

# Probabilistic & Unsupervised Learning

## Exponential families: convexity, duality and free energies

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## Exponential families: the log partition function

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

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

where  $\Phi(\theta)$  is the [log partition function](#)

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

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

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

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

The second derivative is thus positive semi-definite, and so  $\Phi(\theta)$  is [convex in  \$\theta\$](#) .

## Exponential families: mean parameters and negative entropy

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

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

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

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

so

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

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

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

## Exponential families: duality

In fact, the log partition function and negative entropy are [Legendre dual](#) or [convex conjugate](#) functions.

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

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

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

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

$$\Psi(\mu) = \sup_{\theta'} [\theta'^T \mu - \Phi(\theta')] \quad \text{and, if finite} \quad \theta(\mu) = \operatorname{argmax}_{\theta'} [\theta'^T \mu - \Phi(\theta')]$$

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

Continuous functions are reciprocally dual, so we also have:

$$\Phi(\theta) = \sup_{\mu'} [\theta^T \mu' - \Psi(\mu')] \quad \text{and, if finite} \quad \mu(\theta) = \operatorname{argmax}_{\mu'} [\theta^T \mu' - \Psi(\mu')]$$

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

## Duality, inference and the free energy

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

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

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

The likelihood is

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

So we can write the log-likelihood as

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

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  $\mu$  directly?

$$\mu_z^* = \operatorname{argmax}_{\mu_z} [\theta^\top \mu_z - \Psi(\mu_z)]$$

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Concave maximisation(!), but two complications:

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

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



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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  $\mu \in \operatorname{convex hull}(\mathcal{S})$ .
- ▶ 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  $\Psi(\mu)$  can be challenging.

## Convexity and undirected trees

- ▶ We can parametrise a discrete pairwise MRF as follows:

$$\begin{aligned} p(\mathbf{X}) &= \frac{1}{Z} \prod_i f_i(X) \prod_{(ij)} f_{ij}(X_i, X_j) \\ &= \exp \left( \sum_i \sum_k \theta_i(k) \delta(X_i = k) + \sum_{(ij)} \sum_{k,l} \theta_{ij}(k, l) \delta(X_i = k) \delta(X_j = l) - \Phi(\theta) \right) \end{aligned}$$

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

$$\theta = [\theta_i(k), \theta_{ij}(k, l) \quad \forall i, j, k, l]$$

$$\mu = [p(X_i = k), p(X_i = k, X_j = l) \quad \forall i, j, k, l]$$

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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:

$$\begin{aligned} \Psi(\mu_T) &= \mathbb{E}_{\theta_T} \left[ \log \prod_i p(X_i) \prod_{(ij) \in T} \frac{p(X_i, X_j)}{p(X_i)p(X_j)} \right] \\ &= - \sum_i H(X_i) + \sum_{(ij) \in T} I(X_i, X_j) \end{aligned}$$

## The Bethe free energy again

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

$$\mu_Z^* = \operatorname{argmax}_{\mu_Z \in \mathcal{M}} [\theta^\top \mu_Z - \Psi(\mu_Z)]$$

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2. **Approximate**  $\Psi(\mu_Z)$  by the tree-structured form

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

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

## Convexifying BP

Consider instead an **upper bound** on  $\Phi(\theta)$ :

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

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

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

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

If we were to **tighten** the upper bound we might obtain a good approximation to  $\Phi$ :

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

## Convex Upper Bounds on the Log Partition Function

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

Solve this constrained optimisation problem using Lagrange multipliers:

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

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

$$\begin{aligned} \beta(T)\boldsymbol{\lambda}_T - \beta(T)\boldsymbol{\Pi}_T(\boldsymbol{\lambda}) &= 0 \\ \boldsymbol{\lambda}_T &= \boldsymbol{\Pi}_T(\boldsymbol{\lambda}) \end{aligned}$$

where  $\boldsymbol{\Pi}_T(\boldsymbol{\lambda})$  are the Lagrange multipliers corresponding to vertices and edges on the tree  $T$ .

Although there can be many  $\boldsymbol{\theta}_T$  parameters, at optimum they are all constrained: their corresponding mean parameters are all consistent with each other and with  $\boldsymbol{\lambda}$ .

## Convex Upper Bounds on the Log Partition Function

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

This is a **convexified** Bethe free energy.

## 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 factors have exponential form,  $f_0$  is in a tractable exponential family (possibly uniform) but 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

$$P(\mathcal{Z}) \propto e^{\theta_0^T \mathbf{s}_0(\mathcal{Z})} \prod_i e^{\theta_i^T \mathbf{s}_i(\mathcal{Z}_i)} e^{\mathbf{0}^T \tilde{\mathbf{s}}_i(\mathcal{Z}_i)} = e^{\theta_0^T \mathbf{s}_0(\mathcal{Z}) + \sum_i (\theta_i^T \mathbf{s}_i(\mathcal{Z}_i) + \tilde{\theta}^T \tilde{\mathbf{s}}_i(\mathcal{Z}_i))}$$

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

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

## EP relaxation

The EP algorithm relaxes this optimisation:

- ▶ Relax  $\mathcal{M}$  to **locally consistent** marginals, retaining consistency across each edge connecting  $\{\mu_0, \tilde{\mu}_i\}$  (as in BP on a junction graph); and between pairs  $(\mu_i, \tilde{\mu}_i)$ .
- ▶ Replace negative entropy by  $\Psi_{\text{Bethe}}(\{\mu_0, \tilde{\mu}_i\}) - \sum_i (\mathbf{H}[\mu_i, \tilde{\mu}_i] - \mathbf{H}[\tilde{\mu}_i])$ .
- ▶ In effect, drop links between different  $\mu_i$  and run reparameterisation on a junction graph.

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- ▶ In effect, drop links between different  $\mu_i$  and run reparameterisation on a junction graph.

The free-energy-based approximate marginals include  $\mu_i$  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  $f_i(\mathcal{Z}_i)q_{-i}(\mathcal{Z}_i)$ ).
- ▶ These estimates may yield more accurate results than optimising  $\theta$  according to expectations under the tractable marginals  $\tilde{\mu}_i$ .



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