## Stat 521A <br> Lecture 6

## Outline

- Exponential family: what?(8.2)
- Why? (Extra)
- Connection with GMs (8.3)
- Entropy (8.4)
- Projections (8.5)
- Querying a distribution ("inference") - 2.1.5
- Worst case complexity of exact inference (9.1)


## Exponential family

- Def 8.2.2. The exponential family is a set of distributions of the form

$$
\begin{aligned}
p(\mathbf{x} \mid \boldsymbol{\theta}) & =\frac{1}{Z(\boldsymbol{\theta})} h(\mathbf{x}) \exp \left(\mathbf{t}(\boldsymbol{\theta})^{T} \mathbf{T}(\mathbf{x})\right) \\
Z(\boldsymbol{\theta}) & \left.=\sum_{\mathbf{x} \in S} h(\mathbf{x}) \exp (\mathbf{t} \boldsymbol{\theta})^{T} \mathbf{T}(\mathbf{x})\right)
\end{aligned}
$$

Where $x \in X$ are the variables, $h(x)$ defines the support (must not depend on $\theta$ ), $T(x) \in R^{K}$ are the sufficient statistics, $\theta \in \Theta \subseteq R^{M}$ are the parameters, $\mathrm{t}(\theta)$ in $\mathrm{R}^{\mathrm{K}}$ are the natural parameters, and $\mathrm{Z}(\theta) \in \mathrm{R}^{+}$ is the partition function.
We would like $\Theta$ to be a convex open subset of $R^{M}$, and to be non-redundant (iff $\mathrm{t}(\theta)$ is invertible).

## Examples

- $X \sim \operatorname{Ber}(\theta)$.

$$
\begin{array}{rlr}
\mathbf{T}(x) & =[I(x=0), I(x=1)] & \\
\mathbf{t}(\boldsymbol{\theta}) & =[\log \theta, \log (1-\theta)] & \Theta=[0,1], \mathcal{X}=\{0,1\} \\
Z(\theta) & =1 & \\
p(x) & =\exp \left(\mathbf{T}(x)^{T} \mathbf{t}(\boldsymbol{\theta})\right) &
\end{array}
$$

- $X \sim N\left(\mu, \sigma^{2}\right)$.

$$
\begin{array}{rlr}
p(x) & =\frac{1}{\sqrt{2 \pi} \sigma} \exp \left(-\frac{1}{2 \sigma^{2}} x^{2}+\frac{\mu}{\sigma^{2}} x-\frac{1}{2 \sigma^{2}} \mu^{2}\right) \\
\mathbf{T}(x) & =\left[x, x^{2}\right] \\
\mathbf{t}\left(\mu, \sigma^{2}\right) & =\left[\frac{\mu}{\sigma^{2}},-\frac{1}{2 \sigma^{2}}\right] \\
Z\left(\mu, \sigma^{2}\right) & =\sqrt{2 \pi} \sigma \exp \left(\frac{\mu^{2}}{2 \sigma^{2}}\right) & \Theta=\mathbb{R} \times \mathbb{R}^{+}, \mathcal{X}=\mathbb{R}
\end{array}
$$

## Non-examples

- Let $X$ ~ Unif(a,b). Then

$$
\left.p(x \mid \boldsymbol{\theta})=\frac{1}{b-a} I(a \leq x \leq b)=\exp \left(\log \frac{1}{b-a}\right)\right) I(a \leq x \leq b)
$$

- Support depends on ltheta.
- Let $\mathrm{X} \sim \sum_{\mathrm{k}} \pi_{\mathrm{k}} \mathrm{f}\left(\mathrm{x}, \phi_{\mathrm{k}}\right)$ - mixture model. Cannot be written in required form.


## Linear exponential family

- Consider the set

$$
\Theta=\left\{\boldsymbol{\theta} \in \mathbb{R}^{K}: \int \exp \left(\boldsymbol{\theta}^{T} \mathbf{T}(\mathbf{x})\right) d \mathbf{x}<\infty\right\}
$$

- If $\Theta$ is open and convex, and $t(\theta)=\theta$, we say it is a linear exponential family.
- We write

$$
\begin{aligned}
p(\mathbf{x} \mid \boldsymbol{\eta}) & =\frac{1}{Z(\boldsymbol{\eta})} h(\mathbf{x}) \exp \left[\boldsymbol{\eta}^{T} \mathbf{T}(\mathbf{x})\right] \\
Z(\boldsymbol{\eta}) & =\int h(\mathbf{x}) \exp \left[\boldsymbol{\eta}^{T} \mathbf{T}(\mathbf{x})\right] d \mathbf{x}
\end{aligned}
$$

- Or

$$
\begin{aligned}
p(\mathbf{x} \mid \boldsymbol{\eta}) & =h(\mathbf{x}) \exp \left[\boldsymbol{\eta}^{T} \mathbf{T}(\mathbf{x})-A(\boldsymbol{\eta})\right] \\
A(\boldsymbol{\eta}) & =\log Z(\boldsymbol{\eta})
\end{aligned}
$$

## Bernoulli try 1

$$
\begin{aligned}
\mathbf{T}(x) & =[I(x=0), I(x=1)] \\
\boldsymbol{\eta} & =[\log \theta, \log (1-\theta)] \\
p(x) & =\exp \left(\boldsymbol{\eta}^{T} \mathbf{T}(x)\right)
\end{aligned}
$$

- However, (log \theta, log (1-ltheta)) is a curve, not a convex subset. Also, it is redundant.


## Bernoulli try 2

- Define

$$
\begin{aligned}
T(x) & =[I(x=1)] \\
\eta & =\log \frac{\theta}{1-\theta} \\
Z(\eta) & =1+\frac{\theta}{1-\theta}=\frac{1}{1-\theta} \\
p(x) & =\frac{1}{Z(\eta)} \exp (\eta T(x))=(1-\theta) \exp \left(x \log \frac{\theta}{1-\theta}\right) \\
p(x=0) & =(1-\theta) \\
p(x=1) & =(1-\theta) \frac{\theta}{1-\theta}=\theta
\end{aligned}
$$

## Gaussian - natural params

$$
\begin{aligned}
\boldsymbol{\eta} & =\left[\frac{\mu}{\sigma^{2}},-\frac{1}{2 \sigma^{2}}\right] \\
\mathbf{T}(x) & =\left[x, x^{2}\right]
\end{aligned}
$$

The natural parameter space is $\mathbb{R} \times \mathbb{R}^{-}$

## Finite sufficient statistics

- Defn. A statistic is a function of the data, T(D), where $\mathrm{D}=(\mathrm{x} 1, \ldots, \mathrm{xn})$. A sufficient statistic is one that contains all the information in the data. More formally, $T$ is sufficient for $\theta$ if $\theta->T(D)->D$.
- Let Xi ~ ExpFam. The likelihood is given by

$$
p(\mathcal{D} \mid \boldsymbol{\theta})=\prod_{i=1}^{n} p\left(\mathbf{x}_{i} \mid \boldsymbol{\theta}\right)=\frac{1}{Z(\boldsymbol{\theta})^{n}}\left[\prod_{i} h\left(\mathbf{x}_{i}\right)\right] \exp \left(\mathbf{t}(\boldsymbol{\theta})^{T} \sum_{i=1}^{n} \mathbf{T}\left(\mathbf{x}_{i}\right)\right)
$$

- Hence the distribution has sufficient statistics of size $K$, independent of $n$

$$
\left.\mathbf{T}(D)=\sum_{i=1}^{n} \mathbf{T}\left(\mathbf{x}_{i}\right)\right)
$$

- Thm (Pitman-Koopman-Darmois). The expfam is the only family (amongst those where support is indep of theta) with fixed sized suff stat.

Non-parametric models

- Parametric = fixed sized theta
- Exp fam = fixed size cuff stat



## LogZ is MGF

- Consider a linear expfam

$$
p(\mathbf{x} \mid \boldsymbol{\eta})=\frac{1}{Z(\boldsymbol{\eta})} h(\mathbf{x}) \exp \left[\boldsymbol{\eta}^{T} \mathbf{T}(\mathbf{x})\right]
$$

- Define

$$
\frac{1}{g(\boldsymbol{\eta})} \stackrel{\text { def }}{=} Z(\boldsymbol{\eta})=\int h(\mathbf{x}) \exp \left[\boldsymbol{\eta}^{T} \mathbf{T}(\mathbf{x})\right] d \mathbf{x}
$$

- Then

$$
\begin{aligned}
1 \begin{aligned}
1= & g(\boldsymbol{\eta}) \int h(\mathbf{x}) \exp \left[\boldsymbol{\eta}^{T} \mathbf{T}(x)\right] d \mathbf{x} \\
0= & \nabla g(\boldsymbol{\eta}) \int h(\mathbf{x}) \exp \left[\boldsymbol{\eta}^{T} \mathbf{T}(x)\right] d \mathbf{x} \\
& +g(\boldsymbol{\eta}) \int h(\mathbf{x}) \exp \left[\boldsymbol{\eta}^{T} \mathbf{T}(\mathbf{x})\right] \mathbf{T}(\mathbf{x}) d \mathbf{x} \\
\int p(\mathbf{x} \mid \boldsymbol{\eta}) \mathbf{T}(\mathbf{x}) d \mathbf{x}= & -\nabla g(\boldsymbol{\eta}) \int h(\mathbf{x}) \exp \left[\boldsymbol{\eta}^{T} \mathbf{T}(x)\right] d \mathbf{x}
\end{aligned}
\end{aligned}
$$

## LogZ is MGF

$$
\begin{aligned}
\int p(\mathbf{x} \mid \boldsymbol{\eta}) \mathbf{T}(\mathbf{x}) d \mathbf{x} & =-\nabla g(\boldsymbol{\eta}) \int h(\mathbf{x}) \exp \left[\boldsymbol{\eta}^{T} \mathbf{T}(x)\right] d \mathbf{x} \\
-\nabla \log g(\boldsymbol{\eta}) & =-\frac{\nabla g(\boldsymbol{\eta})}{g(\boldsymbol{\eta})}=-(\nabla g(\boldsymbol{\eta}))\left(\int h(\mathbf{x}) \exp \left[\boldsymbol{\eta}^{T} \mathbf{T}(\mathbf{x})\right] d \mathbf{x}\right) \\
E[\mathbf{T}(\mathbf{X})] & =-\nabla \log g(\boldsymbol{\eta})=\nabla \log Z(\boldsymbol{\eta})
\end{aligned}
$$

## MLE is moment matching

- Proof

$$
\begin{aligned}
\log p(\mathcal{D} \mid \boldsymbol{\theta}) & =-n \log Z(\boldsymbol{\theta})+\boldsymbol{\theta}^{T} \mathbf{T}(\mathcal{D}) \\
\nabla_{\boldsymbol{\theta}} \ell(\boldsymbol{\theta}) & =-n \nabla_{\boldsymbol{\theta}} \log Z(\boldsymbol{\theta})+\mathbf{T}(\mathcal{D})=\mathbf{0} \\
E \mathbf{T}(\mathbf{X}) & =\frac{1}{n} \mathbf{T}(\mathcal{D})
\end{aligned}
$$

- Example. Gaussian, $T(X)=\left(X, X^{\wedge} 2\right)$.

$$
\begin{aligned}
E[X] & =\mu=\frac{1}{n} \sum_{i} x_{i} \\
\operatorname{Var}[X] & =\left(E X^{2}\right)-(E X)^{2} \\
E\left[X^{2}\right] & =\sigma^{2}+\mu^{2}=\frac{1}{n} \sum_{i} x_{i}^{2} \\
\sigma^{2} & =\frac{1}{n} \sum_{i} x_{i}^{2}-\mu^{2}
\end{aligned}
$$

## Conjugate priors

- Defn. A prior $p(\theta) \in F$ is conjugate to a likelihood $p(D \mid \theta)$ if the posterior satistifes $p(\theta \mid D) \in F$, i.e., has the same functional form as the prior.
- Thm. All dist in expfam have conj prior.
- Most distrib with conj prior are in exp fam.


## Maximum entropy principle

- Defn. The entropy of a pmf is

$$
H(p) \stackrel{\text { def }}{=}-\sum_{x} p(x) \log p(x), H(p) \geq 0
$$

- The differential entropy of a pdf can be -ve

$$
h(p) \stackrel{\text { def }}{=}-\int_{S} p(x) \log p(x) d x
$$

- The relative entropy, or KL divergence, from $p$ to $q$ is given by

$$
K L(p, q) \stackrel{\text { def }}{=} \sum_{x} p(x) \log \frac{p(x)}{q(x)}
$$

- KL is always $>=0$, even for pdf's.


## Maxent principle

- Suppose we want to pick the most uncertain distribution (principle of least commitment) subject to the constraints that

$$
\sum_{x} f_{k}(x) p(x)=F_{k}
$$

- Optimize the Lagrangian

$$
\begin{aligned}
J(p) & =-\sum_{x} p(x) \log p(x)+\lambda_{0}\left(1-\sum_{x} p(x)\right)+\sum_{k} \lambda_{k}\left(F_{k}-\sum_{x} p(x) f_{k}(x)\right) \\
\frac{\partial J}{\partial p(x)} & =-1-\log p(x)-\lambda_{0}-\sum_{k} \lambda_{k} f_{k}(x)=0 \\
p(x) & =\frac{1}{Z} \exp \left(-\sum_{k} \lambda_{k} f_{k}(x)\right) \\
Z & =e^{1+\lambda_{0}} \\
1 & =\sum_{x} p(x)=\frac{1}{Z} \sum_{x} \exp \left(-\sum_{k} \lambda_{k} f_{k}(x)\right) \\
Z & =Z(\boldsymbol{\lambda})=\sum_{x} \exp \left(-\sum_{k} \lambda_{k} f_{k}(x)\right)
\end{aligned}
$$

## Gaussian maximizes entropy

- MVN is in expfam. $\quad p(\mathbf{x})=\frac{1}{Z} \exp \left(-\frac{1}{2} \mathbf{x}^{T} \mathbf{K} \mathbf{x}\right)=\frac{1}{Z} \exp \left(\sum_{k} \lambda_{k} f_{k}(\mathbf{x})\right)$

$$
f_{i j}(\mathbf{x})=x_{i} x_{j}, \lambda_{i j}=\frac{1}{2} K_{i j}
$$

Theorem 0.1. Let $g(\mathbf{x})$ be any density satisfying $\int g(\mathbf{x}) x_{i} x_{j}=\Sigma_{i j}$. Let $\phi=\mathcal{N}(\mathbf{0}, \boldsymbol{\Sigma})$. Then $h(g) \leq h(\phi)$.

Proof. (From (?, p234).) We have

$$
\begin{align*}
0 & \leq K L(g \| \phi)  \tag{1}\\
& =\int g(\mathbf{x}) \log \frac{g(\mathbf{x})}{\phi(\mathbf{x})} d \mathbf{x}  \tag{2}\\
& =-h(g)-\int g(\mathbf{x}) \log \phi(\mathbf{x}) d \mathbf{x}  \tag{3}\\
& \left.=-h(g)-\int \phi(\mathbf{x}) \log \phi(\mathbf{x}) d \mathbf{x} \mathbf{( * *}^{*}\right)  \tag{4}\\
& =-h(g)+h(\phi) \tag{5}
\end{align*}
$$

where the line marked (**) follows since $g$ and $\phi$ yield the same moments for the quadratic form $\log \phi(\mathbf{x})$.

## Some GMs are expfam models

- We showed earlier that many +ve UGM can be represented as an expfam

$$
p(\mathbf{x})=\frac{1}{Z} \exp \left(\sum_{i} \boldsymbol{\theta}_{i}^{T} f_{i}(\mathbf{x})\right)
$$

- Most CPDs can be represented as expfam
- Eg table $p(X \mid U)$. $T(X, U)=[I(X=x), I(U=u)]$, $t($ theta $)=[\backslash \log p(x \mid u)]$.
- Eg lingauss.

$$
\begin{aligned}
p(x \mid \mathbf{u}) & =\frac{1}{\sqrt{2 \pi} \sigma} \exp \left(-\frac{1}{2 \sigma^{2}}\left(x-\left(w_{0}+w_{1} u_{1}+\cdots+w_{k} u_{k}\right)\right)^{2}\right) \\
\mathbf{T}(x, \mathbf{u}) & =\left[1, x, u_{1}, \ldots, u_{k}, x u_{1}, \ldots, x u_{k}, u_{1}^{2}, u_{1} u_{2}, \ldots, u_{k}^{2}\right]
\end{aligned}
$$

- Product of expfam is expfam.


## DGMs are curved expfam

- In general, the fact that CPDs sum to 1 locally means that they are not linear expfam
- See p248 of K\&F
- Geiger'01 shows that DGMs are curved expfam models (curved means the params are not linearly indep, so \theta is smaller than $t($ (theta)).
- Geiger'01 also shows that GMs with hidden variables are stratified exponential families (SEFs) a finite union of CEFs of various dimensions satisfying some regularity conditions.

Stratified exponential families: Graphical models and model selection Dan Geiger, David Heckerman, Henry King, and Christopher Meek Source: Ann. Statist. Volume 29, Number 2 (2001), 505-529.

## Entropy of an expfam model

- Thm 8.4.1. If $X \sim \operatorname{ExpFam}($ theta), then

$$
H\left(P_{\boldsymbol{\theta}}(\mathbf{x})\right)=\log Z(\boldsymbol{\theta})-E\left[\mathbf{T}(\mathbf{x})^{T} \mathbf{t}(\boldsymbol{\theta})\right]
$$

- Ex 8.4.2. Gaussian.

$$
\begin{aligned}
p(x) & =\frac{1}{\sqrt{2 \pi} \sigma} \exp \left(-\frac{1}{2 \sigma^{2}} x^{2}+\frac{\mu}{\sigma^{2}} x-\frac{1}{2 \sigma^{2}} \mu^{2}\right) \\
\mathbf{T}(x) & =\left[x, x^{2}\right] \\
\mathbf{t}\left(\mu, \sigma^{2}\right) & =\left[\frac{\mu}{\sigma^{2}},-\frac{1}{2 \sigma^{2}}\right] \\
Z\left(\mu, \sigma^{2}\right) & =\sqrt{2 \pi} \sigma \exp \left(\frac{\mu^{2}}{2 \sigma^{2}}\right) \\
H & =\frac{1}{2} \ln \left(2 \pi \sigma^{2}\right)+\frac{\mu^{2}}{2 \sigma^{2}}-\frac{\mu}{\sigma^{2}} E[x]+\frac{1}{2 \sigma^{2}} E\left[x^{2}\right] \\
& =\frac{1}{2} \ln \left(2 \pi \sigma^{2}\right)+\frac{\mu^{2}}{2 \sigma^{2}}-\frac{2 \mu^{2}}{2 \sigma^{2}}+\frac{1}{2 \sigma^{2}}\left(\mu^{2}+\sigma^{2}\right) \\
& =\frac{1}{2} \ln \left(2 \pi \sigma^{2}\right)+\frac{1}{2}=\frac{1}{2} \ln \left(2 \pi \sigma^{2}\right)+\frac{1}{2} \ln e=\frac{1}{2} \ln \left(2 \pi \sigma^{2} e\right) \quad 25
\end{aligned}
$$

## Entropy of a GM

- Thm 8.4.3. If $P(X)=1 / Z \prod_{c} \phi_{c}(X)$ is a UGM, then

$$
H\left(P_{\boldsymbol{\theta}}(\mathbf{x})\right)=\log Z(\boldsymbol{\theta})+\sum_{c} E\left[-\ln \phi_{c}\left(\mathbf{x}_{c}\right)\right]
$$

- Thm 8.4.5. If $P(X)$ is a $D G M$, then
- Pf.

$$
H(P(\mathbf{X}))=\sum_{i} H\left(P\left(X_{i} \mid X_{\pi_{i}}\right)\right)
$$

$$
\begin{aligned}
H(P(\mathbf{X})) & =E[-\log p(\mathbf{X})]=E\left[-\sum_{i} \log p\left(X_{i} \mid \mathbf{X}_{\pi_{i}}\right)\right] \\
& =\sum_{i} E\left[-\log p\left(X_{i} \mid \mathbf{X}_{\pi_{i}}\right)\right]=\sum_{i} H\left(P\left(X_{i} \mid \mathbf{X}_{\pi_{i}}\right)\right) \\
& =\sum_{i} \sum_{\mathbf{X}_{\pi_{i}}} p\left(\mathbf{x}_{\pi_{i}}\right) H\left(P\left(X_{i} \mid \mathbf{x}_{\pi_{i}}\right)\right)
\end{aligned}
$$

- Thm 8.4.6. If $\mathrm{P}(\mathrm{X})$ is a DGM , then

$$
\sum_{i} \min _{\mathbf{x}_{\pi_{i}}} H\left(P\left(X_{i} \mid \mathbf{x}_{\pi_{i}}\right)\right) \leq H(P(\mathbf{X})) \leq \sum_{i} \max _{\mathbf{x}_{\pi_{i}}} H\left(P\left(X_{i} \mid \mathbf{x}_{\pi_{i}}\right)\right)
$$

## Projections

- Def 8.5.1. Let Pba distribution and $Q$ a convex set of distributions.
- The I-projection (information) is

$$
Q^{I}=\arg \min _{Q \in \mathcal{Q}} D(Q \| P) \quad \text { Zero forcing: } \mathrm{P}=0=>\mathrm{Q}=0 \quad \text { Mode seeking }
$$

- The M-projection (moment) is

$$
Q^{M}=\arg \min _{Q \in \mathcal{Q}} D(P \| Q) \quad \mathrm{Q}=0=>\mathrm{P}=0 \quad \text { High variance }
$$



## M-projection is moment matching

- Thm 8.5.5. Let $P$ be any distrib over $X$, and let $Q$ be expfam. If there is a set of params $\theta$ st $\mathrm{E}_{\mathrm{Q}}(\theta)[\tau(\mathrm{X})]=$ $\mathrm{E}_{\mathrm{P}}[\tau(\mathrm{X})]$, then the M -projection of P onto Q is $\mathrm{Q}_{\theta}$.
- Ex. Let $Q=$ fully factorized distribution. Then $Q^{\wedge} M$ is given by product of marginals.

$$
Q^{M}(\mathbf{x})=p\left(X_{1}\right) \ldots p\left(X_{d}\right)
$$

- Ex. Let $P=$ mix Gaussians, $Q=$ single Gaussian.

$$
\begin{aligned}
p(\mathbf{x}) & =\sum_{k} \pi_{k} \mathcal{N}\left(\mathbf{x} \mid \boldsymbol{\mu}_{k}, \boldsymbol{\Sigma}_{k}\right) \\
Q^{M}(\mathbf{x}) & =\mathcal{N}\left(\mathbf{x} \mid \boldsymbol{\mu}_{Q}, \boldsymbol{\Sigma}_{Q}\right) \\
\boldsymbol{\mu}_{Q} & =\sum_{k} \pi_{k} \boldsymbol{\mu}_{k} \\
\boldsymbol{\Sigma}_{Q} & =\sum_{k} \pi_{k}\left(\boldsymbol{\Sigma}_{k}+\left(\boldsymbol{\mu}_{k}-\boldsymbol{\mu}_{Q}\right)\left(\boldsymbol{\mu}_{k}-\boldsymbol{\mu}_{Q}\right)^{T}\right)
\end{aligned}
$$

## I-projection

- I-projection requires computing expectations of $\log (P)$ - which often factorizes - wrt Q, and the entropy of Q.

$$
Q^{I}=\arg \min _{Q \in \mathcal{Q}} D(Q \| P)=\arg \min \sum_{x} Q(x) \log \frac{Q(x)}{P(x)}
$$

- We can choose $Q$ to be "simple", so that it is easy to compute these expectations and entropy terms.
- This is the basis of variational inference.
- By contrast, M-projections require expectations wrt P. Usually this can only be done locally, as in expectation propagation.


## Querying a distribution ("inference")

- Suppose we have a joint $p\left(X_{1}, \ldots, X_{d}\right)$. Partition the variables into $E$ (evidence), $Q$ (query), and $H$ (hidden/ nuisance). We might pose the following queries
- Conditional probability (posterior):

$$
p\left(\mathbf{X}_{Q} \mid \mathbf{x}_{E}\right) \propto \sum_{\mathbf{x}_{H}} p\left(\mathbf{X}_{Q}, \mathbf{x}_{E}, \mathbf{x}_{H}\right)
$$

- MAP estimate $(\mathrm{H}=\emptyset)$ (posterior mode)

$$
\mathbf{x}_{Q}^{*}=\arg \max _{\mathbf{x}_{Q}} p\left(\mathbf{x}_{Q} \mid \mathbf{x}_{E}\right)=\arg \max _{\mathbf{x}_{Q}} p\left(\mathbf{x}_{Q}, \mathbf{x}_{E}\right)
$$

- Marginal MAP estimate (mode of marginal post):

$$
\mathbf{x}_{Q}^{*}=\arg \max _{\mathbf{x}_{Q}} p\left(\mathbf{x}_{Q} \mid \mathbf{x}_{E}\right)=\arg \max _{\mathbf{x}_{Q}} \sum_{\mathbf{x}_{H}} p\left(\mathbf{x}_{Q}, \mathbf{x}_{E}, \mathbf{x}_{H}\right)
$$

## MAP vs marginal MAP

- Max max $=$ max sum
- Ex 2.1.12. Joint is

$$
\begin{aligned}
a^{*}=\arg \max _{a} \sum_{b} p(a, b)=1 & \left.B=0 \left\lvert\, \begin{array}{|c|c|}
\hline 0.04 & 0.3 \\
b^{*} & =\arg \max _{b} \sum_{a} p(a, b)=1 \\
(a, b)^{*} & =\arg \max _{a, b} p(a, b)=(0,1) \\
\hline 0.36 & B=1 \\
0.3 \\
0.66 \\
0.4 & 0.6
\end{array}\right.\right)
\end{aligned}
$$

- One can show that max sum is strictly computationally harder than sum, which is in turn harder than max


## Speech recognition

- Eg speech recognition. Let $\mathrm{Q}=$ words, $\mathrm{H}=$ pronunciation (phonemes sequence), $\mathrm{E}=$ signal.
- We often make the following approximation, which lets us use the Viterbi algorithm

$$
\mathbf{w}^{*}=\arg \max _{\mathbf{W}} \sum_{\mathbf{h}} p(\mathbf{w}, \mathbf{h} \mid \mathbf{e}) \approx \arg \max _{\mathbf{w}} \max _{\mathbf{h}} p(\mathbf{w}, \mathbf{h} \mid \mathbf{e})
$$

- Eg. Consider W1="a back", vs W2="aback". There might be 10 alternative state sequences for W 1 , each with prob 0.03, but just one sequence for W 2 , with prob 0.2. Viterbi would choose W2, but W1 is actually more likely.


## Bayesian statistics

- Bayesian statistics amounts to defining a single joint distribution for both "variables" - latent and observed - and "parameters" (often fixed in number), and then querying the parameters.

$$
p(\boldsymbol{\theta} \mid \mathbf{X}, \mathbf{Y}) \propto p(\boldsymbol{\theta}) \prod_{i} \int p\left(\mathbf{z}_{i} \mid \boldsymbol{\theta}\right) p\left(\mathbf{y}_{i} \mid \mathbf{x}_{i}, \mathbf{z}_{i}, \boldsymbol{\theta}\right) d \mathbf{z}_{i}
$$



## Probability of evidence

- To compute conditional queries, we need to evaluate $\mathrm{p}\left(\mathrm{x}_{\mathrm{E}}\right)$

$$
\begin{aligned}
p\left(\mathbf{X}_{Q} \mid \mathbf{x}_{E}\right) & =\frac{\sum_{\mathbf{x}_{H}} p\left(\mathbf{X}_{Q}, \mathbf{x}_{E}, \mathbf{x}_{H}\right)}{p\left(\mathbf{x}_{E}\right)} \\
p\left(\mathbf{x}_{E}\right) & =\sum_{\mathbf{x}_{Q}} \sum_{\mathbf{x}_{H}} p\left(\mathbf{x}_{Q}, \mathbf{x}_{E}, \mathbf{x}_{H}\right)
\end{aligned}
$$

- This may be a high dimensional integral

$$
\begin{aligned}
p(\boldsymbol{\theta} \mid \mathbf{X}, \mathbf{Y}) & =\frac{p(\boldsymbol{\theta}) \prod_{i} \int p\left(\mathbf{z}_{i} \mid \boldsymbol{\theta}\right) p\left(\mathbf{y}_{i} \mid \mathbf{x}_{i}, \mathbf{z}_{i}, \boldsymbol{\theta}\right) d \mathbf{z}_{i}}{p(\mathbf{X}, \mathbf{Y})} \\
p(\mathbf{X}, \mathbf{Y}) & =\int p(\boldsymbol{\theta})\left[\prod_{i} \int p\left(\mathbf{z}_{i} \mid \boldsymbol{\theta}\right) p\left(\mathbf{y}_{i} \mid \mathbf{x}_{i}, \mathbf{z}_{i}, \boldsymbol{\theta}\right) d \mathbf{z}_{i}\right] d \boldsymbol{\theta}
\end{aligned}
$$

- $p\left(x_{E}\right)$ can be used to decide how likely $x_{E}$ is to have come from this model (classification and model selection)


## Sampling

- Often the posterior is too big to even store explicitly.
- Marginals and MAP estimates are one summary, but may be unrepresentative.
- Samples may provide a better summary.
- eg Attractive Ising model has 2 modes, all 0 and all 1. The marginals are [0.5, 0.5].
- We want to be able to sample from $p(x Q \mid x E)$
- Sometimes we can do this even if we cannot evaluate $p(x E)$ - this is the key idea behind MCMC


## Monte Carlo integration

- Sometimes we want to $E[f(x Q) \mid x E]$, where $f()$ depends on global properties of $Q$, so we cannot use marginal distributions.
- However, if we sample from $p(X Q \mid x E)$, we can use

$$
E\left[f\left(\mathbf{X}_{Q}\right) \mid \mathbf{x}_{E}\right]=\int f\left(\mathbf{x}_{Q}\right) p\left(\mathbf{x}_{Q} \mid \mathbf{x}_{E}\right) d \mathbf{x}_{Q} \approx \frac{1}{N} \sum_{i=1}^{n} f\left(\mathbf{x}_{Q}^{i}\right)
$$

## Inference in discrete state spaces

- We will mostly focus on the case where $Q$ and $H$ are discrete rv's (E can be cts or discrete).
- Thus everything amounts to computing a large number of sums as quickly as possible.
- We will also consider the case where Q, H and E are all jointly Gaussian, where exact answers can also be obtained.
- For general distributions (eg for applications in Bayesian statistics), exact inference is usually not possible (except 1 layer of parameters with conjugate priors and no latent variables).


## Complexity of inference

- Consider computing p(X_Q), p(X_Q|x_E), or p(x_E) for a discrete state space.
- Later we will show that if $P$ is representable by a GM, then we can compute these quantities efficiently, if the graph has special properties.
- However, in general, the problem is computationally expensive.


## Complexity of exact inference

- Thm 9.1.1. Given a DGM, deciding if $p(X=x)>0$ is NP-complete.
- Pf. Easy to see is in NP (linear time to check if $p(x)>0$.) Can show is NP-hard by showing how to reduce 3-SAT to a poly-sized DGM.


$$
X=\left(Q_{1} \vee \neg Q_{2} \vee Q_{3}\right) \wedge\left(Q_{2} \vee Q_{5} \vee Q_{3}\right) \cdots
$$

## Complexity of exact inference

- Defn. NP is the class of problems of the form "are there any solutions $x$ such that $f(x)$ is true". \#P is the class of problems "Count the number of solutions x st $\mathrm{f}(\mathrm{x})$ is true".
- Thm 9.1.2. Given a $D G M$, computing $p(X=x)$ is \#Pcomplete.


## Complexity of approximate inference

- Def 9.1.3. A estimate $\rho$ has absolute error $\varepsilon$ if

$$
\left|p\left(\mathbf{x}_{Q} \mid \mathbf{x}_{e}\right)-\rho\right| \leq \epsilon
$$

- Def 9.1.4. An estimate $\rho$ has relative error $\varepsilon$ if

$$
\frac{\rho}{1+\epsilon} \leq p\left(\mathbf{x}_{Q} \mid \mathbf{x}_{e}\right) \leq \rho(1+\epsilon)
$$

- Thm 9.1.5. Given a DGM, finding a number $\rho$ which as relative error $\varepsilon$ for $p(X=x)$ is NP-hard.
- Thm 9.1.6. Given a DGM, finding a number $\rho$ that has absolute error $\varepsilon$ for $p(X \mid e)$ is NP-hard for any $0 \leq \varepsilon \leq 0.5$.

