Probabilistic & Unsupervised Learning
Approximate Inference

Exponential families: convexity, duality and free energies

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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

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

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

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

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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

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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

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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

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

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\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}')
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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.

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Continuous functions are reciprocally dual, so we also have:

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

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 $\mathbf{z}$.

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

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

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The likelihood is

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

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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?

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

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  - Feasible means are convex combinations of all the single-configuration sufficient statistics.

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    - Take a Boltzmann machine on two variables, x_1, x_2.
    - The sufficient stats are $s(\mathbf{x}) = [x_1, x_2, x_1 x_2]$.
    - Clearly only the stats $\mathcal{S} = \{[0, 0, 0], [0, 1, 0], [1, 0, 0], [1, 1, 1]\}$ are possible.
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    - Thus $\boldsymbol{\mu} \in$ 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:

$$
\begin{aligned}
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)
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- So discrete MRFs are always exponential family, with natural and mean parameters:

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

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- 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:

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$\mathcal{L}$ 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 $\mathbb{E}_\beta[\boldsymbol{\theta}_T] = \boldsymbol{\theta}$.

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

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

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

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

Convex Upper Bounds on the Log Partition Function

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

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

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

- 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

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

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.

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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 $\tilde{\boldsymbol{\mu}}_i$.

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