Clustering Part 2

EECS 349 Spring 2016
Expectation Maximization

- Learning parameters in Bayes Nets is easy if data is complete
  - Just counting
- But what about missing data?
  - We could use our standard “missing data” techniques (use mean, median, etc.)
  - But when lots of data is missing, we want to infer missing data and parameters simultaneously
    - We can use **Expectation Maximization**
Gaussian Mixtures

- K classes, each class $\omega_i$ produces Gaussian observations with mean $\mu_i$ with variance $\sigma^2 I$
- Assume $\sigma^2 I$ given (for now), and we have lots of observations
- Task: estimate $\mu_i$
- But, none of the data points are labeled…
Gaussian Mixtures

- **Know**
  - $K$
  - Data
  - $\sigma^2$
  - $P(\omega_i)$

- **Don't know**
  - Data label

- **Objective**
  - Estimate the $\mu_i$
The GMM assumption

- There are $k$ components. The $i$'th component is called $\omega_i$.
- Component $\omega_i$ has an associated mean vector $\mu_i$. 
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- Each component generates data from a Gaussian with mean $\mu_i$ and covariance matrix $\sigma^2 I$.

Assume that each datapoint is generated according to the following recipe:
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Assume that each datapoint is generated according to the following recipe:

1. Pick a component at random. Choose component $i$ with probability $P(\omega_i)$. 

Most slides from http://www.autonlab.org/tutorials/
The GMM assumption

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- Component $\omega_i$ has an associated mean vector $\mu_i$
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Assume that each datapoint is generated according to the following recipe:

1. Pick a component at random. Choose component $i$ with probability $P(\omega_i)$.
2. Datapoint $\sim N(\mu_i, \sigma^2 I)$
The data generated

Most slides from http://www.autonlab.org/tutorials/
Computing the likelihood

Remember:
We have unlabeled data \( x_1 \ x_2 \ldots \ x_R \)
We know there are \( k \) classes
We know \( P(w_1) \ P(w_2) \ P(w_3) \ldots \ P(w_k) \)
We don’t know \( \mu_1 \ \mu_2 \ldots \ \mu_k \)

We can write \( P(\text{data} \mid \mu_1, \ldots, \mu_k) \)

\[
= p(x_1 \ldots x_R \mid \mu_1 \ldots \mu_k) \\
= \prod_{i=1}^{R} p(x_i \mid \mu_1 \ldots \mu_k) \\
= \prod_{i=1}^{R} \sum_{j=1}^{k} p(x_i \mid w_j, \mu_1 \ldots \mu_k) P(w_j) \\
= \prod_{i=1}^{R} \sum_{j=1}^{k} K \exp\left( -\frac{1}{2\sigma^2} (x_i - \mu_j)^2 \right) P(w_j)
\]
EM for GMMs

For Max likelihood we know \[ \frac{\partial}{\partial \mu_i} \log \text{Pr ob}(\text{data} | \mu_1 \ldots \mu_k) = 0 \]

Some wild'n'crazy algebra turns this into: "For Max likelihood, for each j,

\[ \mu_j = \frac{\sum_{i=1}^{R} P(w_j | x_i, \mu_1 \ldots \mu_k) x_i}{\sum_{i=1}^{R} P(w_j | x_i, \mu_1 \ldots \mu_k)} \]

This is n nonlinear equations in \( \mu_j \)'s."
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This is n nonlinear equations in \( \mu_j \)'s."

If, for each \( x_i \) we knew that for each \( w_j \) the prob that \( \mu_j \) was in class \( w_j \) is \( P(w_j|x_i,\mu_1...\mu_k) \) Then... we would easily compute \( \mu_j \).

If we knew each \( \mu_j \) then we could easily compute \( P(w_j|x_i,\mu_1...\mu_j) \) for each \( w_j \) and \( x_i \).
EM for GMMs

Iterate. On the $t$th iteration let our estimates be
\[
\lambda_t = \{ \mu_1(t), \mu_2(t) \ldots \mu_c(t) \}
\]

E-step

Compute “expected” classes of all datapoints for each class
\[
P(w_i|x_k, \lambda_t) = \frac{p(x_k|w_i, \lambda_t)P(w_i|\lambda_t)}{p(x_k|\lambda_t)} = \frac{p(x_k|w_i, \mu_i(t), \sigma^2 I)p_i(t)}{\sum_{j=1}^c p(x_k|w_j, \mu_j(t), \sigma^2 I)p_j(t)}
\]

M-step.

Compute Max. like $\mu$ given our data’s class membership distributions
\[
\mu_i(t+1) = \frac{\sum_k P(w_i|x_k, \lambda_t)x_k}{\sum_k P(w_i|x_k, \lambda_t)}
\]
Gaussian Mixture Example: Start

Advance apologies: in Black and White this example will be incomprenhensible

Most slides from http://www.autonlab.org/tutorials/
After first iteration

Most slides from http://www.autonlab.org/tutorials/
After 2nd iteration
After 3rd iteration
After 4th iteration

Most slides from http://www.autonlab.org/tutorials/
After 5th iteration

Most slides from http://www.autonlab.org/tutorials/
After 6th iteration
After 20th iteration

Most slides from http://www.autonlab.org/tutorials/
EM at the 10,000 foot level

- Guess some parameters, then
  - Use your parameters to get a distribution over hidden variables
  - Re-estimate the parameters as if your distribution over hidden variables is correct
- Seems magical. When/why does this work?
Underlying EM: The basic idea

- EM: Given a guess $\theta_{old}$ for $\theta$, improve it.
- Idea: construct lower bound that equals the true log likelihood at $\theta_{old}$.

![Graph showing LL(\theta_{new}) and LL(\theta_{old}) with \theta_{new} and \theta_{old} axes. The graph illustrates the improvement in the lower bound.]
For exponential family

- **E step:**
  - Use $\theta_n$ to estimate **expected** sufficient statistics over **complete** data

- **M step**
  - Set $\theta_{n+1} = \text{ML parameters given sufficient statistics}$
    - (Or MAP parameters)
EM in practice

- **Local maxima**
  - Random re-starts, simulated annealing…

- **Variants**
  - Hard EM: set unknown vars to most likely value (e.g. k-means)
  - Generalized EM: increase (not nec. maximize) lower bound in each step
  - Approximate E-step (e.g. sampling)
Seeking Life’s Bare (Genetic) Necessities

COLD SPRING HARBOR, NEW YORK—How many genes does an organism need to survive? Last week at the genome meeting here, two genome researchers with radically different approaches presented complementary views of the basic genes needed for life. One research team, using computer analyses to compare known genomes, concluded that today’s organisms can be sustained with just 250 genes, and that the earliest life forms required a mere 128 genes. The other researcher mapped genes in a simple parasite and estimated that for this organism, 800 genes are plenty to do the job—but that anything short of 100 wouldn’t be enough.

Although the numbers don’t match precisely, those predictions “are not all that far apart,” especially in comparison to the 75,000 genes in the human genome, notes Siv Andersson of Uppsala University in Sweden, who arrived at the 800 number. But coming up with a consensus answer may be more than just a genetic numbers game, particularly as more and more genomes are completely mapped and sequenced. “It may be a way of organizing any newly sequenced genome,” explains Arcady Mushegian, a computational molecular biologist at the National Center for Biotechnology Information (NCBI) in Bethesda, Maryland. Comparing an


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Simple intuition: Documents exhibit multiple topics.
Each topic is a distribution over words

Each document is a mixture of corpus-wide topics

Each word is drawn from one of those topics
In reality, we only observe the documents

The other structure are **hidden variables**
LDA: Math Version

- For each topic $t$
  Choose distribution $\phi_t \sim \text{Dirichlet}(\beta)$

- For each doc
  Choose $\theta \sim \text{Dirichlet}(\alpha)$
  For each token $i$
    choose topic $z_i \sim \text{Mult}(\theta)$
    choose word $w_i \sim \text{Mult}(\phi_{z_i})$

- Exact inference is intractable
  - We will use a collapsed sampler that integrates out $\phi$ and $\theta$

[Griffiths and Steyvers, 2007]
Inference

- Variational and sampling-based methods exist

- Simple collapsed Gibbs sampling approach:
  - Initialize all topic variables $z_i$ randomly to one of $K$ topics
  - For each sampling pass
    - For each token $i$
      - Sample a new value for $z_i$ given all other topic variable assignments
Sampling Distribution

- \( P(\text{topic } z \mid \text{word } w, \text{doc } d) \propto \frac{n^d_z + \alpha}{n^d + \alpha K} \cdot \frac{n^w_z + \beta}{n^w + \beta V} \)

- \( n^d_z = \) number of times topic \( z \) assigned in doc \( d \)
- \( n^w_z = \) number of times topic \( z \) assigned for word \( w \)
- \( K = \) number of topics
- \( V = \) number of unique words
- \( \alpha, \beta : \) Dirichlet prior hyperparameters
Example Inference

human, genome, dna, genetic, genes, sequence, gene, molecular, sequencing, map, information, genetics, mapping, project, sequences, evolution, evolutionary, species, organisms, life, origin, biology, groups, phylogenetic, living, diversity, group, new, two, common, disease, host, bacteria, diseases, resistance, bacterial, new, strains, control, infectious, malaria, parasite, parasites, united, tuberculosis, computer, models, information, data, computers, system, network, systems, model, parallel, methods, networks, software, new, simulations

From David Blei’s 2012 ICML tutorial
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