DeepMP derivation

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1 Derivation of the BP equations

$$\prod_{\ell=0}^{L}\prod_{k} P^{\ell+1}\left(x_{kn}^{\ell+1}\;\middle|\;\sum_i W_{ki}^{\ell}x_{in}^{\ell}\right) \quad \text{where } \boldsymbol{x}_n^0=\boldsymbol{x}_n,\ \boldsymbol{x}_n^{L+1}=y_n. \tag{1}$$

Remember that x_{kn}^{ℓ} the activation output of neuron's k in layer ℓ in correspondence of input example n, we now analyze the single factor

$$P^{\ell+1}\left(x_{kn}^{\ell+1}\;\middle|\;\sum_i W_{ki}^{\ell}x_{in}^{\ell}\right) \tag{2}$$

Factor to variable W messages

$$\hat{\nu}_{kn\to ki}^{\ell+1}(W_{ki}^{\ell}) \propto \int \prod_{i'\neq i} d\nu_{ki'\to n}^{\ell}(W_{ki'}^{\ell}) \prod_{i'} d\nu_{i'n\to k}^{\ell}(x_{i'n}^{\ell})\ d\nu_{\downarrow}(x_{kn}^{\ell+1})\ P^{\ell+1}\left(x_{kn}^{\ell+1}\;\middle|\;\sum_{i'} W_{ki'}^{\ell}x_{i'n}^{\ell}\right) \tag{3}$$

We denote the mean and variance of the incoming messages with

$$m_{ki\to n}^{\ell} = \int d\nu_{ki\to n}^{\ell}(W_{ki}^{\ell})\ W_{ki}^{\ell} \tag{4}$$

$$\sigma_{ki\to n}^{\ell} = \int d\nu_{ki\to n}^{\ell}(W_{ki}^{\ell})\ \left(W_{ki}^{\ell}-m_{ki\to n}^{\ell}\right)^2 \tag{5}$$

$$\hat{x}_{in\to k}^{\ell} = \int d\nu_{in\to k}^{\ell}(x_{in}^{\ell})\ x_{in}^{\ell} \tag{6}$$

$$\Delta_{in\to k}^{\ell} = \int d\nu_{in\to k}^{\ell}(x_{in}^{\ell})\ \left(x_{in}^{\ell}-\hat{x}_{in\to k}^{\ell}\right)^2 \tag{7}$$

We use the central limit theorem to observe that with the respect to the incoming message distributions, messages that we assume to be independent, the preactivation is in the large input limit a Gaussian random variable

$$\sum_{i'\neq i} W_{ki'}^{\ell}x_{i'n}^{\ell} \sim \mathcal{N}(\omega_{kn\to i}^{\ell}, V_{kn\to i}^{\ell}) \tag{8}$$

with

$$\omega^{\ell}_{kn\to i} = \mathbb{E}_{\nu}\left[\sum_{i'\neq i} W^{\ell}_{ki'} x^{\ell}_{i'n}\right] = \sum_{i'\neq i} m^{\ell}_{ki'\to n}\, \hat{x}^{\ell}_{i'n\to k} \tag{9}$$

$$V^{\ell}_{kn\to i} = Var_{\nu}\left[\sum_{i'\neq i} W^{\ell}_{ki'} x^{\ell}_{i'n}\right] = \sum_{i'\neq i}\left(\sigma^{\ell}_{ki'\to n}\,\Delta^{\ell}_{i'n\to k} + \left(m^{\ell}_{ki'\to n}\right)^2\,\Delta^{\ell}_{i'n\to k} + \sigma^{\ell}_{ki'\to n}\,\left(\hat{x}^{\ell}_{i'n\to k}\right)^2\right) \tag{10}$$

Therefore we can rewrite the outgoing messages as

$$\hat{\nu}^{\ell+1}_{kn\to i}(W^{\ell}_{ki}) \propto \int dz\, d\nu^{\ell}_{in\to k}(x^{\ell}_{in})\, d\nu_{\downarrow}(x^{\ell+1}_{kn})\, e^{-\frac{(z-\omega_{kn\to i}-W^{\ell}_{ki}x^{\ell}_{in})^2}{2V_{kn\to i}}}\, P^{\ell+1}\left(x^{\ell+1}_{kn}\,\middle|\, z\right)$$

We now assume $W^{\ell}_{ki}x^{\ell}_{in}$ to be small compare to the other terms. With a second order Taylor expansion we obtain

$$\hat{\nu}^{\ell+1}_{kn\to i}(W^{\ell}_{ki}) \propto \int dz\;\; d\nu_{\downarrow}(x^{\ell+1}_{kn})\; e^{-\frac{(z-\omega_{kn\to i})^2}{2V_{kn\to i}}}\, P^{\ell+1}\left(x^{\ell+1}_{kn}\,\middle|\, z\right) \tag{11}$$

$$\times\left(1 + \frac{z-\omega_{kn\to i}}{V_{kn\to i}}\hat{x}^{\ell}_{in\to k}W^{\ell}_{ki} + \frac{(z-\omega_{kn\to i})^2 - V_{kn\to i}}{2V_{kn\to i}}\left(\Delta + \left(\hat{x}^{\ell}_{in\to k}\right)^2\right)\left(W^{\ell}_{ki}\right)^2\right) \tag{12}$$

Introducing the function

$$\varphi^{\ell}(B, A, \omega, V) = \log\int \mathrm{d}x\,\mathrm{d}z\; e^{-\frac{1}{2}Ax^2+Bx}\, P^{\ell}\left(x|z\right) e^{-\frac{(\omega-z)^2}{2V}} \tag{13}$$

and defining

$$g^{\ell+1}_{kn\to i} = \partial_{\omega}\varphi^{\ell+1}(B, A, \omega^{\ell}_{kn\to i}, V^{\ell}_{kn\to i}) \tag{14}$$

$$\Gamma^{\ell+1}_{kn\to i} = -\partial^2_{\omega}\varphi^{\ell+1}(B, A, \omega^{\ell}_{kn\to i}, V^{\ell}_{kn\to i}) \tag{15}$$

the expansion for the log-message reads:

$$\log\hat{\nu}^{\ell+1}_{kn\to i}(W^{\ell}_{ki}) \approx const + \hat{x}^{\ell}_{in\to k}\, g^{\ell+1}_{kn\to i}W^{\ell}_{ki} - \frac{1}{2}\left(\left(\Delta^{\ell}_{in\to k} + \left(\hat{x}^{\ell}_{in\to k}\right)^2\right)\Gamma^{\ell+1}_{kn\to i} - \Delta^{\ell}_{in\to k}\left(g^{\ell+1}_{kn\to i}\right)^2\right)\left(W^{\ell}_{ki}\right)^2 \tag{16}$$

Factor to variable x messages Derivations of this messages is specular to the preceding one. The result is

$$\log\hat{\nu}^{\ell+1}_{kn\to i}(x^{\ell}_{in}) \approx const + m^{\ell}_{ki\to n}\, g^{\ell+1}_{kn\to i}x^{\ell}_{in} - \frac{1}{2}\left(\left(\sigma^{\ell}_{ki\to n} + \left(m^{\ell}_{ki\to n}\right)^2\right)\Gamma^{\ell+1}_{kn\to i} - \sigma^{\ell}_{ki\to n}\left(g^{\ell+1}_{kn\to i}\right)^2\right)\left(x^{\ell}_{in}\right)^2 \tag{17}$$

Variable W to output factor messages The message from variable W^ℓ_{ki} to the output factor kn reads:

$$\nu^\ell_{ki\to n}(W^\ell_{ki}) \propto P^\ell_{\theta_{ki}}(W^\ell_{ki}) e^{\sum_{n'\neq n}\log\hat{\nu}^{\ell+1}_{kn\to i}(W^\ell_{ki})} \tag{18}$$

$$\approx P^\ell_{\theta_{ki}}(W^\ell_{ki}) e^{H^\ell_{ki\to n}W^\ell_{ki} - \frac{1}{2}G^\ell_{ki\to n}\left(W^\ell_{ki}\right)^2} \tag{19}$$

where we defined

$$H^\ell_{ki\to n} = \sum_{n'\neq n} \hat{x}^\ell_{in'\to k}\, g^{\ell+1}_{kn'\to i} \tag{20}$$

$$G^\ell_{ki\to n} = \sum_{n'\neq n} \left(\left(\Delta^\ell_{in'\to k} + \left(\hat{x}^\ell_{in'\to k}\right)^2\right)\Gamma^{\ell+1}_{kn'\to i} - \Delta^\ell_{in'\to k}\left(g^{\ell+1}_{kn'\to i}\right)^2\right) \tag{21}$$

Introducing the effective free energy

$$\psi^\ell(H,G,\theta) = \log\int \mathrm{d}W\;\; P^\ell_\theta\left(W\right) e^{HW-\frac{1}{2}GW^2} \tag{22}$$

we can then express the first two cumulants of $\nu^\ell_{ki\to n}(W^\ell_{ki})$ as

$$m^\ell_{ki\to n} = \partial_H\psi^\ell(H^\ell_{ki\to n}, G^\ell_{ki\to n}, \theta_{ki}) \tag{23}$$

$$\sigma^\ell_{ki\to n} = \partial^2_H\psi^\ell(H^\ell_{ki\to n}, G^\ell_{ki\to n}, \theta_{ki}) \tag{24}$$

Variable x to input factor messages The downgoing message

$$\nu_\downarrow(x^\ell_{in}) \propto e^{\sum_k \log\hat{\nu}^{\ell+1}_{kn\to i}(x^\ell_{in})} \tag{25}$$

$$\approx e^{B^\ell_{kn}x - \frac{1}{2}A^\ell_{kn}x^2} \tag{26}$$

With

$$B^\ell_{in} = \sum_n m^\ell_{ki\to n}\, g^{\ell+1}_{kn\to i} \tag{27}$$

$$A^\ell_{in} = \sum_n \left(\left(\sigma^\ell_{ki\to n} + \left(m^\ell_{ki\to n}\right)^2\right)\Gamma^{\ell+1}_{kn\to i} - \sigma^\ell_{ki\to n}\left(g^{\ell+1}_{kn\to i}\right)^2\right) \tag{28}$$

Variable x to output factor messages Defining also the cavity quantities

$$B^\ell_{in\to k} = B^\ell_{in\to k} - m^\ell_{ki\to n}\, g^{\ell+1}_{kn\to i} \tag{29}$$

$$A^\ell_{in\to k} = A^\ell_{in\to k} - \left(\left(\sigma^\ell_{ki\to n} + \left(m^\ell_{ki\to n}\right)^2\right)\Gamma^{\ell+1}_{kn\to i} - \sigma^\ell_{ki\to n}\left(g^{\ell+1}_{kn\to i}\right)^2\right) \tag{30}$$

and the non-cavity ones

$$\omega^{\ell}_{kn} = \sum_{i} m^{\ell}_{ki\to n}\, \hat{x}^{\ell}_{in\to k} \tag{31}$$

$$V^{\ell}_{kn} = \sum_{i} \left(\sigma^{\ell}_{ki\to n}\, \Delta^{\ell}_{in\to k} + \left(m^{\ell}_{ki\to n}\right)^2 \Delta^{\ell}_{in\to k} + \sigma^{\ell}_{ki\to n} \left(\hat{x}^{\ell}_{i'n\to k}\right)^2 \right) \tag{32}$$

we can express the first 2 cumulants of the upgoing messages as

$$\hat{x}^{\ell}_{in\to k} = \partial_B \varphi^{\ell}(B^{\ell}_{in\to k}, A^{\ell}_{in\to k}, \omega^{\ell-1}_{in}, V^{\ell-1}_{in}) \tag{33}$$

$$\sigma^{\ell}_{in\to k} = \partial^2_B \varphi^{\ell}(B^{\ell}_{in\to k}, A^{\ell}_{in\to k}, \omega^{\ell-1}_{in}, V^{\ell-1}_{in}) \tag{34}$$

Wrapping it up Additional considerations but straightforward considerations are required for the input and output layers ($\ell = 0$ and $\ell = L+1$ respectively), since they do not receive messages from below and above respectively. In the end, and thanks to indipendence assumptions and central limit theorem that we used throughout the derivation, we arrive to a closed set of equations involving mean and variance (or the corresponding natural parameters) of the messages.

2 Derivation of the AMP equations