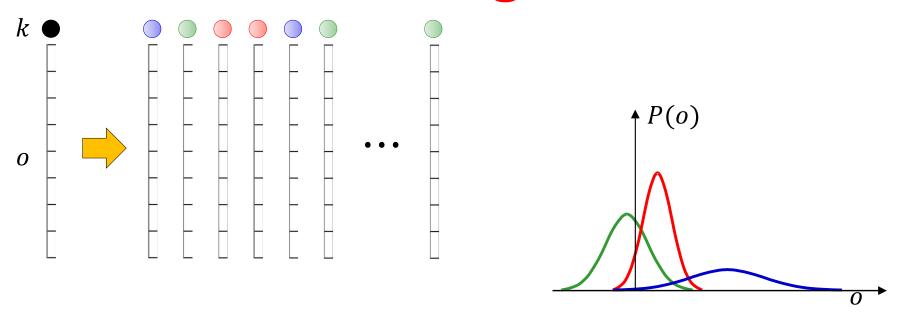
- Every Gaussian is capable of generating this vector
 - With different probabilities

Consider a single vector



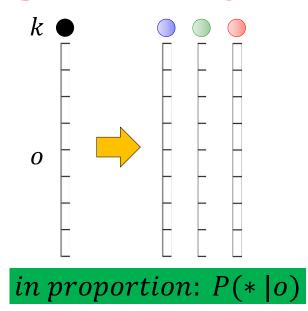
- Every Gaussian is capable of generating this vector
 - With different probabilities
- If we saw a large number of these vectors, how many of these would have come from each Gaussian?

Consider a single vector



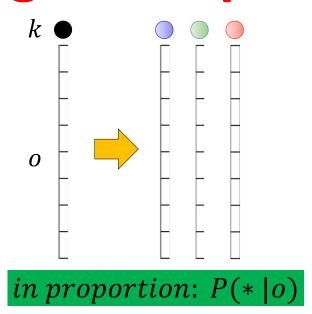
- Every Gaussian is capable of generating this vector
 - With different probabilities
- If we saw a large number of these vectors, how many of these would have come from each Gaussian
- All of them, but in proportion to P(k|o)

Completing incomplete vectors



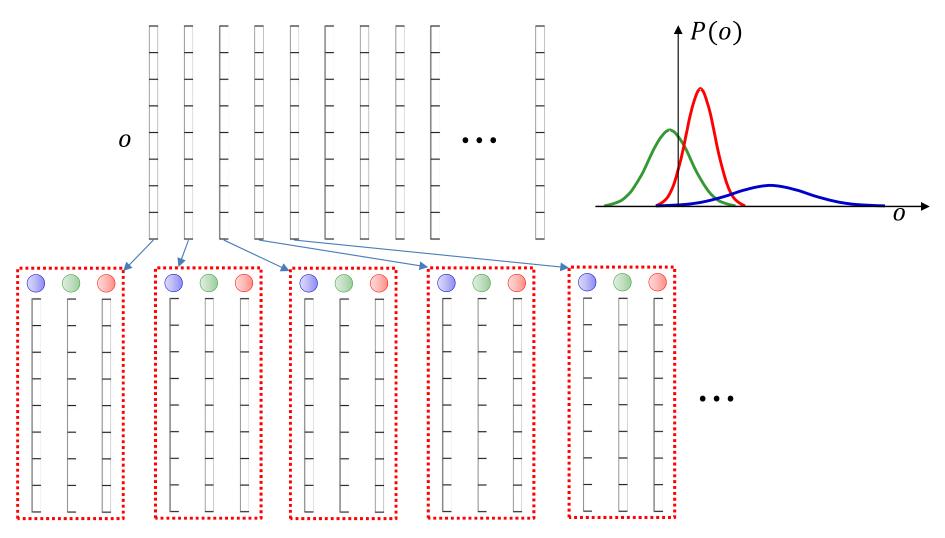
- Complete the data by attributing to every Gaussian
 - I.e. make many complete "clones" of the data
- But assign a proportion to each completed vector
 - Proportion is P(k|o)
 - Which can be computed if we know P(k) and P(o|k)
- Then estimate the parameters using the complete data

Completing incomplete vectors

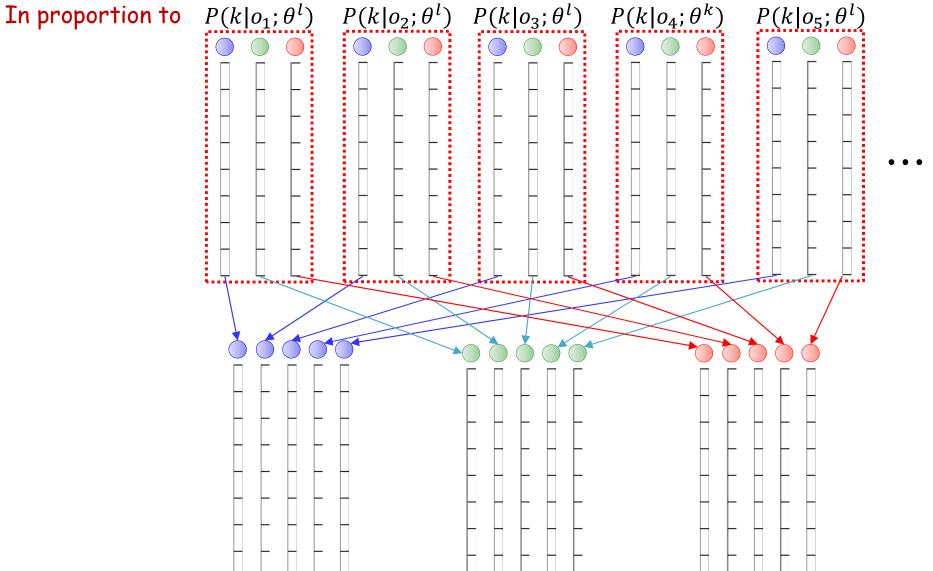


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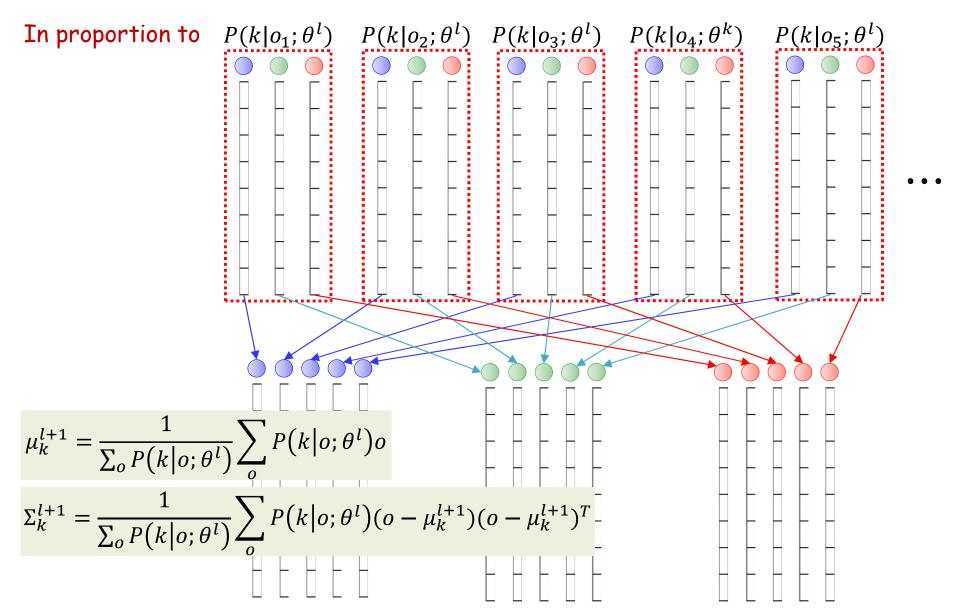
From previous estimate of model



- "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

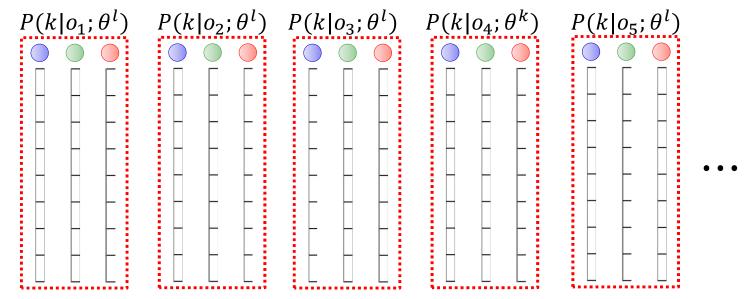


- Now you can segregate the vectors by Gaussian
 - The number of segregated complete vectors from each observation will be in proportion to $P(k|o;\theta^l)$



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 - The number of segregated complete vectors from each observation will be in proportion to $P(k|o;\theta^l)$

In proportion to $P(k|o_1; \theta^l)$

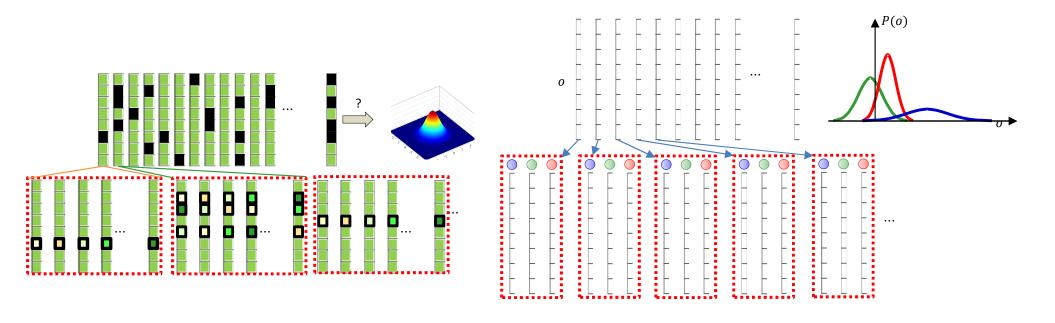


- Initialize μ_k^0 and Σ_k^0 for all k
- Iterate (over *l*):
 - Compute $P(k|o; \theta^l)$ for all o
 - Compute the proportions by which o is assigned to all Gaussians
 - Update:

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

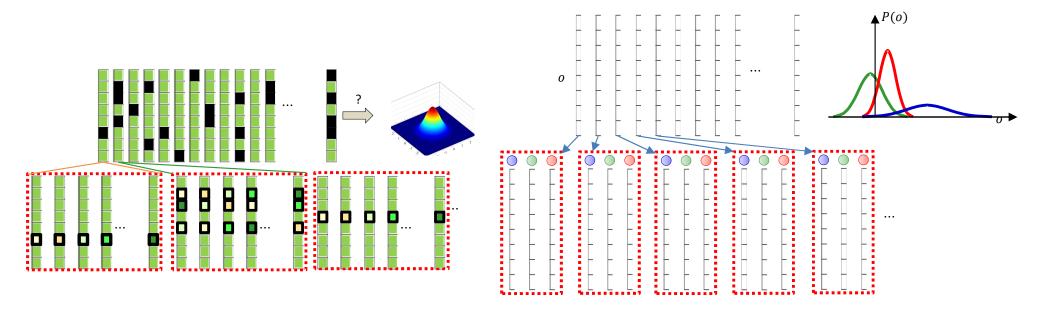
$$- \Sigma_k^{l+1} = \frac{1}{\sum_{o} P(k|o; \theta^l)} \sum_{o} P(k|o; \theta^l) (o - \mu_k^{l+1}) (o - \mu_k^{l+1})^T$$

General EM principle



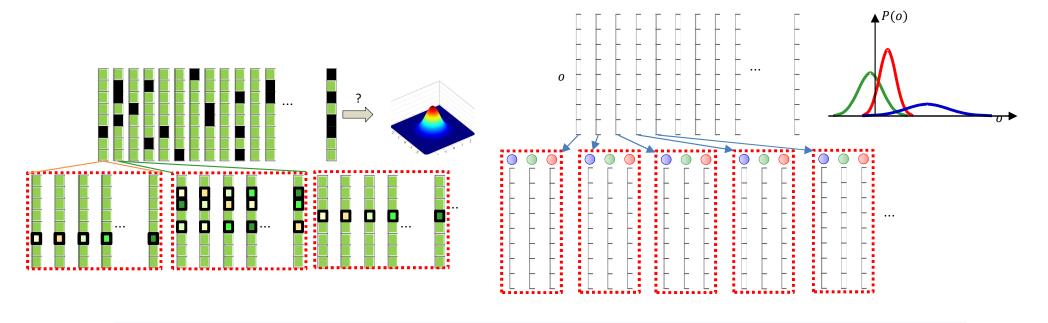
- "Complete" the data by considering every possible value for missing data/variables
 - In proportion to their posterior probability, given the observation, P(m|o) (or P(k|o))
- Reestimate parameters from the "completed" data

General EM principle



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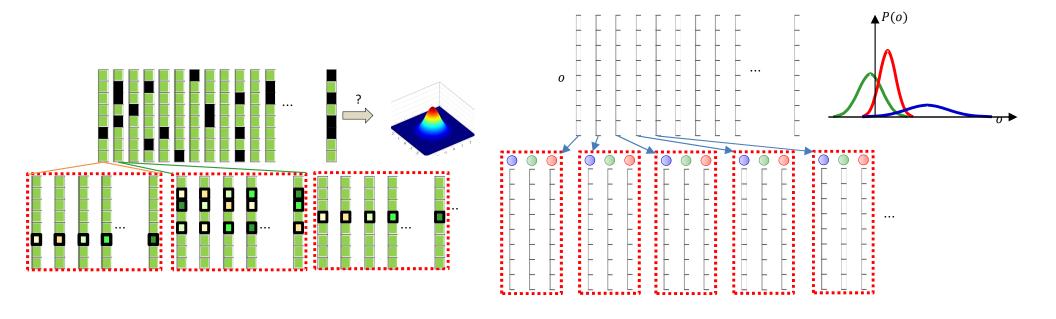
General EM principle



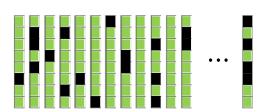
- "Complete" the data by considering every possible value for missing data/variables
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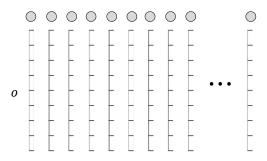
Sufficient to "complete" the data by sampling missing values from the posterior P(m|o) (or P(k|o)) instead

Alternate EM principle

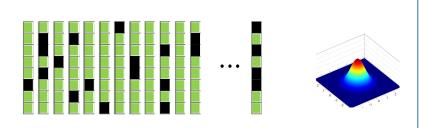


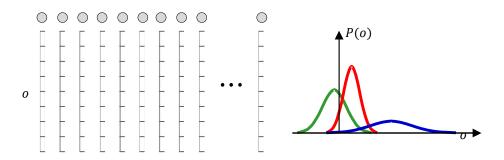
- "Complete" the data by sampling possible value for missing data/variables from P(m|o) (or P(k|o))
- Reestimate parameters from the "completed" data



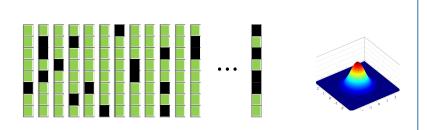


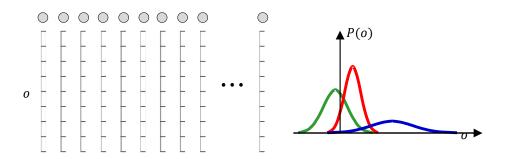
Initially, some data/information are missing



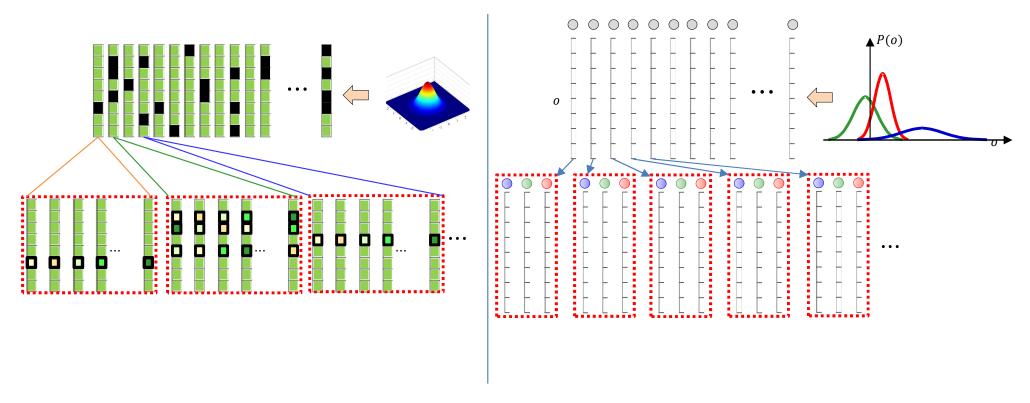


- Initially, some data/information are missing
- Initialize model parameters

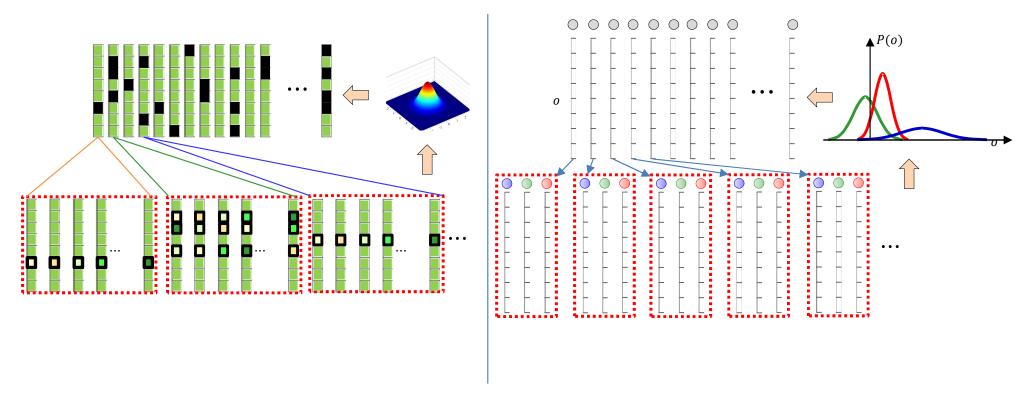




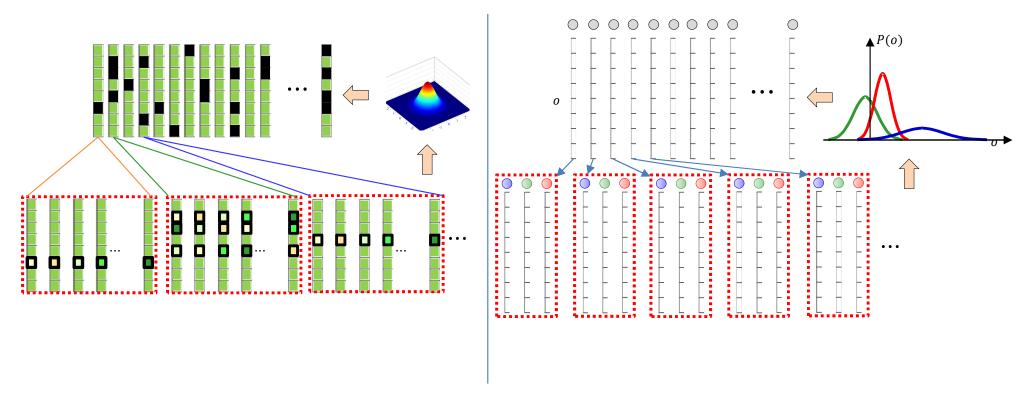
- Initially, some data/information are missing
- Initialize model parameters
- Iterate:



- 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

Poll 2: tinyurl.com/mlsp22-20221110-2

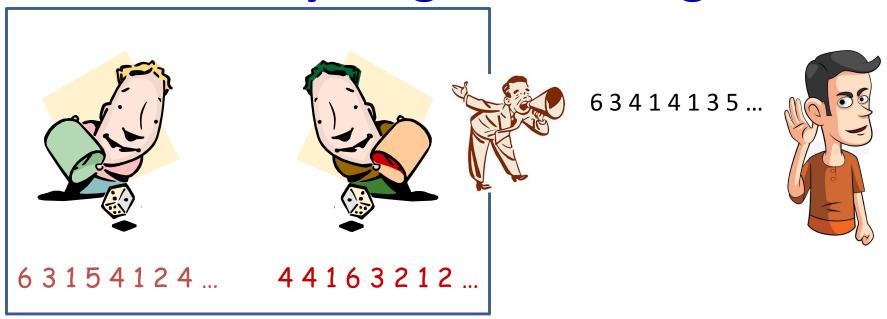
- EM attempts to "complete" the data, and estimate the model parameters with the now completed data
 - True
 - False
- It completes the data by drawing missing values in proportion to P(m|o), where o are the observed data
 - True
 - False
- Instead of attempting to complete the data with every possible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

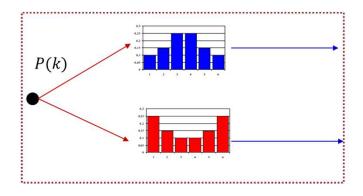
Your friendly neighborhood gamblers



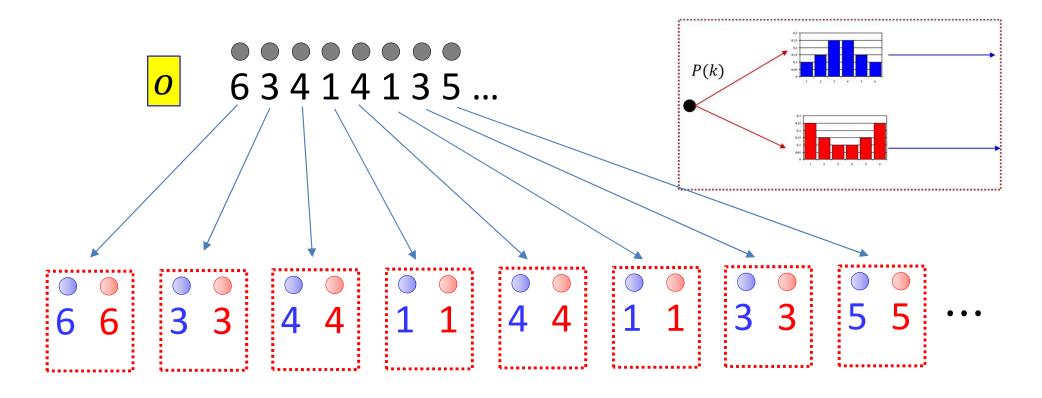
- Two gamblers shoot dice in a closed room
 - The dice are differently loaded for the two of them
- A crazy crier randomly select one of the them and calls out his number
 - But doesn't mention whose number he chose
- You only see the numbers
 - But do not know which of them rolled the number.
- How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

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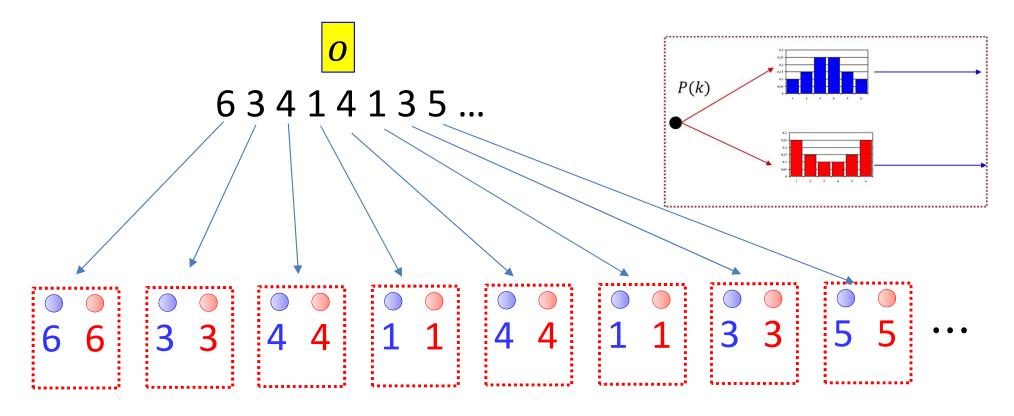
0 63414135...



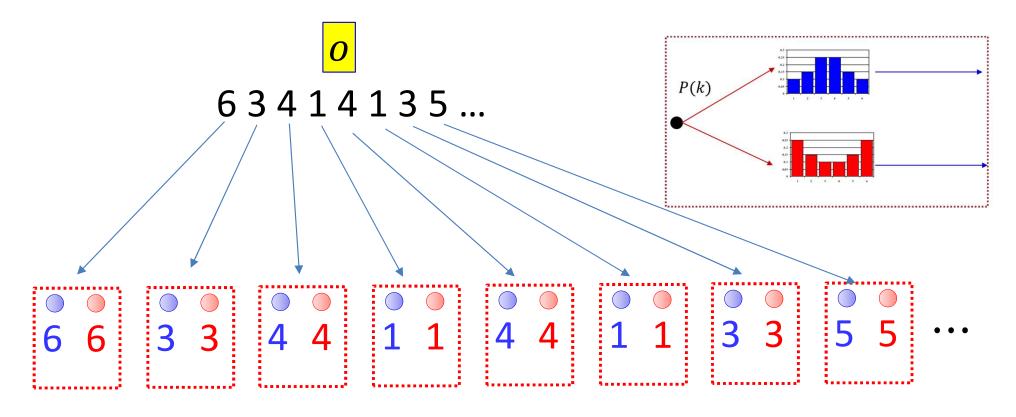
• The "color" of the dice (multinomial) is missing



- 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



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



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

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

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

But now for something somewhat different

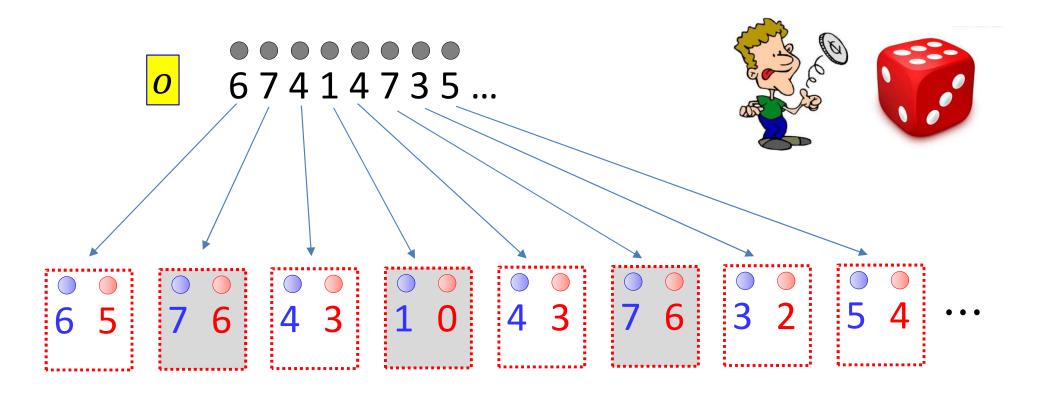


- Caller rolls a dice and flips a coin
- He calls out the number rolled if the coin shows head
- Otherwise he calls the number+1
- Can we estimate p(heads) and p(number) for the dice from a collection of outputs

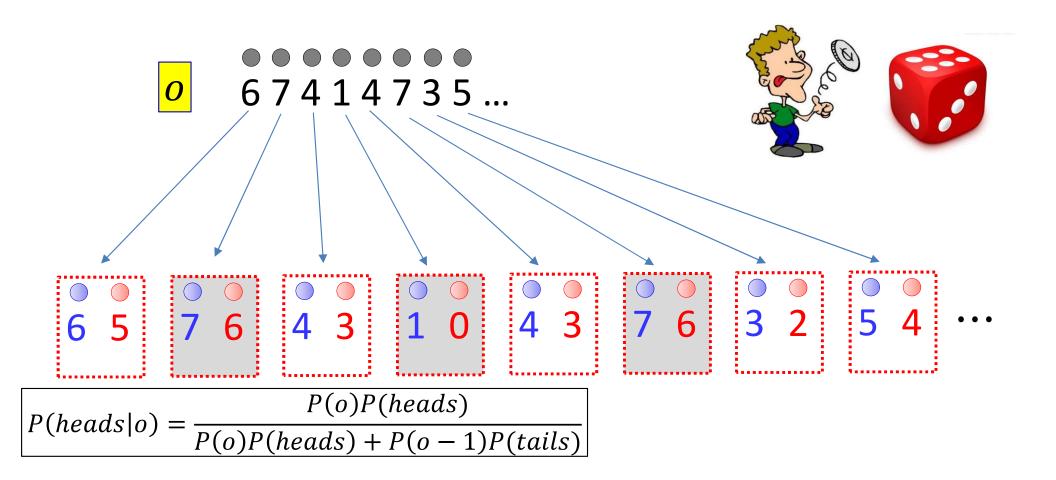
0 67414735...

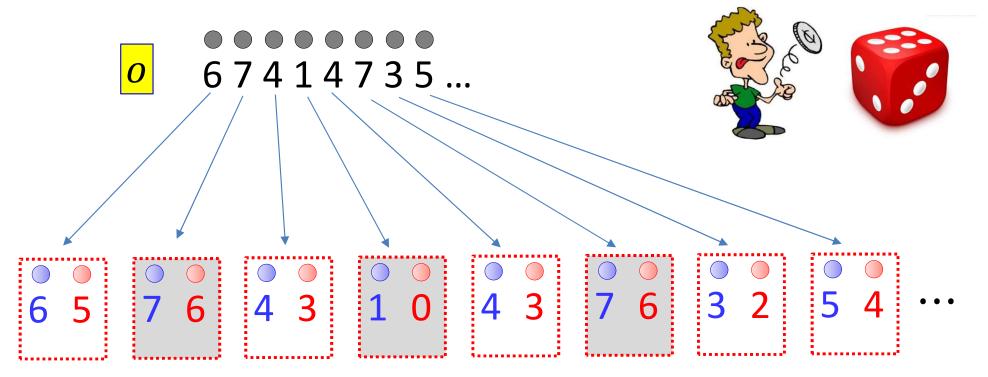


• The "face" of the coin is missing



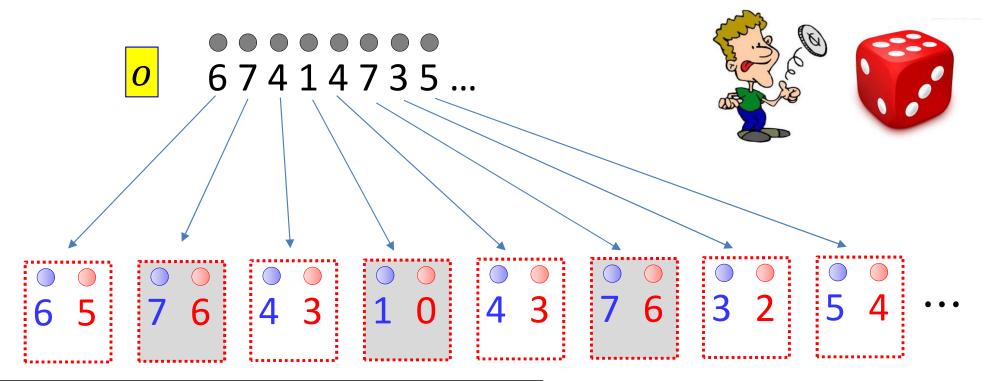
- The "face" of the coin is missing
- "Complete" each observation in every possible way:
 - assign each vector to every face
 - In proportion $P(f|o;\theta^l)$ (computed from current model estimate)
- Compute statistics from "completed" data





$$P(heads|o) = \frac{P(o)P(heads)}{P(o)P(heads) + P(o-1)P(tails)}$$

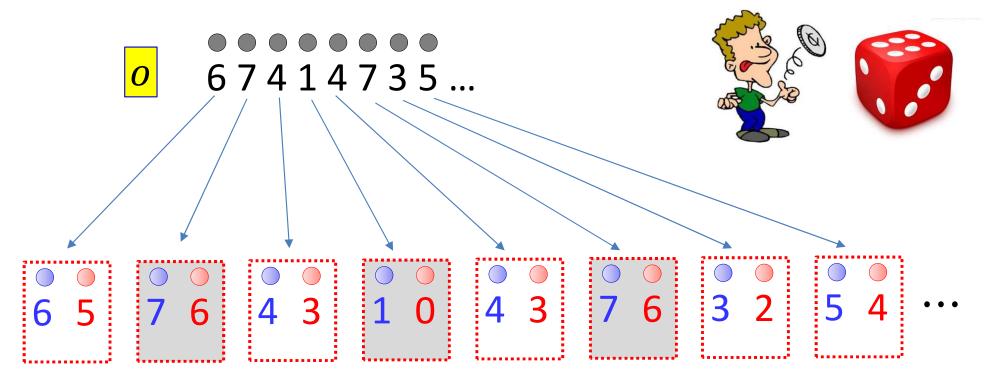
$$P(tails|o) = \frac{P(o-1)P(tails)}{P(o)P(heads) + P(o-1)P(tails)}$$



$$P(heads|o) = \frac{P(o)P(heads)}{P(o)P(heads) + P(o-1)P(tails)}$$

$$P(tails|o) = \frac{P(o-1)P(tails)}{P(o)P(heads) + P(o-1)P(tails)}$$

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



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

 $P(heads) \propto \sum_{i=0}^{n} N_o P(heads|o)$

But now for something somewhat different

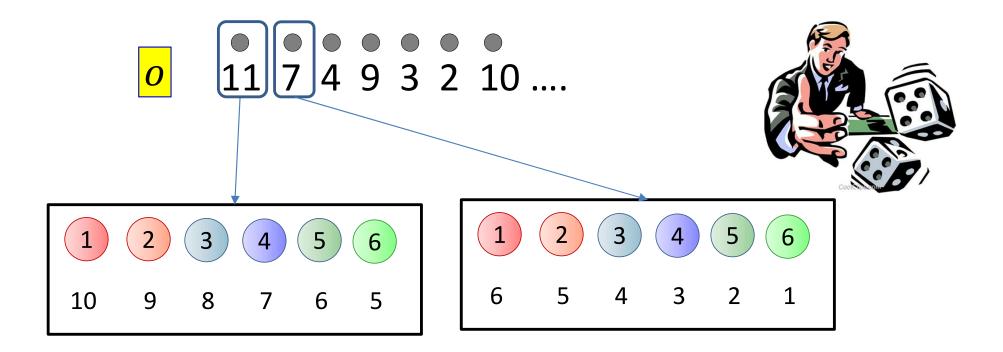


- Roller rolls two dice
- He calls out the sum
- Determine P(dice) from a collection of outputs

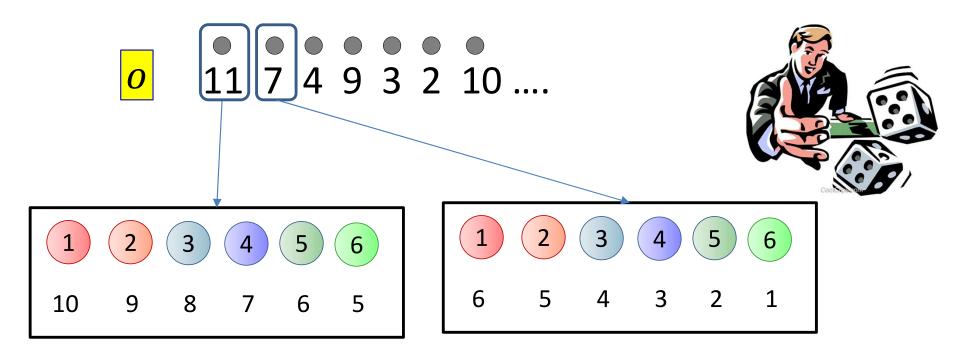
0
11 7 4 9 3 2 10



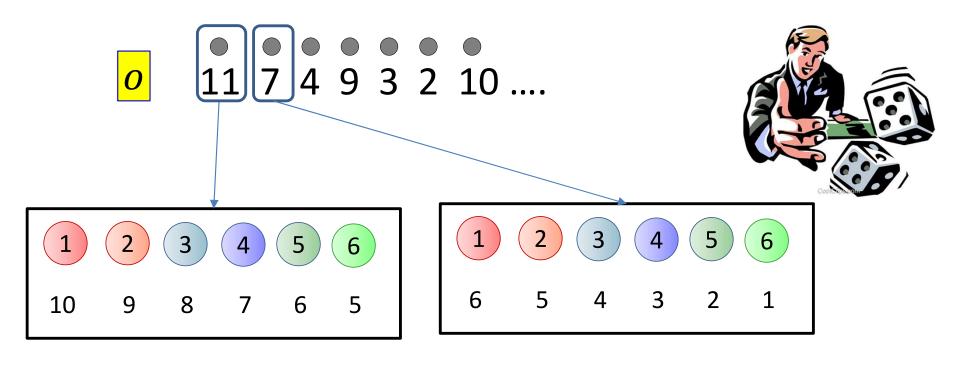
• The "first" dice info is missing



- 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/mlsp22-20221110-3

- 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