Probabilistic & Unsupervised Learning
Approximate Inference

Exponential families: convexity, duality and free energies

Maneesh Sahani
`maneesh@gatsby.ucl.ac.uk`

Gatsby Computational Neuroscience Unit, and
MSc ML/CSML, Dept Computer Science
University College London

Term 1, Autumn 2020

Exponential families: the log partition function

Consider an exponential family distribution with sufficient statistic $s(X)$ and natural parameter $\boldsymbol{\theta}$ (and no base factor in X alone). We can write its probability or density function as

$$p(X|\boldsymbol{\theta}) = \exp\left(\boldsymbol{\theta}^{\mathsf{T}} s(X) - \Phi(\boldsymbol{\theta})\right)$$

where $\Phi(\boldsymbol{\theta})$ is the log partition function

$$\Phi(\boldsymbol{\theta}) = \log \sum_x \exp\left(\boldsymbol{\theta}^{\mathsf{T}} s(x)\right)$$

$\Phi(\boldsymbol{\theta})$ plays an important role in the theory of the exponential family. For example, it maps natural parameters to the moments of the sufficient statistics:

$$\frac{\partial}{\partial\boldsymbol{\theta}}\Phi(\boldsymbol{\theta}) = e^{-\Phi(\boldsymbol{\theta})}\sum_x s(x)e^{\boldsymbol{\theta}^{\mathsf{T}} s(x)} = \mathbb{E}_{\boldsymbol{\theta}}\left[s(X)\right] = \boldsymbol{\mu}(\boldsymbol{\theta}) = \boldsymbol{\mu}$$

$$\frac{\partial^2}{\partial\boldsymbol{\theta}^2}\Phi(\boldsymbol{\theta}) = e^{-\Phi(\boldsymbol{\theta})}\sum_x s(x)^2 e^{\boldsymbol{\theta}^{\mathsf{T}} s(x)} - e^{-2\Phi(\boldsymbol{\theta})}\left[\sum_x s(x)e^{\boldsymbol{\theta}^{\mathsf{T}} s(x)}\right]^2 = \mathbb{V}_{\boldsymbol{\theta}}\left[s(X)\right]$$

The second derivative is thus positive semi-definite, and so $\Phi(\boldsymbol{\theta})$ is convex in $\boldsymbol{\theta}$.

Exponential families: mean parameters and negative entropy

A (minimal) exponential family distribution can also be parameterised by the means of the sufficient statistics.

$$\boldsymbol{\mu}(\boldsymbol{\theta}) = \mathbb{E}_{\boldsymbol{\theta}}\left[s(X)\right]$$

Consider the negative entropy of the distribution as a function of the mean parameter:

$$\Psi(\boldsymbol{\mu}) = \mathbb{E}_{\boldsymbol{\theta}}\left[\log p(X|\boldsymbol{\theta}(\boldsymbol{\mu}))\right] = \boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{\mu} - \Phi(\boldsymbol{\theta})$$

so

$$\boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{\mu} = \Phi(\boldsymbol{\theta}) + \Psi(\boldsymbol{\mu})$$

The negative entropy is dual to the log-partition function. For example,

$$\begin{aligned}\frac{d}{d\boldsymbol{\mu}}\Psi(\boldsymbol{\mu}) &= \frac{\partial}{\partial\boldsymbol{\mu}}\left(\boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{\mu} - \Phi(\boldsymbol{\theta})\right) + \frac{d\boldsymbol{\theta}}{d\boldsymbol{\mu}}\frac{\partial}{\partial\boldsymbol{\theta}}\left(\boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{\mu} - \Phi(\boldsymbol{\theta})\right)\\ &= \boldsymbol{\theta} + \frac{d\boldsymbol{\theta}}{d\boldsymbol{\mu}}(\boldsymbol{\mu} - \boldsymbol{\mu}) = \boldsymbol{\theta}\end{aligned}$$

Exponential families: duality

The log partition function and negative entropy are Legendre dual or convex conjugate functions.

Consider the KL divergence between distributions with natural parameters $\boldsymbol{\theta}$ and $\boldsymbol{\theta}'$:

$$\begin{aligned}\mathbf{KL}\left[\boldsymbol{\theta}\middle\|\boldsymbol{\theta}'\right] = \mathbf{KL}\left[p(X|\boldsymbol{\theta})\middle\|p(X|\boldsymbol{\theta}')\right] &= \mathbb{E}_{\boldsymbol{\theta}}\left[-\log p(X|\boldsymbol{\theta}') + \log p(X|\boldsymbol{\theta})\right]\\ &= -\boldsymbol{\theta}'^{\mathsf{T}}\boldsymbol{\mu} + \Phi(\boldsymbol{\theta}') + \Psi(\boldsymbol{\mu}) \geq 0\\ \Rightarrow \Psi(\boldsymbol{\mu}) &\geq \boldsymbol{\theta}'^{\mathsf{T}}\boldsymbol{\mu} - \Phi(\boldsymbol{\theta}')\end{aligned}$$

where $\boldsymbol{\mu}$ are the mean parameters corresponding to $\boldsymbol{\theta}$.

Now, the minimum KL divergence of zero is reached iff $\boldsymbol{\theta} = \boldsymbol{\theta}'$, so

$$\Psi(\boldsymbol{\mu}) = \sup_{\boldsymbol{\theta}'}\left[\boldsymbol{\theta}'^{\mathsf{T}}\boldsymbol{\mu} - \Phi(\boldsymbol{\theta}')\right] \qquad \text{and, if finite} \qquad \boldsymbol{\theta}(\boldsymbol{\mu}) = \operatorname*{argmax}_{\boldsymbol{\theta}'}\left[\boldsymbol{\theta}'^{\mathsf{T}}\boldsymbol{\mu} - \Phi(\boldsymbol{\theta}')\right]$$

The left-hand equation is the definition of the conjugate dual of a convex function.

Continuous functions are reciprocally dual, so we also have:

$$\Phi(\boldsymbol{\theta}) = \sup_{\boldsymbol{\mu}'}\left[\boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{\mu}' - \Psi(\boldsymbol{\mu}')\right] \qquad \text{and, if finite} \qquad \boldsymbol{\mu}(\boldsymbol{\theta}) = \operatorname*{argmax}_{\boldsymbol{\mu}'}\left[\boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{\mu}' - \Psi(\boldsymbol{\mu}')\right]$$

Thus, duality gives us another relation between $\boldsymbol{\theta}$ and $\boldsymbol{\mu}$.

Duality, inference and the free energy

Consider a joint exponential family distribution on observed $\mathbf{x}$ and latent $\mathbf{z}$.

$$p(\mathbf{x},\mathbf{z}) = \exp\left[\boldsymbol{\theta}^{\mathsf{T}} s(\mathbf{x},\mathbf{z}) - \Phi_{XZ}(\boldsymbol{\theta})\right]$$

The posterior on $\mathbf{z}$ is also in the exponential family, with the clamped sufficient statistic $s_Z(\mathbf{z};\mathbf{x}) = s_{XZ}(\mathbf{x}^{\mathrm{obs}},\mathbf{z})$; the same (now possibly redundant) natural parameter $\boldsymbol{\theta}$; and partition function $\Phi_Z(\boldsymbol{\theta}) = \log\sum_{\mathbf{z}}\exp\boldsymbol{\theta}^{\mathsf{T}} s_Z(\mathbf{z})$.

The likelihood is

$$\mathcal{L}(\boldsymbol{\theta}) = p(\mathbf{x}|\boldsymbol{\theta}) = \sum_{\mathbf{z}} e^{\boldsymbol{\theta}^{\mathsf{T}} s(\mathbf{x},\mathbf{z}) - \Phi_{XZ}(\boldsymbol{\theta})} = \sum_{\mathbf{z}} e^{\boldsymbol{\theta}^{\mathsf{T}} s_Z(\mathbf{z};\mathbf{x})} e^{-\Phi_{XZ}(\boldsymbol{\theta})} = \exp[\Phi_Z(\boldsymbol{\theta}) - \Phi_{XZ}(\boldsymbol{\theta})]$$

So we can write the log-likelihood as

$$\ell(\boldsymbol{\theta}) = \sup_{\boldsymbol{\mu}_Z}[\underbrace{\boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{\mu}_Z - \Phi_{XZ}(\boldsymbol{\theta})}_{\langle\log p(\mathbf{x},\mathbf{z})\rangle_q} - \underbrace{\Psi(\boldsymbol{\mu}_Z)}_{-\mathbf{H}[q]}] = \sup_{\boldsymbol{\mu}_Z}\mathcal{F}(\boldsymbol{\theta},\boldsymbol{\mu}_Z)$$

This is the familiar free energy with $q(\mathbf{z})$ represented by its mean parameters $\boldsymbol{\mu}_Z$!

Inference with mean parameters

We have described inference in terms of the distribution q, approximating as needed, then computing expected suff stats. Can we describe it instead as an optimisation over $\boldsymbol{\mu}$ directly?

$$\boldsymbol{\mu}_Z^* = \operatorname*{argmax}_{\boldsymbol{\mu}_Z}[\boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{\mu}_Z - \Psi(\boldsymbol{\mu}_Z)]$$

Concave maximisation(!), but two complications:

- The optimum must be found over feasible means. Interdependance of the sufficient statistics may prevent arbitrary sets of mean sufficient statistics being achieved
  - Feasible means are convex combinations of all the single-configuration sufficient statistics.

    $$\boldsymbol{\mu} = \sum_{\mathbf{x}}\nu(\mathbf{x})s(\mathbf{x}) \qquad \sum_{\mathbf{x}}\nu(\mathbf{x}) = 1$$

    - Take a Boltzmann machine on two variables, x_1, x_2.
    - The sufficient stats are $s(\mathbf{x}) = [x_1, x_2, x_1x_2]$.
    - Clearly only the stats $\mathcal{S} = \{[0,0,0],[0,1,0],[1,0,0],[1,1,1]\}$ are possible.
    - Thus $\boldsymbol{\mu} \in \text{convex hull}(\mathcal{S})$.
  - For a discrete distribution, this space of possible means is bounded by exponentially many hyperplanes connecting the discrete configuration stats: called the marginal polytope.
- Even when restricted to the marginal polytope, evaluating $\Psi(\boldsymbol{\mu})$ can be challenging.

Convexity and undirected trees

- We can parametrise a discrete pairwise MRF as follows:

$$p(\mathbf{X}) = \frac{1}{Z}\prod_i f_i(X)\prod_{(ij)} f_{ij}(X_i,X_j)$$
$$= \exp\left(\sum_i\sum_k \boldsymbol{\theta}_i(k)\delta(X_i = k) + \sum_{(ij)}\sum_{k,l}\boldsymbol{\theta}_{ij}(k,l)\delta(X_i = k)\delta(X_j = l) - \Phi(\boldsymbol{\theta})\right)$$

- So discrete MRFs are always exponential family, with natural and mean parameters:

$$\boldsymbol{\theta} = \left[\boldsymbol{\theta}_i(k), \boldsymbol{\theta}_{ij}(k,l) \quad \forall i,j,k,l\right]$$
$$\boldsymbol{\mu} = \left[p(X_i = k), p(X_i = k, X_j = l) \quad \forall i,j,k,l\right]$$

  In particular, the mean parameters are just the singleton and pairwise probability tables.
- If the MRF has tree structure T, the negative entropy can be written in terms of the single-site entropies and mutual informations on edges:

$$\Psi(\boldsymbol{\mu}_T) = \mathbb{E}_{\boldsymbol{\theta}_T}\left[\log\prod_i p(X_i)\prod_{(ij)\in T}\frac{p(X_i,X_j)}{p(X_i)p(X_j)}\right]$$
$$= -\sum_i H(X_i) + \sum_{(ij)\in T} I(X_i,X_j)$$

The Bethe free energy again

We can see the Bethe free energy problem as a relaxation of the true free-energy optimisation:

$$\boldsymbol{\mu}_Z^* = \operatorname*{argmax}_{\boldsymbol{\mu}_Z\in\mathcal{M}}[\boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{\mu}_Z - \Psi(\boldsymbol{\mu}_Z)]$$

where $\mathcal{M}$ is the set of feasible means.

1. Relax $\mathcal{M} \to \mathcal{L}$, where $\mathcal{L}$ is the set of locally consistent means (i.e. all nested means marginalise correctly).
2. Approximate $\Psi(\boldsymbol{\mu}_Z)$ by the tree-structured form

$$\Psi_{\text{Bethe}}(\boldsymbol{\mu}_Z) = -\sum_i H(X_i) + \sum_{(ij)\in G} I(X_i,X_j)$$

$\mathcal{L}$ is still a convex set (polytope for discrete problems). However Ψ_{Bethe} is not convex.

Convexifying BP

Consider instead an upper bound on $\Phi(\boldsymbol{\theta})$:

Imagine a set of spanning trees T for the MRF, each with its own parameters $\boldsymbol{\theta}_T, \boldsymbol{\mu}_T$. By padding entries corresponding to off-tree edges with zero, we can assume that $\boldsymbol{\theta}_T$ has the same dimensionality as $\boldsymbol{\theta}$.

Suppose also that we have a distribution β over the spanning trees so that $\mathbb{E}_\beta\left[\boldsymbol{\theta}_T\right] = \boldsymbol{\theta}$.

Then by the convexity of $\Phi(\boldsymbol{\theta})$,

$$\Phi(\boldsymbol{\theta}) = \Phi(\mathbb{E}_\beta\left[\boldsymbol{\theta}_T\right]) \leq \mathbb{E}_\beta\left[\Phi(\boldsymbol{\theta}_T)\right]$$

If we were to tighten the upper bound we might obtain a good approximation to Φ:

$$\Phi(\boldsymbol{\theta}) \leq \inf_{\beta, \boldsymbol{\theta}_T : \mathbb{E}_\beta[\boldsymbol{\theta}_T] = \boldsymbol{\theta}} \mathbb{E}_\beta\left[\Phi(\boldsymbol{\theta}_T)\right]$$

Convex Upper Bounds on the Log Partition Function

$$\Phi(\boldsymbol{\theta}) \leq \inf_{\boldsymbol{\theta}_T : \mathbb{E}_\beta[\boldsymbol{\theta}_T] = \boldsymbol{\theta}} \mathbb{E}_\beta\left[\Phi(\boldsymbol{\theta}_T)\right] \overset{\text{def}}{=} \Phi_\beta(\boldsymbol{\theta})$$

Solve the constrained optimisation problem using Lagrange multipliers:

$$\mathcal{L} = \mathbb{E}_\beta\left[\Phi(\boldsymbol{\theta}_T)\right] - \boldsymbol{\lambda}^{\mathsf{T}}(\mathbb{E}_\beta\left[\boldsymbol{\theta}_T\right] - \boldsymbol{\theta})$$

Setting the derivatives wrt $\boldsymbol{\theta}_T$ to zero, we get:

$$\begin{aligned} \frac{\partial}{\partial \boldsymbol{\theta}_T} \sum_T \beta(T)\Phi(\boldsymbol{\theta}_T) - \boldsymbol{\lambda}^{\mathsf{T}} \frac{\partial}{\partial \boldsymbol{\theta}_T} \sum_T \beta(T)\boldsymbol{\theta}_T &= 0 \\ \beta(T)\boldsymbol{\mu}_T - \beta(T)\Pi_T(\boldsymbol{\lambda}) &= 0 \\ \boldsymbol{\mu}_T &= \Pi_T(\boldsymbol{\lambda}) \end{aligned}$$

where $\Pi_T(\boldsymbol{\lambda})$ selects the Lagrange multipliers corresponding to elements of $\boldsymbol{\theta}$ that are non-zero in the tree T.

Although each tree has its own parameters $\boldsymbol{\theta}_T$, at the optimum they are all constrained: their mean parameters are all consistent with each other (c.f. the tree-reparametrisation view of BP) and with the Lagrange multipliers $\boldsymbol{\lambda}$.

Convex Upper Bounds on the Log Partition Function

$$\begin{aligned} \Phi_\beta(\boldsymbol{\theta}) &= \sup_{\boldsymbol{\lambda}} \inf_{\boldsymbol{\theta}_T} \mathbb{E}_\beta\left[\Phi(\boldsymbol{\theta}_T)\right] - \boldsymbol{\lambda}^{\mathsf{T}}(\mathbb{E}_\beta\left[\boldsymbol{\theta}_T\right] - \boldsymbol{\theta}) \\ &= \sup_{\boldsymbol{\lambda}} \boldsymbol{\lambda}^{\mathsf{T}}\boldsymbol{\theta} + \mathbb{E}_\beta\left[\inf_{\boldsymbol{\theta}_T} \Phi(\boldsymbol{\theta}_T) - \boldsymbol{\theta}_T^{\mathsf{T}}\Pi_T(\boldsymbol{\lambda})\right] \\ &= \sup_{\boldsymbol{\lambda}} \boldsymbol{\lambda}^{\mathsf{T}}\boldsymbol{\theta} + \mathbb{E}_\beta\left[-\Psi(\Pi_T(\boldsymbol{\lambda}))\right] \\ &= \sup_{\boldsymbol{\lambda}} \boldsymbol{\lambda}^{\mathsf{T}}\boldsymbol{\theta} + \mathbb{E}_\beta\left[\sum_i H_{\boldsymbol{\lambda}}(X_i) - \sum_{(ij)\in T} I_{\boldsymbol{\lambda}}(X_i, X_j)\right] \\ &= \sup_{\boldsymbol{\lambda}} \boldsymbol{\lambda}^{\mathsf{T}}\boldsymbol{\theta} + \sum_i H_{\boldsymbol{\lambda}}(X_i) - \sum_{(ij)} \beta_{ij} I_{\boldsymbol{\lambda}}(X_i, X_j) \end{aligned}$$

- This is a **convexified** version of the Bethe free energy.
- Optimisation wrt $\boldsymbol{\lambda}$is approximate inference applied to the tighest bound on $\Phi(\theta)$ for fixed β.
- The bound holds for any β and can be tightened by further minimisation.

EP free energy

A Bethe-like approach also casts EP as a variational energy fixed point method.

Consider finding marginals of a (posterior) distribution defined by clique potentials:

$$P(\mathcal{Z}) \propto f_0(\mathcal{Z}) \prod_i f_i(\mathcal{Z}_i)$$

where all factor have exponential form, f_0 is in a tractable exponential family (possibly uniform) bu the f_i are jointly intractable – i.e. product cannot be marginalised, although individual terms may be (numerically) tractable.

Augment by including tractable ExpFam terms with zero natural parameters

$$P(\mathcal{Z}) \propto e^{\boldsymbol{\theta}_0^{\mathsf{T}}\mathbf{s}_0(\mathcal{Z})} \prod_i e^{\boldsymbol{\theta}_i^{\mathsf{T}} s_i(\mathcal{Z}_i)} e^{\mathbf{0}^{\mathsf{T}}\tilde{\mathbf{s}}_i(\mathcal{Z}_i)} = e^{\boldsymbol{\theta}_0^{\mathsf{T}}\mathbf{s}_0(\mathcal{Z}) + \sum_i \left(\boldsymbol{\theta}_i^{\mathsf{T}} s_i(\mathcal{Z}_i) + \tilde{\boldsymbol{\theta}}^{\mathsf{T}}\tilde{\mathbf{s}}(\mathcal{Z}_i)\right)}$$

Now, the variational dual principle tells us that the expected sufficient statistics:

$$\boldsymbol{\mu}_0^* = \langle \mathbf{s}_0 \rangle_P; \quad \boldsymbol{\mu}_i^* = \langle \mathbf{s}_i(\mathcal{Z}_i) \rangle_P; \quad \tilde{\boldsymbol{\mu}}_i^* = \langle \tilde{\mathbf{s}}_i \rangle_P$$

are given by

$$\{\boldsymbol{\mu}_0^*, \boldsymbol{\mu}_i^*, \tilde{\boldsymbol{\mu}}_i^*\} = \underset{\{\boldsymbol{\mu}_0, \boldsymbol{\mu}_i, \tilde{\boldsymbol{\mu}}_i\} \in \mathcal{M}}{\text{argmax}} \left[\boldsymbol{\theta}_0^{\mathsf{T}}\boldsymbol{\mu}_0 + \sum_i \left(\boldsymbol{\theta}_i^{\mathsf{T}}\boldsymbol{\mu}_i + \mathbf{0}^{\mathsf{T}}\tilde{\boldsymbol{\mu}}_i\right) - \Psi(\boldsymbol{\mu}_0, \boldsymbol{\mu}_i, \tilde{\boldsymbol{\mu}}_i)\right]$$

EP relaxation

The EP algorithm relaxes this optimisation:

- Relax $\mathcal{M}$ to locally consistent marginals, retaining consistency across each edge connecting $\{\boldsymbol{\mu}_0, \tilde{\boldsymbol{\mu}}_i\}$ (as in BP on a junction graph); and between pairs $(\boldsymbol{\mu}_i, \tilde{\boldsymbol{\mu}}_i)$.
- Replace negative entropy by $\Psi_{\text{Bethe}}(\{\boldsymbol{\mu}_0, \tilde{\boldsymbol{\mu}}_i\}) - \sum_i (\mathbf{H}[\boldsymbol{\mu}_i, \tilde{\boldsymbol{\mu}}_i] - \mathbf{H}[\tilde{\boldsymbol{\mu}}_i])$.
- In effect, drop links between different $\boldsymbol{\mu}_i$ and run reparameterisation on a junction graph.

The free-energy-based approximate marginals include $\boldsymbol{\mu}_i$ which are refined during updates.

- Direct learning on the EP free-energy would use these marginals rather than the approximate ones (and a local normaliser formed by integrating over $f_i(\mathcal{Z}_i) q_{\neg i}(\mathcal{Z}_i)$).
- These estimates may yield more accurate results than optimising θ according to expectations under the tractable marginals $\tilde{\boldsymbol{\mu}}_i$.

References

- **Graphical Models, Exponential Families, and Variational Inference. Wainwright and Jordan. Foundations and Trends in Machine Learning, 2008 1:1-305.**
- Exact Maximum A Posteriori Estimation for Binary Images. Greig, Porteous and Seheult, Journal of the Royal Statistical Society B, 51(2):271-279, 1989.
- Fast Approximate Energy Minimization via Graph Cuts. Boykov, Veksler and Zabih, International Conference on Computer Vision 1999.
- MAP estimation via agreement on (hyper)trees: Message-passing and linear-programming approaches. Wainwright, Jaakkola and Willsky, IEEE Transactions on Information Theory, 2005, 51(11):3697-3717.
- Learning Associative Markov Networks. Taskar, Chatalbashev and Koller, International Conference on Machine Learning, 2004.
- A New Class of Upper Bounds on the Log Partition Function. Wainwright, Jaakkola and Willsky. IEEE Transactions on Information Theory, 2005, 51(7):2313-2335.
- MAP Estimation, Linear Programming and Belief Propagation with Convex Free Energies. Weiss, Yanover and Meltzer, Uncertainty in Artificial Intelligence, 2007.