Introduction to Graphical Models
lecture 10 - Learning with latent variables (EM)

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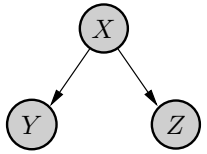
Learning Bach

- An example:
  – a machine "listens" (reads notes of) Bach pieces over and over again
  – it's supposed to learn how to write Bach pieces itself (or at least harmonize them)
- *Harmonizing Chorales in the Style of J S Bach*
  Moray Allan & Chris Williams (NIPS 2004)
  http://www.srcf.ucam.org/~mma29/2002/harmony/
- They learn this by assuming that there is some latent context (the current harmony) implicit in the music

recap: Learning in graphical models I

- Given three random varibles X, Y, Z with structure



$$P(X,Y,Z) = P(X)\ P(Y|X)\ P(Z|X)$$

  – unknown parameters $P(X=x) \equiv \pi_x$, $P(Y=y|X=x) \equiv a_{yx}$, $P(Z=z|X=x) \equiv b_{zx}$
  – Given a data set $\{(x_i, y_i, z_i)\}_{i=1}^N$
  – how can we learn the parameters $\theta = (\boldsymbol{\pi}, \boldsymbol{a}, \boldsymbol{b})$?

- answer:

define counts:	set parameters equal:
$c_x = \sum_{i=1}^N [x_i = x]$	$\pi_x \leftarrow \frac{c_x}{N}$
$c_{yx} = \sum_{i=1}^N [y_i = y][x_i = x]$	$a_{yx} \leftarrow \frac{c_{yx}}{N c_x}$
$c_{zx} = \sum_{i=1}^N [z_i = z][x_i = x]$	$b_{zx} \leftarrow \frac{c_{zx}}{N c_x}$

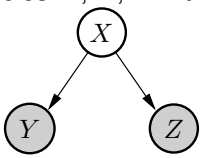
recap: Learning in graphical models II

- why (in what sense) is this the correct answer?
  – these parameters maximize *observed data log-likelihood*

$$L(\theta) = \log \prod_{i=1}^n P(x_i, y_i, z_i\ ; \theta)$$
$$= \sum_{i=1}^n \log P(x_i, y_i, z_i\ ; \theta)$$

Learning with missing data

- Given three random varibles X, Y, Z with structure



$$P(X,Y,Z) = P(X)\ P(Y|X)\ P(Z|X)$$

  – unknown parameters $P(X=x) \equiv \pi_x$, $P(Y=y|X=x) \equiv a_{yx}$, $P(Z=z|X=x) \equiv b_{zx}$
  – Given a partial data set $\{(y_i, z_i)\}_{i=1}^N$ (observations x_i are missing!)
  – how can we learn the parameters θ?

- any ideas?

General ideas for learning with missing data

- We should somehow *fill in the missing data*..

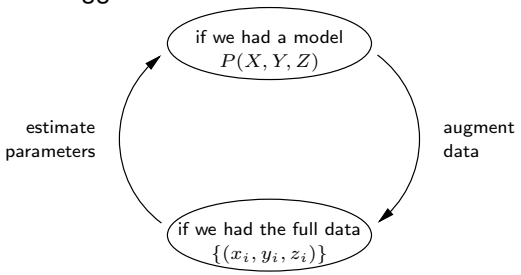
  partial data $\{(y_i, z_i)\}_{i=1}^N$ $\quad\rightarrow\quad$ augmented data $\{(\hat{x}_i, y_i, z_i)\}_{i=1}^N$

- but how should we choose $\hat{x}_i$
  ... invent fictional $\hat{x}_i$??

A chicken and egg problem

- If we knew the model $P(X,Y,Z)$ already, we could use it to invent/estimate an $\hat{x}_i$ for each partial datum (y_i, z_i)
  – then use this "augmented data" to train the model

- the chicken and egg situation:



Viterbi training I

(name Viterbi usually *only* used in context of HMMs, we use it here more generally)

- given partial data $\{(y_i, z_i)\}_{i=1}^N$
- given *some initial* parameters θ^{old} that define a model $P(X,Y,Z\,;\theta^{\text{old}})$
- iterate:
  – for each datum compute $\hat{x}_i = \text{argmax}_x\, P(x, y_i, z_i\,;\theta^{\text{old}})$
  ("data agumentation" using the old parameters)
  – using the augmented data $\{(\hat{x}_i, y_i, z_i)\}_{i=1}^N$, compute new parameters

$$\theta^{\text{new}} = \operatorname*{argmax}_\theta L(\theta)$$

that maximize the (augmented) data log-likelihood

Viterbi training II

- feel uneasy about this algorithm?
  – what if the initial parameters θ^{old} are really bad?
  → very bad augmented data?
  → very bad parameter setting in the next step?

- generally:
  – yes, all these iterative-chicken-and-egg-type algorithms are prone to local minima
  – depend very much on initial choice of parameters

- but we can relax the hard augmentation...

Expectation Maximization I

- instead of the strict augmentation $\hat{x}_i = \text{argmax}_x \, P(x, y_i, z_i \,; \theta^{\text{old}})$
  we can compute the posterior belief over the missing data using the current model

$$q_i(x) = P(x|y_i, z_i \,; \theta^{\text{old}})$$

- but then, how choose new parameters when we have
  – partial data $\{(y_i, z_i)\}_{i=1}^N$ and the posteriors $q_i(x)$ for each i??

  → we can't use complete data log-likelihood (since data is missing)
  → but we can use *expected* data log-likelihood (expectation w.r.t. q)!
  → maximize expected data log-likelihood (=Expectation Maximization)

- switch notation, to derive general algorithms:

  – let X be a (set of) hidden variables
  – let Y be a (set of) observed variables
  – let $P(X, Y \,; \theta)$ be a parameterized probabilistic model

Expected data log-likelihood

- complete data log-likelihood (if X and Y are observed):

$$L(\theta) = \sum_{i=1}^{n} \log P(x_i, y_i \,; \theta)$$

- observed data log-likelihood (if only Y is observed and we can eliminate X analytically):

$$\hat{L}(\theta) = \sum_{i=1}^{n} \log P(y_i \,; \theta) = \sum_{i=1}^{n} \log \sum_x P(x, y_i \,; \theta)$$

- expected data log-likelihood (if only Y is observed and we have a posterior $q_i(x; \theta^{\text{old}})$ over the missing data):

$$Q(\theta, \theta^{\text{old}}) = \sum_{i=1}^{n} \sum_x q_i(x; \theta^{\text{old}}) \, \log P(x, y_i \,; \theta)$$

where $q_i(x; \theta^{\text{old}}) = P(x|y_i \,; \theta^{\text{old}})$

Note: $Q(\theta, \theta^{\text{old}}) \leq \hat{L}(\theta)$ (see later, free energy)

Expectation Maximization II

- given partial data $\{y_i\}_{i=1}^N$
- given *some initial* parameters θ^{old} that define a model $P(X, Y\,;\theta^{\text{old}})$
- iterate:

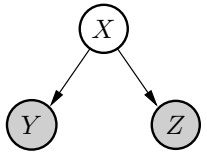
  (E-step) for each datum compute $q_i(x;\theta^{\text{old}}) = P(x|y_i\,;\theta^{\text{old}})$
  ("expected data agumentation" using the old parameters)

  (M-step) compute new parameters

  $$\theta^{\text{new}} = \operatorname*{argmax}_\theta Q(\theta, \theta^{\text{old}})$$

  that maximize expected data log-likelihood

Example



$$P(X, Y, Z) = P(X)\ P(Y|X)\ P(Z|X)$$

- **(E-step)** Compute

  $$q_i(x\,;\theta^{\text{old}}) = P(x|y_i, z_i\,;\theta^{\text{old}})$$
  $$\propto P(x)\ P(y_i\,|\,x)\ P(z_i|x) = \pi_x^{\text{old}}\ a_{y_i x}^{\text{old}}\ b_{z_i x}^{\text{old}}$$

  This is an inference problem! – Naive Bayes!

- **(M-step)** compute *expected* counts:
  $c_x = \sum_{i=1}^N q_i(x)$
  $c_{yx} = \sum_{i=1}^N q_i(x)\ [y_i = y]$
  $c_{zx} = \sum_{i=1}^N q_i(x)\ [z_i = z]$
  and set parameter as before

- EM on an intuitive level:
  – fill in missing data
  – do this by computing the posterior $q_i(x\,;\theta^{\text{old}})$ over missing variables
  – maximized expected data log-likelihood

- now: very elegant and powerful theoretical formulation

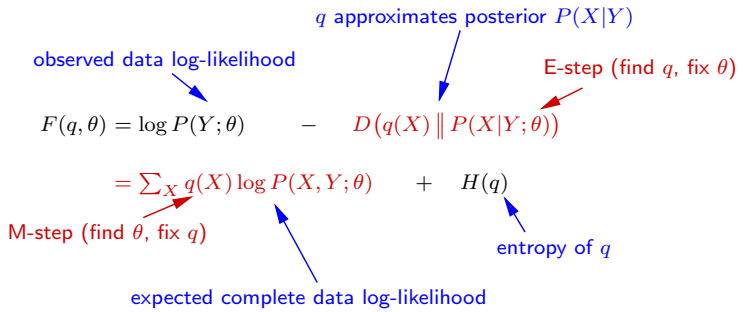
Free energy view on EM I

- Generally,
  – let X be a (set of i.i.d.) hidden variables
  – let Y be a (set of i.i.d.) observed variables
  – let $P(X, Y\,;\theta)$ be a parameterized probabilistic model

- define the function

$$F(q,\theta) = \log P(Y;\theta) - D\big(q(X)\,\big\|\,P(X|Y;\theta)\big) \tag{1}$$
$$= \log P(Y;\theta) - \sum_X q(X) \log \frac{q(X)}{P(X\,|\,Y;\theta)}$$
$$= \sum_X q(X) \log P(Y;\theta) + \sum_X q(X) \log P(X\,|\,Y;\theta) + H(q)$$
$$= \sum_X q(X) \log P(X, Y;\theta) + H(q), \tag{2}$$

Free energy view on EM II



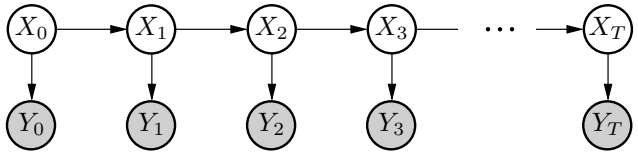
- we actually want to maximize $P(Y;\theta)$ w.r.t. θ → but can't analytically
- instead, maximize lower bound $F(q,\theta) \leq \log P(Y;\theta)$
  - E-step: find q that maximizes $F(q,\theta)$ for fixed θ^{old} using (1)
    (→ find q to minimize KLD, makes lower bound tight for fixed θ)
  - M-step: find θ that maximizes $F(q,\theta)$ for fixed q using (2)
- EM = step-wise coordinate ascent of the function $F(q,\theta)$

⇒ convergence proof: F can only increase!

Example

- next time: learning goal-directed behavior
- today: HMMs again

Example: EM in HMMs



$$P(X_0,..,X_T,Y_0,..,Y_T) = P(X_0) \cdot \prod_{t=1}^{T} P(X_t|X_{t-1}) \cdot \prod_{t=0}^{T} P(Y_t|X_t)$$

- We've done inference in HMMs enough (e.g., lecture 4)
- Assume we don't know the parameters $\theta = (\boldsymbol{\pi}, \boldsymbol{a}, \boldsymbol{b})$ of the model:

$$P(X_0 = x) = \pi_x$$
$$P(X_t = x' | X_{t-1} = x) = a_{xx'}$$
$$P(Y_t = y | X_t = x) = b_{xy}$$

- We have a data set of observation sequences $\{y^i_{0:T}\}_{i=1}^N$
  → use EM to train parameters (old name of EM for HMMs: *Baum-Welch algorithm*)

Example: EM in HMMs

- E-step: compute $q_i(x_{0:T};\theta) = P(x_{0:T} \,|\, y^i_{0:T};\theta)$
- M-step: compute

$$\theta^{\text{new}} = \operatorname*{argmax}_\theta \sum_{i=1}^{N} \sum_{x_{0:T}} q_i(x_{0:T};\theta^{\text{old}}) \;\log P(x_{0:T}, y^i_{0:T};\theta)$$

Again, this optimization ends up assigning *expected counts* to the new parameters:

$$\pi_x^{\text{new}} = \sum_{i=0}^{N} q_i(x_0 = x)$$
$$a_{xx'}^{\text{new}} = \frac{\sum_{i=0}^{N}\sum_{t=1}^{T} q_i(x_t = x', x_{t-1} = x)}{\sum_{i=0}^{N}\sum_{t=1}^{T} q_i(x_{t-1} = x)}$$
$$b_{xy}^{\text{new}} = \frac{\sum_{i=0}^{N}\sum_{t=0}^{T} [y^i_t = y]\; q_i(x_t = x)}{\sum_{i=0}^{N}\sum_{t=0}^{T} q_i(x_t = x)}$$

back to Bach

(Moray Allan & Chris Williams (NIPS 2004)
http://www.srcf.ucam.org/~mma29/2002/harmony/)

- use an HMM
  – observed sequence $Y_{0:T}$ Soprano melody
  – latent sequence $X_{0:T}$ chord & and harmony:

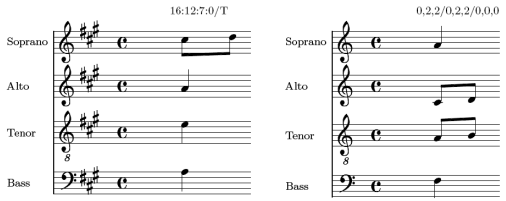


Figure 1: Hidden state representations (a) for harmonisation, (b) for ornamentation.

back to Bach

- results:

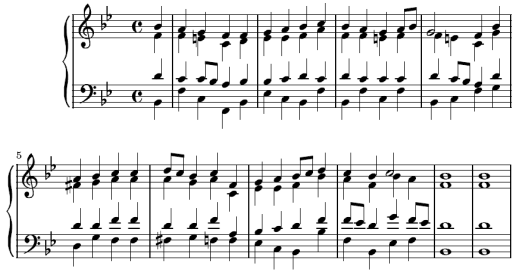


Figure 2: Most likely harmonisation under our model of chorale K4, BWV 48

summary

- EM ↔ idea of *fill in missing data*
  EM ↔ consider *expected* data log-likelihood
  EM ↔ free energy maximization as lower bound of observed data LL

- 2 core computational principles:
  – information processing
  – learning
  → EM combines both for learning with missing data

- next time:
  – learning goal-directed behavior