

LECTURE 10: THE EM ALGORITHM (CONTD)

STAT 545: INTRO. TO COMPUTATIONAL STATISTICS

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EXPONENTIAL FAMILY MODELS

Consider a space \mathbb{X} . E.g. \mathbb{R}, \mathbb{R}^d or \mathbb{N} .

$\phi(x) = [\phi_1(x), \dots, \phi_D(x)] :$ (feature) vector of sufficient statistics

$\theta = [\theta_1, \dots, \theta_D] :$ vector of natural parameters

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$h(x)$ is the base-measure or base distribution.

$Z(\theta) = \int h(x) \exp(\theta^\top \phi(x)) dx$ is the normalization constant.

The normal distribution:

$$\begin{aligned} p(x|\mu, \sigma^2) &= \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2\sigma^2}(x - \mu)^2\right) \\ &= \frac{\exp\left(-\frac{\mu^2}{2\sigma^2}\right)}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2\sigma^2}x^2 + \frac{\mu}{\sigma^2}x\right) \end{aligned}$$

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The Poisson distribution:

$$\begin{aligned} p(x|\lambda) &= \frac{\lambda^x \exp(-\lambda)}{x!} \\ &= \exp(-\lambda) \frac{1}{x!} \exp(\log(\lambda)x) \end{aligned}$$

MINIMAL EXPONENTIAL FAMILY

Sufficient statistics are linearly independent

Consider a K -component discrete distribution $\pi = (\pi_1, \dots, \pi_K)$

$$p(X) = \prod_{c=1}^K \pi_c^{\delta(X=c)} = \exp\left(\sum_{c=1}^K \delta(X=c) \log \pi_c\right)$$

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Is it minimal?

$$\begin{aligned} p(X) &= \pi_K \exp\left(\sum_{c=1}^{K-1} \delta(X=c) \log \pi_c / \pi_K\right) \\ &= \frac{1}{Z} \exp\left(\sum_{c=1}^{K-1} \delta(X=c) \theta_c\right) \end{aligned}$$

Given N i.i.d. observations $X \equiv \{x_1, \dots, x_N\}$, the likelihood is

$$\begin{aligned}\mathcal{L}(X|\boldsymbol{\theta}) &= \prod_{i=1}^N \frac{1}{Z(\boldsymbol{\theta})} h(x_i) \exp(\boldsymbol{\theta}^\top \boldsymbol{\phi}(x_i)) \\ &= \left(\frac{1}{Z(\boldsymbol{\theta})} \right)^N \left(\prod_{i=1}^N h(x_i) \right) \exp(\boldsymbol{\theta}^\top \sum_{i=1}^N \boldsymbol{\phi}(x_i))\end{aligned}$$

MAXIMUM-LIKELIHOOD ESTIMATION

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The log-likelihood $\ell(X|\boldsymbol{\theta}) = \log \mathcal{L}(X|\boldsymbol{\theta})$ is

$$\ell(X|\boldsymbol{\theta}) = \boldsymbol{\theta}^\top \left(\sum_{i=1}^N \boldsymbol{\phi}(x_i)\right) - N \log Z(\boldsymbol{\theta}) + \sum_{i=1}^N \log h(x_i)$$

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To calculate a maximum likelihood estimate, we only need the sum of the suff. statistics.

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At MLE of θ_d , the d th component of $\boldsymbol{\theta}$: $\frac{\partial \ell(X|\boldsymbol{\theta})}{\partial \theta_d} = 0$.

$$\begin{aligned} \sum_{i=1}^N \phi_d(x_i) &= N \frac{\partial \log Z(\boldsymbol{\theta})}{\partial \theta_d} \\ \frac{1}{N} \sum_{i=1}^N \phi_d(x_i) &= \frac{1}{Z(\boldsymbol{\theta})} \frac{\partial Z(\boldsymbol{\theta})}{\partial \theta_d} \\ &= \frac{1}{Z(\boldsymbol{\theta})} \int h(x) \frac{\partial \exp(\boldsymbol{\theta}^\top \boldsymbol{\phi}(x))}{\partial \theta_d} dx \\ &= \int \frac{1}{Z(\boldsymbol{\theta})} h(x) \exp(\boldsymbol{\theta}^\top \boldsymbol{\phi}(x)) \phi_d(x) dx \end{aligned}$$

Match empirical and population averages of $\phi(x)$:

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RHS: ‘moment parameters’ of the exponential distribution.

Thus: θ_{MLE} are natural parameters corresponding to empirical moment parameters (‘moment matching’).

MLE FOR EXPONENTIAL FAMILIES

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Is this a maximum?

- is second derivative (Hessian) negative (negative definite)?

We can show $\frac{\partial^2}{\partial \theta_i \partial \theta_j} \log Z(X|\theta) = \text{Cov}(\phi_i, \phi_j)$, and the Hessian of $\ell(X|\theta)$ is $-N$ times the feature covariance matrix

EXAMPLE

The 1-d Gaussian: $\phi = [x \ x^2]$

Moment parameters are mean and mean squared

Easy to find corresponding natural parameters

Quite often, it is not the case.

However, we will restrict ourselves to cases where it is.

MISSING DATA IN EXPONENTIAL FAMILY DISTRIBUTIONS

Let samples from the exponential family have two parts: $[x \ y]$.

Feature vector $\phi([x \ y]) := \phi(x, y)$.

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We observe only x . What is the posterior over y ?

$$P(y|x, \theta) = \frac{P(x, y|\theta)}{P(x|\theta)} = \frac{h(x, y)}{P(x|\theta)Z(\theta)} \exp(\theta^\top \phi(x, y))$$

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An exponential family distrib. over y (remember x is fixed) with:

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Not necessarily easy to work with, but will restrict to this case.
 y_i with different x_i belong to different exp. fam. distrbs.

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An algorithm for MLE in exp. fam. distrib. with missing data

Problem: Given observations i.i.d. $X = \{x_1, \dots, x_N\}$ from $P(x|\boldsymbol{\theta})$ where $P(X, Y|\boldsymbol{\theta})$ is exponential family, maximize w.r.t. $\boldsymbol{\theta}$

$$\ell(X|\boldsymbol{\theta}) = \log P(X|\boldsymbol{\theta}) = \sum_{i=1}^N \log P(x_i|\boldsymbol{\theta})$$

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MLE IN LATENT VARIABLE MODELS

$$\begin{aligned}\ell(X|\boldsymbol{\theta}) &= \sum_{i=1}^N \log P(x_i|\boldsymbol{\theta}) = \sum_{i=1}^N \log \int P(x_i, y_i|\boldsymbol{\theta}) dy_i \\ &= \sum_{i=1}^N \log \int q_i(y_i) \frac{P(x_i, y_i|\boldsymbol{\theta})}{q_i(y_i)} dy_i \quad (\text{for arbitrary densities } q_i(y_i))\end{aligned}$$

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MLE IN LATENT VARIABLE MODELS

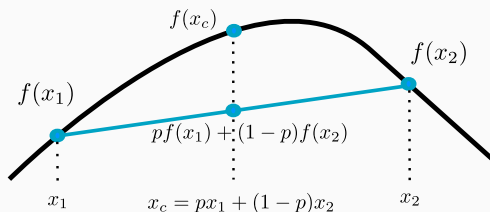
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JENSEN'S INEQUALITY

Let $f(x)$ be a concave real-valued function defined on \mathbb{X} .



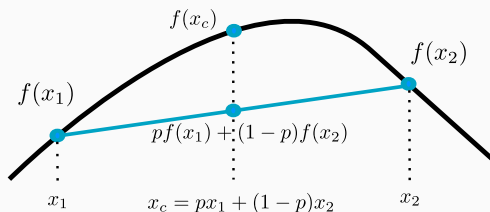
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A chord always lies below the function.

E.g. logarithm (defined on \mathbb{R}^+).

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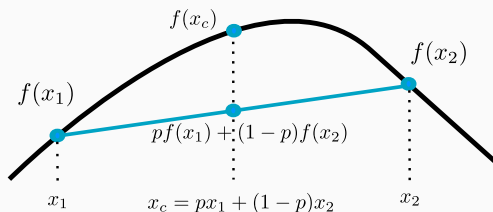
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Jensen: for any prob. vector $p = (p_1, \dots, p_K)$ and any set of points (x_1, \dots, x_K) ,
$$f\left(\sum_{i=1}^K p_i x_i\right) \geq \sum_{i=1}^K p_i f(x_i)$$

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In fact, for a prob. density $p(x)$, $f(\int_{\mathbb{X}} x p(x) dx) \geq \int_{\mathbb{X}} f(x) p(x) dx$

Defining $Q(Y) = \prod_{i=1}^N q_i(y_i)$,

$$\begin{aligned}\ell(X|\boldsymbol{\theta}) &\geq \sum_{i=1}^N \int q_i(y_i) \log P(x_i, y_i|\boldsymbol{\theta}) dy_i + \sum_{i=1}^N H(q_i) \\ &= \sum_{i=1}^N \mathbb{E}_{q_i}[\log P(x_i, y_i|\boldsymbol{\theta})] + \sum_{i=1}^N H(q_i) \\ &= \ell(X|\boldsymbol{\theta}) - \sum_{i=1}^N \text{KL}(q_i(y_i) \| P(y_i|X, \boldsymbol{\theta})) \\ &:= \mathcal{F}_X(\boldsymbol{\theta}, Q(\cdot))\end{aligned}$$

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$\mathcal{F}_X(\boldsymbol{\theta}, Q(\cdot))$ is a lower bound to the log-likelihood $\ell(X|\boldsymbol{\theta})$.

Sometimes called ‘variational free energy’ and is function of $\boldsymbol{\theta}$ and the ‘variational distribution’ $Q(Y)$ (X is fixed).

OPTIMIZING THE VARIATIONAL LOWER BOUND

Our original goal was to maximize the log-likelihood:

$$\theta_{MLE} = \operatorname{argmax} \ell(X|\theta)$$

EM algorithm: maximize the lower-bound instead

$$(\theta^*, Q^*) = \operatorname{argmax} \mathcal{F}_X(\theta, Q(\cdot))$$

Hopefully easier, since all summations are outside logarithms.

Strategy: Coordinate ascent.

Alternately maximize w.r.t Q and θ

First find best lower-bound given the current θ_s .

Optimize this lower-bound to find θ_{s+1} .

Maximizing $\mathcal{F}_X(\boldsymbol{\theta}, Q)$ with $\boldsymbol{\theta}$ fixed:

- Recall $\mathcal{F}_X(\boldsymbol{\theta}, Q) = \ell(X|\boldsymbol{\theta}) - \sum_{i=1}^N \text{KL}(q_i(y_i) \| P(y_i|x_i, \boldsymbol{\theta}))$

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- Solution: set $q_i(y_i) = P(y_i|x_i, \boldsymbol{\theta})$ for $i = 1, \dots, N$
- Recall: $P(\cdot|x_i, \boldsymbol{\theta})$ is an exponential family distribution with natural parameters $\boldsymbol{\theta}$ and feature vector $\boldsymbol{\phi}(x_i, \cdot)$

Maximizing $\mathcal{F}_X(\boldsymbol{\theta}, Q)$ with Q fixed:

$$\mathcal{F}_X(\boldsymbol{\theta}, Q) = \sum_{i=1}^N \mathbb{E}_{q_i}[\log P(x_i, y_i | \boldsymbol{\theta})] + \sum_{i=1}^N H(q_i)$$

The entropy terms $H(q_i)$ don't depend on $\boldsymbol{\theta}$. Ignore.

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$$\log P(x_i, y_i | \boldsymbol{\theta}) = \boldsymbol{\theta}^\top \boldsymbol{\phi}(x_i, y_i) + \log h(x_i) - \log Z(\boldsymbol{\theta})$$

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THE EXPECTATION-MAXIMIZATION ALGORITHM

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Compare with the fully observed log-likelihood:

$$\ell(X|\boldsymbol{\theta}) = \boldsymbol{\theta}^\top \left(\sum_{i=1}^N \boldsymbol{\phi}(x_i) \right) - N \log Z(\boldsymbol{\theta}) + \text{const}$$

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To maximize \mathcal{F}_X w.r.t. θ_d , solve $\frac{\partial}{\partial \theta_d} \mathcal{F}_X(\boldsymbol{\theta}, Q) = 0$:

- Solution: set $\boldsymbol{\theta}^*$ to match moments

$$\mathbb{E}_{\boldsymbol{\theta}^*}[\boldsymbol{\phi}_d(x, y)] = \frac{1}{N} \sum_{i=1}^N \mathbb{E}_{q_i}[\boldsymbol{\phi}_d(x_i, y_i)]$$

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Compare with the fully observed log-likelihood:

$$\ell(X|\boldsymbol{\theta}) = \boldsymbol{\theta}^\top \left(\sum_{i=1}^N \boldsymbol{\phi}(x_i) \right) - N \log Z(\boldsymbol{\theta}) + \text{const}$$

To maximize \mathcal{F}_X w.r.t. θ_d , solve $\frac{\partial}{\partial \theta_d} \mathcal{F}_X(\boldsymbol{\theta}, Q) = 0$:

- Solution: set $\boldsymbol{\theta}^*$ to match moments

$$\mathbb{E}_{\boldsymbol{\theta}^*}[\boldsymbol{\phi}_d(x, y)] = \frac{1}{N} \sum_{i=1}^N \mathbb{E}_{q_i}[\boldsymbol{\phi}_d(x_i, y_i)]$$

$q_i(y_i) = P(y_i|X, \boldsymbol{\theta}^{old})$, an exponential family distribution whose moment parameters can be calculated (by assumption).

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M-step (Maximization):

- Set θ^{s+1} so that $\mathbb{E}_{\theta^{s+1}}[\phi(x, y)] = \frac{1}{N} \sum_{i=1}^N \mathbb{E}_{q_i^s}[\phi(x_i, y_i)]$.

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After the E-step, $Q^s(Y) = P(Y|X, \boldsymbol{\theta}^{s-1})$

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Can also show that local maxima of \mathcal{F}_X are local maxima of ℓ .

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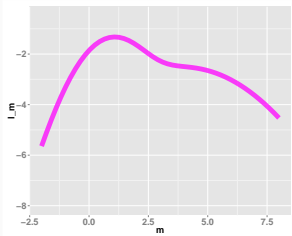
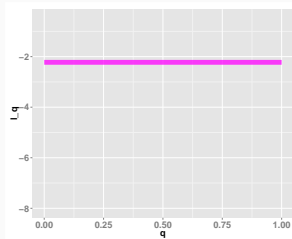
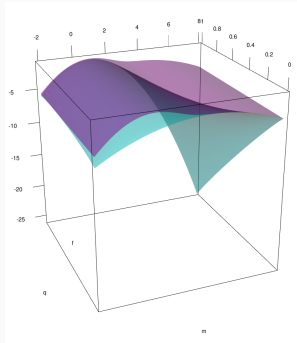
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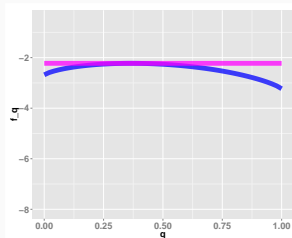
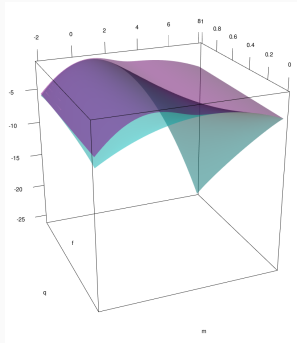
What is the posterior distribution over the hidden variable?

If we knew the hidden variable, what is the MLE?

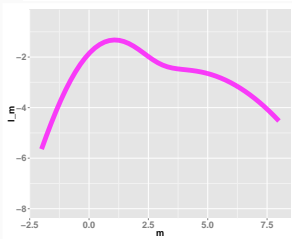
THE EM ALGORITHM



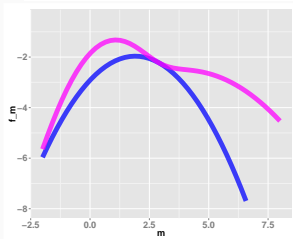
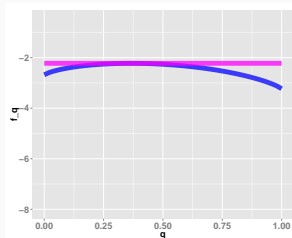
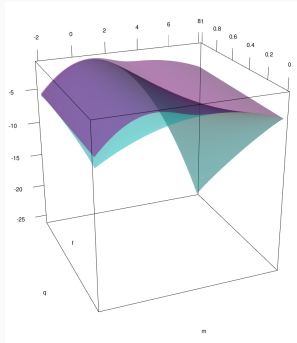
THE EM ALGORITHM



Initialize $m = 2.9$.



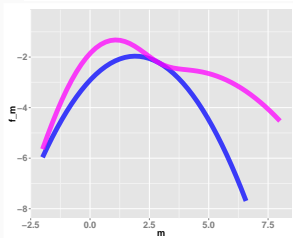
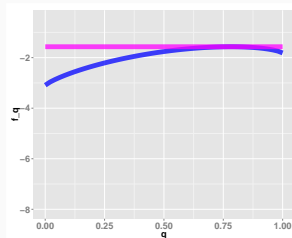
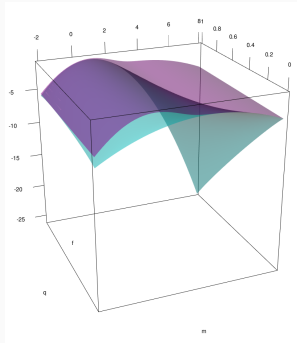
THE EM ALGORITHM



Initialize $m = 2.9$.

Set $q = 0.37$.

THE EM ALGORITHM

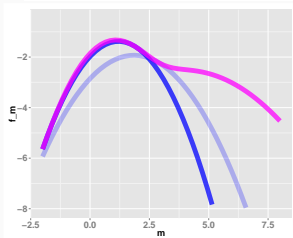
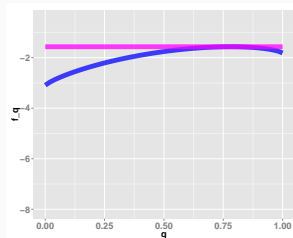
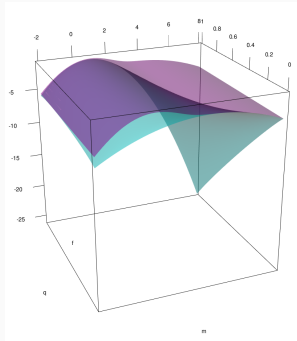


Initialize $m = 2.9$.

Set $q = 0.37$.

Set $m = 1.88$.

THE EM ALGORITHM



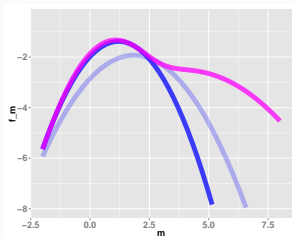
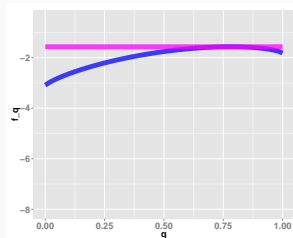
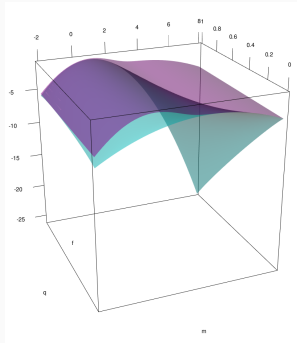
Initialize $m = 2.9$.

Set $q = 0.37$.

Set $m = 1.88$.

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THE EM ALGORITHM



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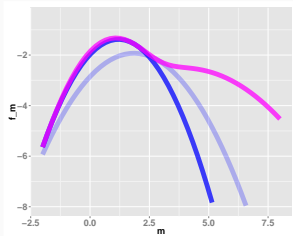
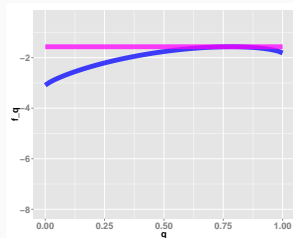
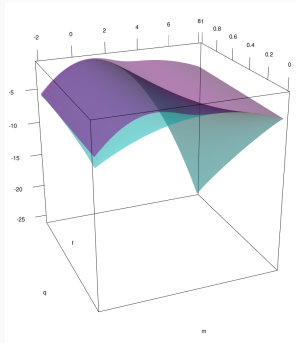
Set $q = 0.37$.

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THE EM ALGORITHM



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Repeat till convergence