We recall that the partition function $Z(\lambda)$ or the moment-generating function $M(\lambda) = \frac{Z(\lambda)}{Z(0)}$ entirely (though implicitly) determines the density $p(x) \propto e^{-S(x)}$.

We consider below two standard approximation schemes.

1 Saddle-Point Approximation

A simple approximation for the partition function $Z(\lambda)$ is achieved by performing a quadratic expansion around the local maxima of the integrand. This results in a Gaussian integral, that can be solved exactly:

$$\begin{aligned} Z(\lambda) &= \int dx\, e^{-S(x)+\lambda^T x} \\ &\approx \int dx\, e^{-S(x^\star)+\lambda^T x - \frac{1}{2}(x-x^\star)^T H(x^\star)(x-x^\star)} \\ &= e^{-S(x^\star)} \int dx\, e^{\lambda^T x - \frac{1}{2}(x-x^\star)^T H(x^\star)(x-x^\star)} \\ &= e^{-S(x^\star)+\lambda^T x^\star + \frac{1}{2}\lambda^T H(x^\star)^{-1}\lambda} \int dx\, e^{-\frac{1}{2}(x-\mu)^T H(x^\star)(x-\mu)} \\ &= e^{-S(x^\star)+\lambda^T x^\star + \frac{1}{2}\lambda^T H(x^\star)^{-1}\lambda} \det\left(\frac{H(x^\star)}{2\pi}\right)^{-\frac{1}{2}}, \end{aligned}$$

where $x^\star$ is such that $\frac{\partial S(x^\star)}{\partial x^\star} = 0$ and $H(x^\star) = \frac{\partial S^2(x^\star)}{\partial x^\star x^{\star T}}$ is the Hessian matrix around $x^\star$.

This approximation is also known as *semi-classical* approximation, since it can be interpreted as assuming that the variable $x = x^\star + z$ is made of a "classical" part $x^\star$, satisfying the classical equations of motion $\frac{\partial S(x^\star)}{\partial x^\star} = 0$, and a "quantum" or random part z which fluctuates around zero with covariance matrix $\Sigma = H(x^\star)^{-1}$.

If $-S(x)$ has multiple local minima, we maybe have to sum over then to obtain an accurate approximation.

A great advantage of this approximation is that computing n-point functions is trivial when combined with Wick's theorem, explained below.

1.1 Wick's Theorem

Wick's theorem allow us to compute the n-point functions in terms of combinations of 2-point functions and it is the key ingredient to build Feynman diagrams in the next sections [7, 1, 8, 4].

In order derive the most basic version of Wick's theorem we assume that our action $S(x)$ has been decomposed as a zero-mean Gaussian action plus higher-order interaction terms, $S(x) = -\frac{1}{2}x^T\Sigma^{-1}x + V(x)$. n-point functions of the Gaussian part $p_0(x) \propto e^{-\frac{1}{2}x^T\Sigma^{-1}x}$ can be easily written as

$$\mathbb{E}_{p_0}[x_{a_1}...x_{a_n}] = \frac{\partial^n}{\partial\lambda_{a_1}...\lambda_{a_n}} e^{\frac{1}{2}\lambda^T\Sigma\lambda}.$$

In its simplest form, Wick's theorem can be enunciated as

Theorem 1. *(Wick)*

The expectation $\mathbb{E}_{p_0}[x_{a_1}...x_{a_n}]$ *under* $p_0(x) \propto e^{-\frac{1}{2}x^T\Sigma^{-1}x}$ *is given by*

$$\mathbb{E}_{p_0}[x_{a_1}...x_{a_n}] = \begin{cases} \sum_{\{(i_l,j_l)\}} \prod_{l=1}^{k} \Sigma_{i_l j_l} & n = 2k \\ 0 & n = 2k+1 \end{cases},$$

where $\sum_{\{(i_l,j_l)\}}$ *indicates a summation of all possible pairwise groupings of the indexes* $\{a_1...a_n\}$.

2 Perturbative Expansion

Roughly speaking, a perturbative expansion is simply a series expansion inside the partition function. The expansion is in general performed assuming a weak coupling between variables [10, 3, 6, 5].

We start by splitting the action functional $S(x) = S_0(x) + V(x)$ into a "free-field" term $S_0(x)$, which induces the distribution $p_0(x) \propto e^{-S_0(x)}$ where all the variables are independent of each other, and the "coupling" terms $V(x)$ which makes the variables dependent on each other (hence coupling them). The partition function can then be rewritten in terms of an expectation under p_0,

$$Z(\lambda) = \int dx e^{-S(x)+\lambda^T x} = \int dx e^{-S_0(x)} e^{-V(x)+\lambda^T x} = Z_0 \mathbb{E}_{p_0}\big[e^{-V(x)+\lambda^T x}\big].$$

This separation is convenient because moments are easy to compute under the free-field distribution $p_0(x)$.

The next step in the perturbative expansion is to expand the term $e^{-V(x)}$ in a power series around $V(x) = 0$,

$$e^{-V(x)} = \sum_{k=0}^{\infty} \sum_{|a|=k} \frac{\alpha_{k,a}}{k!} \prod_{i=1}^{d} x_i^{a_i},$$

where $\sum_{|a|=k}$ is a summation over all integer sequences of length d that sum up to k. Substituting this back in the partition function we get

$$\begin{aligned} Z(\lambda) &= Z_0 \sum_{k=0}^{\infty} \sum_{|a|=k} \frac{\alpha_{k,a}}{k!} \mathbb{E}_{p_0}\left[e^{\lambda^T x} \prod_{i=1}^{d} x_i^{a_i} \right] \\ &= Z_0 \sum_{k=0}^{\infty} \sum_{|a|=k} \frac{\alpha_{k,a}}{k!} \frac{\partial^k}{\partial \lambda_1^{a_1} ... \lambda_d^{a_d}} \mathbb{E}_{p_0}\big[e^{\lambda^T x}\big]. \end{aligned}$$

The n-point functions can be computed as

$$\mathbb{E}_p[x_{a_1}...x_{a_N}] = \sum_{k=0}^{\infty} \sum_{|a|=k} \frac{\alpha_{k,a}}{k!} \mathbb{E}_{p_0}\left[x_{a_1}...x_{a_N} \prod_{i=1}^{d} x_i^{a_i} \right]. \tag{1}$$

Note that every term in the expansion above can be computed analytically, since they only involve expectations under the simple distribution p_0 where all variables are independent.

2.1 Concrete Example: Boltzmann Machines

Boltzmann Machines are distributions over binary variables $x \in \{0,1\}^d$ defined by the unnormalized distribution

$$p(x) \propto e^{\frac{1}{2}x^T W x + b^T x},$$

where we assume $\text{diag}(W) = 0$ and $W = W^T$.

We can split the "negative energy" $S(x) = \frac{1}{2}x^T W x + b^T x$ as $S(x) = S_0(x) + V(x)$, where $S_0(x) = b^T x$ and $V(x) = \frac{1}{2}x^T W x$. Note that $S_0(x)$ corresponds to the energy of d independent Bernoulli random variables with probability $p(x_i = 1) = \text{sigmoid}(b_i) = \mu_i$.

For this Boltzmann Machine we have $Z_0 = \prod_{i=1}^{d} (1+e^{b_i})$ and $\mathbb{E}_{p_0}\left[e^{\lambda^T x}\right] = \frac{1}{Z_0}\prod_{i=1}^{d}(1+e^{b_i+\lambda_i})$.

The partition function up to first order in W is given by

$$Z(\lambda) \;= \prod_{i=1}^{d} (1+e^{b_i+\lambda_i})\left[1+\frac{1}{2}\sum_{ij} W_{ij} m_i m_j\right],$$

where $m_i = \text{sigmoid}(\lambda_i)$.

We can now use $Z(\lambda)$ to compute corrections to the mean and other moments

$$\begin{aligned}
\mathbb{E}_p[x_i] \;&= \frac{1}{Z}\frac{\partial}{\partial \lambda_i} Z(\lambda) \\
&\approx \mu_i + \frac{\mu_i(1-\mu_i)\sum_k W_{ki}\mu_k}{\left[1+\frac{1}{2}\sum_{ij} W_{ij}\mu_i\mu_j\right]} \\
&\approx \mu_i + \mu_i(1-\mu_i)\sum_j W_{ji}\mu_j,
\end{aligned}$$

where we have used $x/(1+r^T x) \approx x$ and $\mu_i = \text{sigmoid}(b_i)$.

The second-order correction to the second moments is given by

$$\begin{aligned}
\mathbb{E}_p[x_i x_k] \;&= \frac{1}{Z}\frac{\partial^2}{\partial \lambda_i \lambda_k} Z(\lambda) \\
&\approx \mu_i\mu_k + \mu_i\mu_k\left[(1-\mu_k)\sum_j W_{kj}\mu_j + (1-\mu_i)\sum_j W_{ij}\mu_j\right] \\
&+ \mu_i(1-\mu_i)\mu_k(1-\mu_k)W_{ik},
\end{aligned}$$

and the central second-moment is approximated by

$$\text{Cov}_p[x_i x_k] \;\approx \mu_i(1-\mu_i)\mu_k(1-\mu_k)W_{ik}.$$

A much more detailed perturbation analysis and higher-order computations from a physics perspective can be found in [3, 9].

For a more modern application of these methods to Restricted Boltzmann Machines, see [2].

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