COMP 543: Tools & Models for Data Science

Optimization–Expectation Maximization

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Missing Data

- First, a few words...
  - EM is a very widely-used MLE algorithm for dealing with missing data
  - Perhaps the most intense thing we'll discuss this semester?
  - But definitely understandable to a Rice UG/MCS/PhD
  - So pay attention carefully!

Missing Data

- Often, one has an optimization problem that would be easy...
  - Except that some of the data are missing
- Why might data be missing?
  - They were never recorded
  - Wrong values recorded
  - They are imaginary

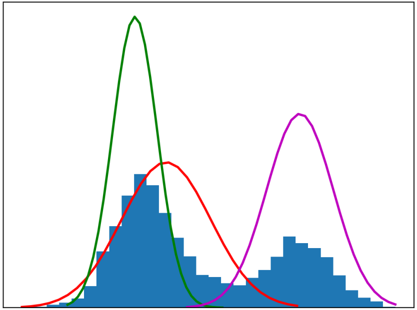
  ? When might data be imaginary?

Imaginary or Hidden data

- Complex models
- Imagine the process for generating the data
- Common models with hidden parameters
  - Gaussian Mixture Model
  - Hidden Markov Model
- intermediate steps & parameters are needed in the data generation process
- The values of these parameters are hidden from the observer
- For example
  1. Roll a die to choose a Gaussian
  2. Use that Gaussian to produce the data
- Common first steps are rolling a die or flipping a coin

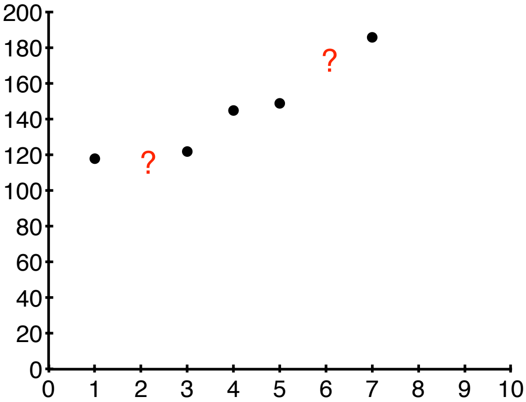
Gaussian Mixture Model

- Often used when we have a complex multi-variate distribution
- With weird shapes and many modes
- Hierarchical model
- K different Gaussians in our mixture
- Builds the distribution by mixing together K Gaussian distributions



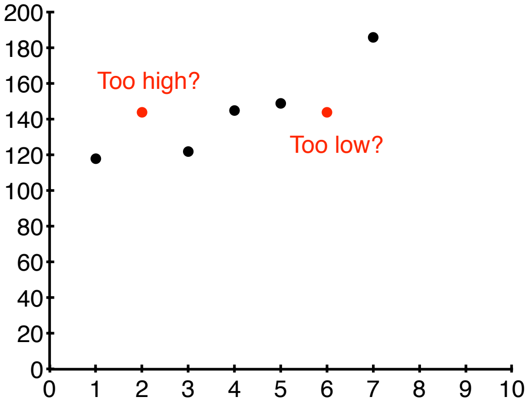
Why Can't We Do Something Simple?

- Like replace with the mean?
  - Back to the regression example
  - Want a line to fit points $\langle 118, ?, 122, 145, 149, ?, 186 \rangle$
  - Mean of observed data is 144



Why Can't We Do Something Simple?

- Like replace with the mean?
  - Back to the regression example
  - Want a line to fit points $\langle 118, ?, 122, 145, 149, ?, 186 \rangle$
  - Mean of observed data is 144
  - Does $\langle 118, 144, 122, 145, 149, 144, 186 \rangle$ make sense?
  - No: given our regression model, we expect values in-keeping with model



- EM lets us learn the model & integrate over all possible values in a fancy way

Can't We Just Drop the Data?

- In our example, why not just learn from $\langle 118, 122, 145, 149, 186 \rangle$?
  - Might make sense here...
  - But not in general
  - We can bias our data
  - Or discard a lot of useful information if just one bit is missing

Hierarchical Models

- In data science, often impossible to drop missing data
- Because the data are missing (or hidden) by design
- Happens with “hierarchical models”

Hierarchical Model Example

- Have a bag with two coins
- First has probability p_1 of heads
- Second has probability p_2 of heads
- I repeatedly reach in, pull out a coin
- Identity is $z_i \in \{1,2\}$
- Flip it 10 times and observe x_i heads
  - How do we compute $\Theta = \{p_1, p_2\}$?
  - Each z_i is missing: we don't know identity of coin
  - ? How could we just drop missing data in this case?

- This is a trial over a RV
- Represents coin selected at trial i
- Full dataset is $\{x_i, z_i\}$ pairs

Formal Problem Definition

- Formally: we want to compute an MLE for $L(\Theta|x_1, x_2, \ldots, z_1, z_2, \ldots)$
  - $x_1, x_2, \ldots$ are observed data
  - $z_1, z_2, \ldots$ are missing data
- Recall
  - This is just like computing the PDF
  - The Likelihood function flips the parameters
  - Measures how likely the parameters are given the data

Formal Problem Definition

- Recall that:
  - $L(\Theta | x_1, x_2, ..., z_1, z_2, ...) = f(x_1, x_2, ..., z_1, z_2, ... | \Theta)$
- When the z's are missing, choose Θ to max

$$\int_{\langle z_1, z_2, ... \rangle} f(x_1, x_2, ..., z_1, z_2, ... | \Theta) d\langle z_1, z_2, ... \rangle$$

“Integrating out” a Variable

$$\int_{\langle z_1, z_2, \ldots \rangle} f(x_1, x_2, \ldots, z_1, z_2, \ldots | \Theta) d\langle z_1, z_2, \ldots \rangle$$

- Sum over all possible values of the variable you are integrating out
- Example: say we have (height, weight) pairs
- Probabilities are:

$$\langle(\text{short}, \text{light}), 0.3\rangle, \langle(\text{short}, \text{heavy}), 0.1\rangle, \langle(\text{tall}, \text{light}), 0.2\rangle, \langle(\text{tall}, \text{heavy}), 0.4\rangle$$

- Probability they are “tall” is $0.6 = \sum_{\text{weight } w} Pr[(\text{tall}, w)]$
- Easy here, but difficult in the general case!

Expectation Maximization

- Is an iterative algorithm for difficult missing-data MLEs
- Basic idea...
  - Have an estimate Θ^{iter} for each iteration
  - Repeatedly update Θ^{iter} until convergence
  - Looks a lot like gradient descent, right?
- But EM is unique in how it deals with missing data points
  - The famous "Q function"

$$Q(\Theta^{\text{iter}}, \Theta^{\text{iter}-1}) = E\left[\log f(x_1, x_2, \ldots, z_1, z_2, \ldots | \Theta^{\text{iter}}) | x_1, x_2, \ldots, \Theta^{\text{iter}-1}\right]$$

Expectation Maximization

- How to interpret the Q function?
  - Q function is:

$$Q(\Theta^{\text{iter}}, \Theta^{\text{iter}-1}) = E\left[\log f(x_1, x_2, ..., z_1, z_2, ...|\Theta^{\text{iter}})|x_1, x_2, ..., \Theta^{\text{iter}-1}\right]$$

  - Treat $z_1, z_2, ...$ as random variables
  - With distribution $f(z_1, z_2, ...|x_1, x_2, ..., \Theta^{\text{iter}-1})$
  - Kind of like Bayesian approach
  - We're going to get something that looks like a posterior distribution over the zs
  - The Q-function is the expected value of the LLH wrt this distribution

- What is expected value?
  - Recall: expected value of $g(z)$ when z has distribution (PDF) $f(z)$ is $\sum_z f(z)g(z)$ or $\int_z f(z)g(z)dz$
  - When z is discrete, $f(z)$ is a probability
  - Example: If we sample (A,B) from

$$\langle(1,2),.3\rangle, \langle(3,5),0.1\rangle, \langle(2,6),0.2\rangle, \langle(-3,6),0.4\rangle$$

  - $E[A+B] = 0.3\times(1+2)+0.1\times(3+5)+0.2\times(2+6)+0.4\times(-3+6)$

Discrete and Continuous Q Function

- Continuous version is:

$$Q(\Theta^{\text{iter}}, \Theta^{\text{iter}-1}) = E\left[\log f(x_1, x_2, \ldots, z_1, z_2, \ldots | \Theta^{\text{iter}}) | x_1, x_2, \ldots, \Theta^{\text{iter}-1}\right]$$

- If zs are discrete (usually are):

$$Q(\Theta^{\text{iter}}, \Theta^{\text{iter}-1}) = \sum_{\langle z_1, z_2, \ldots \rangle} f(z_1, z_2, \ldots | x_1, x_2, \ldots, \Theta^{\text{iter}-1}) \log f(x_1, x_2, \ldots, z_1, z_2, \ldots | \Theta^{\text{iter}})$$

What are the Values of Z?

- The zs are often useful
  - In a GMM, they tell you which cluster each data point belongs to
- Running EM doesn't actually tell you the values of the zs
- But, once you have Θ it's often easy to get the values
- E.g. Use Bayes rule to find the posterior probability for each cluster

Basic EM Algorithm

- It is an iterative algorithm
  - Start with a reasonable guess as to best Θ, call this Θ^0
- In each iteration:
  - Choose Θ^{iter} to maximize the expected value of the log-likelihood
- Stop when you can't improve any more

Back to the Example

- Best to return to our example...
  - Bag with two coins
  - $\Theta = \{p_1, p_2\}$: probability of each coin being heads
  - $z_i \in \{1, 2\}$: identity of coin flip the ith time I reach in the bag
  - $x_i \in \{0, ..., 10\}$: number of heads for the ith trial
- So where do we start?

Back to the Example

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  - $z_i \in \{1, 2\}$: identity of coin flip the ith time I reach in the bag
  - $x_i \in \{0, ..., 10\}$: number of heads for the ith trial
- So where do we start?
- With the likelihood function!

$$
\begin{aligned}
L(\Theta | x_1, x_2, ..., z_1, z_2, ...) &= f(x_1, x_2, ..., z_1, z_2, ... | \Theta) \\
&= \prod_i f(x_i, z_i | \Theta) \\
&= \prod_i \frac{1}{2} \text{Binomial}(x_i | p_{z_i}, 10)
\end{aligned}
$$

- Assume each action is independent
- $f()$ is the density function given our parameter set
- x_i is the ith # of heads and z_i is the identity of the ith coin selected

Unpack the Equation

$$= \prod_i \frac{1}{2} \text{Binomial}(x_i | p_{z_i}, 10)$$

- $\frac{1}{2}$ is the 50/50 chance of pulling out each coin
- Binomial because it models coin flips
- 10 coin flips
- p_{z_i} = Probability of Heads for each z_i (Recall: $z_i = \{1, 2\}$)
- We're using the identity of the coin to choose the right probability

What About the Posterior for the Missing Data

- Need $f(z_1, z_2, \ldots | x_1, x_2, \ldots, \Theta^{\text{iter}-1}) = \prod_i f(z_i | x_i, \Theta^{\text{iter}-1})$
- Can take product because we assume independence
  - Use Bayes' rule!

$$f(z_i | x_i, \Theta^{\text{iter}-1}) = \frac{f(x_i, z_i | \Theta^{\text{iter}-1})}{f(x_i | \Theta^{\text{iter}-1})}$$
$$= \frac{\frac{1}{2}\text{Binomial}(x_i | p_{z_i}^{\text{iter}-1}, 10)}{f(x_i | \Theta^{\text{iter}-1})}$$

- Joint distribution of x_i, z_i given the parameters
- Divided by a normalizing constant

- What is $f(x_i | \Theta^{\text{iter}-1})$?

What About the Posterior for the Missing Data

- What is $f(x_i|\Theta^{\text{iter}-1})$?

$$f(x_i|\Theta^{\text{iter}-1}) = \frac{1}{2}\text{Binomial}(x_i|p_1^{\text{iter}-1}, 10) + \frac{1}{2}\text{Binomial}(x_i|p_2^{\text{iter}-1}, 10)$$

- So, plug in these values to the equation on the previous slide to get:

$$f(z_i|x_i, \Theta^{\text{iter}-1}) = \frac{\frac{1}{2}\text{Binomial}(x_i|p_{z_i}^{\text{iter}-1}, 10)}{\frac{1}{2}\text{Binomial}(x_i|p_1^{\text{iter}-1}, 10) + \frac{1}{2}\text{Binomial}(x_i|p_2^{\text{iter}-1}, 10)}$$

- Cannot discard the denominator in this case, because with need the values to sum to 1
- Computing $f(z_i|x_i, \Theta^{\text{iter}-1})$ requires a pass over the data: called "E-Step"

OK, got the E-Step, Now What?

Now we need the M-Step, where we **maximize** Q **wrt.** $\boldsymbol{\Theta^{\text{iter}}}$

- Back to the Q function:

$$Q(\Theta^{\text{iter}}, \Theta^{\text{iter}-1}) = \sum_{\langle z_1, z_2, \ldots \rangle} f(z_1, z_2, \ldots | x_1, x_2, \ldots, \Theta^{\text{iter}-1}) \log f(x_1, x_2, \ldots, z_1, z_2, \ldots | \Theta^{\text{iter}})$$

- Let $c_{i,j}$ denote $f(z_i = j | x_i, \Theta^{\text{iter}-1})$

$$Q(\Theta^{\text{iter}}, \Theta^{\text{iter}-1}) = \sum_{z_1} \sum_{z_2} \sum_{z_3} \ldots \left(\prod_i c_{i,z_i} \right) \log f(x_1, x_2, \ldots, z_1, z_2, \ldots | \Theta^{\text{iter}})$$

OK, got the E-Step, Now What?

$$\sum_{z_1}\sum_{z_2}\sum_{z_3}\cdots\left(\prod_i c_{i,z_i}\right)\log f(x_1,x_2,\ldots,z_1,z_2,\ldots|\Theta^{\text{iter}})$$

- Where $\log f(x_1,x_2,\ldots,z_1,z_2,\ldots|\Theta^{\text{iter}})$ is:

$$\begin{aligned}\log\prod_i \text{Binomial}(x_i|p_{z_i}^{\text{iter}}) &= \sum_i \log \text{Binomial}(x_i|p_{z_i}^{\text{iter}})\\ &\propto \sum_i \log\left((p_{z_i}^{\text{iter}})^{x_i}\times(1-p_{z_i}^{\text{iter}})^{10-x_i}\right)\\ &= \sum_i x_i\log(p_{z_i}^{\text{iter}})+(10-x_i)\log(1-p_{z_i}^{\text{iter}})\end{aligned}$$

- log of products = sum of logs
- Binomial PMF $\left(\binom{n}{k}p^k(1-p)^{n-k}\right)$ has a combinatorial term, drop and switch to $\propto$
- Distribute the log function

OK, got the E-Step, Now What?

- Dropping the “iter” on $p_{z_i}^{\text{iter}}$ (since both terms have it), the Q function becomes:

$$\sum_{z_1}\sum_{z_2}\sum_{z_3}\cdots\left(\prod_i c_{i,z_i}\right)\sum_i x_i \log(p_{z_i}) + (10 - x_i)\log(1 - p_{z_i})$$

- Note: We are summing over an exponential number of items

The M-Step

- Now, we need to maximize:

$$\sum_{z_1}\sum_{z_2}\sum_{z_3}\cdots\left(\prod_i c_{i,z_i}\right)\sum_i x_i \log(p_{z_i}) + (10 - x_i)\log(1 - p_{z_i})$$

- Ugly! Or is it? Consider just one variable, z_1. Write as:

$$\sum_{z_1}\sum_{\langle z_2,z_3,\ldots\rangle} c_{1,z_1} a(\langle z_2, z_3, \ldots\rangle)\left(x_1 \log(p_{z_1}) + (10 - x_1)\log(1 - p_{z_1}) + \sum_{i=2}^{n} b(\langle z_2, z_3, \ldots\rangle)\right)$$

$$= \sum_{\langle z_2,z_3,\ldots\rangle} c_{1,1} a(\langle z_2, z_3, \ldots\rangle)\left(x_1 \log(p_1) + (10 - x_1)\log(1 - p_1) + \sum_{i=2}^{n} b(\langle z_2, z_3, \ldots\rangle)\right)$$

$$+ \sum_{\langle z_2,z_3,\ldots\rangle} c_{1,2} a(\langle z_2, z_3, \ldots\rangle)\left(x_1 \log(p_2) + (10 - x_1)\log(1 - p_2) + \sum_{i=2}^{n} b(\langle z_2, z_3, \ldots\rangle)\right)$$

- where a is the terms in $\prod_i c_{i,z_i}$ except for the current coin flip
- where b is the terms in the sum over the x_i except for the current coin flip

The M-Step

$$c_{1,1} \sum_{\langle z_2, z_3, \ldots \rangle} a(\langle z_2, z_3, \ldots \rangle) \left(x_1 \log(p_1) + (10 - x_1) \log(1 - p_1) + \sum_{i=2}^{n} b(\langle z_2, z_3, \ldots \rangle) \right)$$

$$+ c_{1,2} \sum_{\langle z_2, z_3, \ldots \rangle} a(\langle z_2, z_3, \ldots \rangle) \left(x_1 \log(p_2) + (10 - x_1) \log(1 - p_2) + \sum_{i=2}^{n} b(\langle z_2, z_3, \ldots \rangle) \right)$$

- Continuing, split into the actual two terms, one for each coin, then distribute the c terms:

$$= c_{1,1} \left(x_1 \log(p_1) + (10 - x_1) \log(1 - p_1) \right) \sum_{\langle z_2, z_3, \ldots \rangle} a(\langle z_2, z_3, \ldots \rangle)$$

$$+ c_{1,1} \sum_{\langle z_2, z_3, \ldots \rangle} a(\langle z_2, z_3, \ldots \rangle) \sum_{i=2}^{n} b(\langle z_2, z_3, \ldots \rangle)$$

$$+ c_{1,2} \left(x_1 \log(p_2) + (10 - x_1) \log(1 - p_2) \right) \sum_{\langle z_2, z_3, \ldots \rangle} a(\langle z_2, z_3, \ldots \rangle)$$

$$+ c_{1,2} \sum_{\langle z_2, z_3, \ldots \rangle} a(\langle z_2, z_3, \ldots \rangle) \sum_{i=2}^{n} b(\langle z_2, z_3, \ldots \rangle)$$

The M-Step

- Continuing, recombine in a simpler way & drop the $\sum_{\langle z_2,z_3,\ldots\rangle} a(\langle z_2,z_3,\ldots\rangle)$ from the first term:

$$
\begin{aligned}
& c_{1,1}\left(x_1\log(p_1)+(10-x_1)\log(1-p_1)\right)\sum_{\langle z_2,z_3,\ldots\rangle} a(\langle z_2,z_3,\ldots\rangle) \\
& + c_{1,1}\sum_{\langle z_2,z_3,\ldots\rangle} a(\langle z_2,z_3,\ldots\rangle)\sum_{i=2}^{n} b(\langle z_2,z_3,\ldots\rangle) \\
& + c_{1,2}\left(x_1\log(p_2)+(10-x_1)\log(1-p_2)\right)\sum_{\langle z_2,z_3,\ldots\rangle} a(\langle z_2,z_3,\ldots\rangle) \\
& + c_{1,2}\sum_{\langle z_2,z_3,\ldots\rangle} a(\langle z_2,z_3,\ldots\rangle)\sum_{i=2}^{n} b(\langle z_2,z_3,\ldots\rangle) \\
& = c_{1,1}\left(x_1\log(p_1)+(10-x_1)\log(1-p_1)\right)+ \\
& + c_{1,2}\left(x_1\log(p_2)+(10-x_1)\log(1-p_2)\right)+ \\
& + \sum a(\langle z_2,z_3,\ldots\rangle)\sum^{n} b(\langle z_2,z_3,\ldots\rangle)
\end{aligned}
$$

The M-Step

- Question: why can we drop $\sum_{\langle z_2, z_3, \ldots \rangle} a(\langle z_2, z_3, \ldots \rangle)$ from:

$$c_{1,1}\left(x_1 \log(p_1) + (10 - x_1)\log(1 - p_1)\right) \sum_{\langle z_2, z_3, \ldots \rangle} a(\langle z_2, z_3, \ldots \rangle)$$

- Answer: $a(\langle z_2, z_3, \ldots \rangle)$ is the posterior probability of flip sequence 2 coming from coin z_2 and flip sequence 3 coming from coin z_3 and flip sequence 4 coming from coin z_4 and so on.
- Since we sum over all possible $\langle z_2, z_3, \ldots \rangle$, we are summing the probability all possible identities for coins $2, 3, 4 \ldots$
- This has to equal 1!
- Why? By definition, when you sum the probability of all possibilities, you get 1

The M-Step

- Note the last term in

$$
\begin{aligned}
& c_{1,1}\left(x_1 \log(p_1) + (10 - x_1)\log(1 - p_1)\right) + \\
& + c_{1,2}\left(x_1 \log(p_2) + (10 - x_1)\log(1 - p_2)\right) + \\
& + \sum_{\langle z_2, z_3, \ldots \rangle} a(\langle z_2, z_3, \ldots \rangle) \sum_{i=2}^{n} b(\langle z_2, z_3, \ldots \rangle)
\end{aligned}
$$

- This is like a "littler" Q-function, or what we get after removing the first coin flip (z_1). So we have shown the Q-function is just:

$$
\begin{aligned}
& c_{1,1}\left(x_1 \log(p_1) + (10 - x_1)\log(1 - p_1)\right) + \\
& c_{1,2}\left(x_1 \log(p_2) + (10 - x_1)\log(1 - p_2)\right) + \\
\sum_{z_2}\sum_{z_3}\ldots & \left(\prod_{i \geq 2} c_{i,z_i}\right) \sum_{i \geq 2} x_i \log(p_{z_i}) + (10 - x_i)\log(1 - p_{z_i})
\end{aligned}
$$

The M-Step

- So we've shown we can remove z_1 from the nasty summation $\sum_{z_1}\sum_{z_2}\sum_{z_3}$ ...
- We can use the same algebraic manipulations to get rid of z_2, then z_3, etc., giving us:

$$\sum_i c_{i,1}\left(x_i \log(p_1) + (10 - x_i)\log(1 - p_1)\right) + c_{i,2}\left(x_i \log(p_2) + (10 - x_i)\log(1 - p_2)\right)$$

The M-Step

- Now we maximize wrt p_1, p_2
- Partial derivative wrt p_1:

$$\sum_i c_{i,1} x_i \frac{1}{p_1} - \sum_i c_{i,1}(10 - x_i)\frac{1}{1-p_1}$$

- Set to zero:

$$\sum_i c_{i,1} x_i \frac{1}{p_1} - \sum_i c_{i,1}(10 - x_i)\frac{1}{1-p_1} = 0$$

$$\frac{1}{p_1}\sum_i c_{i,1} x_i - \frac{1}{1-p_1}\sum_i 10 c_{i,1} + \frac{1}{1-p_1}\sum_i c_{i,1} x_i = 0$$

$$(1-p_1)\sum_i c_{i,1} x_i - p_1 \sum_i 10 c_{i,1} + p_1 \sum_i c_{i,1} x_i = 0$$

$$\sum_i c_{i,1} x_i - p_1 \sum_i 10 c_{i,1} = 0$$

$$p_1 = \frac{\sum_i c_{i,1} x_i}{\sum_i 10 c_{i,1}}$$

The M-Step

- Recall: $c_{i,j}$ denotes $f(z_i = j | x_i, \Theta^{\text{iter}-1})$
- Let's consider

$$p_1 = \frac{\sum_i c_{i,1} x_i}{\sum_i 10 c_{i,1}}$$

- We are taking a weighted sum that looks at how many times, out of 10, we got heads
- Taking into account a weighting factor that each data point was effected by c_1
- We can repeat for c_2

The M-Step

- So, $p_2 = \frac{\sum_i c_{i,2} x_i}{\sum_i 10 c_{i,2}}$
- Very simple!!

```
set p_1 = 0.8, p_2 = 0.2
while (p_1, p_2 still change) do
  compute c_{i,1}, c_{i,2} for each i
  set p_1 = (Σ_i c_{i,1} x_i) / (Σ_i 10 c_{i,1})
  set p_2 = (Σ_i c_{i,2} x_i) / (Σ_i 10 c_{i,2})
end while
```

- But a long way to get there

A Quick Review

- Goal: Find the model parameters, p_1 and p_2
- Given: Observations of the number of heads in 10 coin tosses, over a number of trials
- It's (relatively) easy if we know which coin was selected during each trial

$$p_1 = \frac{\text{\# of heads using coin 1}}{\text{total \# of flips using coin 1}}$$

$$p_2 = \frac{\text{\# of heads using coin 2}}{\text{total \# of flips using coin 2}}$$

A Quick Review

- If we don't know which coin was selected for each trial, we need to estimate it
- We could do this by
  1. Computing the most likely coin selected for each observation, given an estimate of p_1 and p_2
  2. Then use these assignments to compute a revised MLE estimate of the parameters
  3. Repeat until p_1 and p_2 converge

A Quick Review

- Alternatively, we could
  - Compute the probability for each possible combination of the selected coins
  - Use these probabilities to build a weighted function of the data to determine the probabilities
  - And re-estimate the parameters, using the weighted functions in an MLE

  - Alternate between guessing the distribution of the missing data (the E-step)
  - And re-estimating the parameter values (the M-step)

Thoughts about EM

- EM requires a lot of thinking and a lot of math
- It's very efficient (great for big data)
- However, if you have a lot of missing data
  - Use Markov Chain Monte Carlo (MCMC) / Bayesian methods
  - Easier than EM
  - Not as efficient

Questions?