Detailed derivation of Belief Propagation algorithm on Pairwise Markov Random Fields

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By definition of probability density function:

(1)
$$\sum_{x_1} \sum_{x_2} \cdots \sum_{x_n} p(x_1, x_2, \dots x_n) = 1$$

We are interested in "single-node" marginal probabilities:

$$(2) p_{i}(x_{i}) = \sum_{x_{1}} \cdots \sum_{x_{i-1}} \sum_{x_{i+1}} \cdots \sum_{x_{n}} p(x_{1}, x_{2}, \dots x_{n})$$

$$p_{j}(x_{i}) = \sum_{x_{1}} \cdots \sum_{x_{j-1}} \sum_{x_{j+1}} \cdots \sum_{x_{n}} p(x_{1}, x_{2}, \dots x_{n})$$

For nodes, which are connected - we, also interested in "pairwise" marginal probabilities:

(3)
$$p_{ij}(x_i, x_j) = \sum_{x_1} \cdots \sum_{x_{i-1}} \sum_{x_{i+1}} \cdots \sum_{x_{j-1}} \sum_{x_{j+1}} \cdots \sum_{x_n} p(x_1, x_2, \dots x_n)$$

Also, the following equalities for marginal probabilities – are obvious (keeping in mind Equation (1)):

$$\sum_{x_{i}} p_{i}(x_{i}) = \sum_{x_{i}} \left(\sum_{x_{1}} \cdots \sum_{x_{i-1}} \sum_{x_{i+1}} \cdots \sum_{x_{n}} p(x_{1}, x_{2}, \dots x_{n}) \right) =$$

$$= \sum_{x_{1}} \sum_{x_{2}} \cdots \sum_{x_{n}} p(x_{1}, x_{2}, \dots x_{n}) = 1$$

$$(4)$$

$$\sum_{x_{j}} p_{j}(x_{j}) = \sum_{x_{j}} \left(\sum_{x_{1}} \cdots \sum_{x_{j-1}} \sum_{x_{j+1}} \cdots \sum_{x_{n}} p(x_{1}, x_{2}, \dots x_{n}) \right) =$$

$$= \sum_{x_{1}} \sum_{x_{2}} \cdots \sum_{x_{n}} p(x_{1}, x_{2}, \dots x_{n}) = 1$$

(5)
$$\sum_{x_i} \sum_{x_j} p_{ij}(x_i, x_j) = \sum_{x_i} \sum_{x_j} \left(\sum_{x_1} \cdots \sum_{x_{i-1}} \sum_{x_{i+1}} \cdots \sum_{x_{j-1}} \sum_{x_{j+1}} \cdots \sum_{x_n} p(x_1, x_2, \dots x_n) \right) =$$

$$= \sum_{x_1} \sum_{x_2} \cdots \sum_{x_n} p(x_1, x_2, \dots x_n) = 1$$

Lets represent single-node marginal probabilities, using pairwise marginal probabilities (keeping in mind Equation (3)):

$$p_{i}(x_{i}) = \sum_{x_{1}} \cdots \sum_{x_{i-1}} \sum_{x_{i+1}} \cdots \sum_{x_{n}} p(x_{1}, x_{2}, \dots x_{n}) =$$

$$= \sum_{x_{j}} \left(\sum_{x_{1}} \cdots \sum_{x_{i-1}} \sum_{x_{i+1}} \cdots \sum_{x_{j-1}} \sum_{x_{j+1}} \cdots \sum_{x_{n}} p(x_{1}, x_{2}, \dots x_{n}) \right) =$$

$$= \sum_{x_{j}} p_{ij}(x_{i}, x_{j})$$

$$p_{j}(x_{j}) = \sum_{x_{1}} \cdots \sum_{x_{j-1}} \sum_{x_{j+1}} \cdots \sum_{x_{n}} p(x_{1}, x_{2}, \dots x_{n}) =$$

$$= \sum_{x_{i}} \left(\sum_{x_{1}} \cdots \sum_{x_{i-1}} \sum_{x_{i+1}} \cdots \sum_{x_{j-1}} \sum_{x_{j+1}} \cdots \sum_{x_{n}} p(x_{1}, x_{2}, \dots x_{n}) \right) =$$

$$= \sum_{x_{i}} p_{ij}(x_{i}, x_{j})$$

Lets consider summation over all edges - of some functions $f_i(x_i)$ and $f_j(x_j)$ (these functions depends only on states of single nodes: i and j), also lets denote q_i - as a number of edges, which connected to node i ("degree" of node i), and q_j - "degree" of node j. So, in this case - we can represent summations over all edges, as summations over nodes, multiplied by node-degrees:

(7)
$$\sum_{(i,j)} f_i(x_i) = \sum_i (q_i \times f_i(x_i))$$
$$\sum_{(i,j)} f_j(x_j) = \sum_j (q_j \times f_j(x_j))$$

Hammersley-Clifford Theorem [2, 3, 4] states, that probability distribution of configurations of Markov Random Field can be factorized into product of non-negative functions ("potentials") – defined over maximal cliques of graph:

(8)
$$p(x_1, x_2, \dots x_n) = \frac{1}{Z} \times \left(\prod_{(i,j)} \psi_{ij}(x_i, x_j) \right) \times \left(\prod_i \phi_i(x_i) \right) \times \left(\prod_j \phi_j(x_j) \right)$$

Boltzmann's Law:

$$p(x_1, x_2, \dots x_n) = \frac{1}{Z} \times \exp\left(\frac{-E(x_1, x_2, \dots x_n)}{T}\right)$$

We can treat T just as a scaling coefficient, and for simplicity lets assume that T = 1:

(9)
$$p(x_1, x_2, \dots x_n) = \frac{1}{Z} \times \exp(-E(x_1, x_2, \dots x_n))$$

From (8) and (9):

$$\exp\left(-E(x_1, x_2, \dots x_n)\right) = \left(\prod_{(i,j)} \psi_{ij}(x_i, x_j)\right) \times \left(\prod_i \phi_i(x_i)\right) \times \left(\prod_j \phi_j(x_j)\right)$$

So:

$$(10) \quad E(x_1, x_2, \dots x_n) = -\left(\sum_{(i,j)} \ln(\psi_{ij}(x_i, x_j))\right) - \left(\sum_{i} \ln(\phi_i(x_i))\right) - \left(\sum_{j} \ln(\phi_j(x_j))\right)$$

Lets, assume that we have function $b(x_1, x_2, ... x_n)$, which approximates real probability density function $p(x_1, x_2, ... x_n)$. It means, that Equations (1)–(6) the same for $b(x_1, x_2, ... x_n)$:

(11)
$$\sum_{x_1} \sum_{x_2} \cdots \sum_{x_n} b(x_1, x_2, \dots x_n) = 1$$

(12)
$$b_{i}(x_{i}) = \sum_{x_{1}} \cdots \sum_{x_{i-1}} \sum_{x_{i+1}} \cdots \sum_{x_{n}} b(x_{1}, x_{2}, \dots x_{n})$$
$$b_{j}(x_{i}) = \sum_{x_{1}} \cdots \sum_{x_{j-1}} \sum_{x_{j+1}} \cdots \sum_{x_{n}} b(x_{1}, x_{2}, \dots x_{n})$$

$$(13) \quad b_{ij}(x_i, x_j) = \sum_{x_1} \cdots \sum_{x_{i-1}} \sum_{x_{i+1}} \cdots \sum_{x_{j-1}} \sum_{x_{j+1}} \cdots \sum_{x_n} b(x_1, x_2, \dots x_n)$$

(14)
$$\sum_{x_i} b_i(x_i) = 1$$
$$\sum_{x_j} b_j(x_j) = 1$$

(15)
$$\sum_{x_i} \sum_{x_j} b_{ij}(x_i, x_j) = 1$$

(16)
$$b_{i}(x_{i}) = \sum_{x_{j}} b_{ij}(x_{i}, x_{j})$$
$$b_{j}(x_{j}) = \sum_{x_{i}} b_{ij}(x_{i}, x_{j})$$

Lets use Kullback-Leibler divergence for measurement of "difference" between real and approximated functions:

$$D_{KL}(b||p) = \sum_{x_1} \sum_{x_2} \cdots \sum_{x_n} \left(b(x_1, x_2, \dots x_n) \times \ln \left(\frac{b(x_1, x_2, \dots x_n)}{p(x_1, x_2, \dots x_n)} \right) \right) =$$

$$= \left(\sum_{x_1} \sum_{x_2} \cdots \sum_{x_n} b(x_1, x_2, \dots x_n) \times \ln \left(b(x_1, x_2, \dots x_n) \right) \right) -$$

$$- \left(\sum_{x_1} \sum_{x_2} \cdots \sum_{x_n} b(x_1, x_2, \dots x_n) \times \ln \left(p(x_1, x_2, \dots x_n) \right) \right)$$

Lest substitute $p(x_1, x_2, \dots x_n)$ using expression from equation (9):

$$D_{KL}(b||p) = \left(\sum_{x_1} \sum_{x_2} \cdots \sum_{x_n} b(x_1, x_2, \dots x_n) \times \ln(b(x_1, x_2, \dots x_n))\right) - \left(\sum_{x_1} \sum_{x_2} \cdots \sum_{x_n} b(x_1, x_2, \dots x_n) \times \ln\left(\frac{1}{Z} \times \exp(-E(x_1, x_2, \dots x_n))\right)\right) = \left(\sum_{x_1} \sum_{x_2} \cdots \sum_{x_n} b(x_1, x_2, \dots x_n) \times \ln(b(x_1, x_2, \dots x_n))\right) - \left(\sum_{x_1} \sum_{x_2} \cdots \sum_{x_n} b(x_1, x_2, \dots x_n) \times (-\ln(Z) - E(x_1, x_2, \dots x_n))\right) = \left(\sum_{x_1} \sum_{x_2} \cdots \sum_{x_n} b(x_1, x_2, \dots x_n) \times \ln(b(x_1, x_2, \dots x_n))\right) + \left(\sum_{x_1} \sum_{x_2} \cdots \sum_{x_n} b(x_1, x_2, \dots x_n) \times \ln(Z)\right) + \left(\sum_{x_1} \sum_{x_2} \cdots \sum_{x_n} b(x_1, x_2, \dots x_n) \times E(x_1, x_2, \dots x_n)\right)$$

As far, as Z is just a constant – it doesn't depend on $x_1, x_2 \dots x_n$, so we can move ln(Z) out of summations:

$$D_{KL}(b||p) = \left(\sum_{x_1} \sum_{x_2} \cdots \sum_{x_n} b(x_1, x_2, \dots x_n) \times \ln(b(x_1, x_2, \dots x_n))\right) + \left(\sum_{x_1} \sum_{x_2} \cdots \sum_{x_n} b(x_1, x_2, \dots x_n)\right) \times \ln(Z) + \left(\sum_{x_1} \sum_{x_2} \cdots \sum_{x_n} b(x_1, x_2, \dots x_n) \times E(x_1, x_2, \dots x_n)\right)$$

Taking into account equation (11), we can substitute multiplier near ln(Z) – to 1:

(20)
$$D_{KL}(b||p) = \left(\sum_{x_1} \sum_{x_2} \cdots \sum_{x_n} b(x_1, x_2, \dots x_n) \times \ln(b(x_1, x_2, \dots x_n))\right) + \left(\sum_{x_1} \sum_{x_2} \cdots \sum_{x_n} b(x_1, x_2, \dots x_n) \times E(x_1, x_2, \dots x_n)\right) + \ln(Z)$$

Lets use following notation:

$$U(b(x_1, x_2, \dots x_n)) = \sum_{x_1} \sum_{x_2} \dots \sum_{x_n} (b(x_1, x_2, \dots x_n) \times E(x_1, x_2, \dots x_n))$$

$$(21) \quad -H(b(x_1, x_2, \dots x_n)) = \sum_{x_1} \sum_{x_2} \dots \sum_{x_n} (b(x_1, x_2, \dots x_n) \times \ln(b(x_1, x_2, \dots x_n)))$$

$$G(b(x_1, x_2, \dots x_n)) = U(b(x_1, x_2, \dots x_n)) - H(b(x_1, x_2, \dots x_n))$$

$$-F(b(x_1, x_2, \dots x_n)) = -F = \ln(Z)$$

So:

(22) $D_{KL}(b||p) = G(b(x_1, x_2, \dots x_n)) - F = U(b(x_1, x_2, \dots x_n)) - H(b(x_1, x_2, \dots x_n)) + ln(Z)$ Let's transform $U(b(x_1, x_2, \dots x_n))$, using expression for energy (10):

$$\begin{aligned} &U(b(x_1,x_2,\ldots x_n)) = \sum_{x_1} \sum_{x_2} \cdots \sum_{x_n} \left(b(x_1,x_2,\ldots x_n) \times E(x_1,x_2,\ldots x_n) \right) = \\ &= \sum_{x_1} \sum_{x_2} \cdots \sum_{x_n} \left(b(x_1,x_2,\ldots x_n) \times \left(-\left(\sum_{i,j} ln(\psi_{ij}(x_i,x_j)) \right) - \left(\sum_{i} ln(\phi_{i}(x_i)) \right) - \left(\sum_{j} ln(\phi_{j}(x_j)) \right) \right) \right) = \\ &= -\left(\sum_{x_1} \sum_{x_2} \cdots \sum_{x_n} \left(b(x_1,x_2,\ldots x_n) \times \sum_{i} ln(\psi_{ij}(x_i,x_j)) \right) \right) - \\ &- \left(\sum_{x_1} \sum_{x_2} \cdots \sum_{x_n} \left(b(x_1,x_2,\ldots x_n) \times \sum_{i} ln(\phi_{i}(x_i)) \right) \right) - \\ &- \left(\sum_{x_1} \sum_{x_2} \cdots \sum_{x_n} \left(b(x_1,x_2,\ldots x_n) \times \sum_{j} ln(\phi_{j}(x_j)) \right) \right) = \\ &= -\left(\sum_{i} \sum_{x_1} \sum_{x_2} \cdots \sum_{x_n} \left(b(x_1,x_2,\ldots x_n) \times ln(\psi_{ij}(x_i,x_j)) \right) \right) - \\ &- \left(\sum_{i} \sum_{x_1} \sum_{x_2} \cdots \sum_{x_n} \left(b(x_1,x_2,\ldots x_n) \times ln(\phi_{i}(x_i)) \right) \right) - \\ &- \left(\sum_{j} \sum_{x_1} \sum_{x_2} \cdots \sum_{x_n} \left(b(x_1,x_2,\ldots x_n) \times ln(\phi_{j}(x_j)) \right) \right) = \\ &= -\left(\sum_{i,j} \sum_{x_1} \sum_{x_2} \sum_{x_1} \cdots \sum_{x_{i-1}} \sum_{x_{i+1}} \cdots \sum_{x_{j-1}} \sum_{x_{j+1}} \cdots \sum_{x_n} \left(b(x_1,x_2,\ldots x_n) \times ln(\psi_{ij}(x_i,x_j)) \right) \right) - \\ &- \left(\sum_{j} \sum_{x_1} \sum_{x_1} \cdots \sum_{x_{i-1}} \sum_{x_{i+1}} \cdots \sum_{x_n} \left(b(x_1,x_2,\ldots x_n) \times ln(\phi_{i}(x_i)) \right) \right) - \\ &- \left(\sum_{j} \sum_{x_1} \sum_{x_1} \cdots \sum_{x_{i-1}} \sum_{x_{i+1}} \cdots \sum_{x_n} \left(b(x_1,x_2,\ldots x_n) \times ln(\phi_{i}(x_i)) \right) \right) - \\ &- \left(\sum_{j} \sum_{x_1} \sum_{x_1} \cdots \sum_{x_{i-1}} \sum_{x_{i+1}} \cdots \sum_{x_n} \left(b(x_1,x_2,\ldots x_n) \times ln(\phi_{i}(x_i)) \right) \right) - \\ &- \left(\sum_{j} \sum_{x_1} \sum_{x_1} \cdots \sum_{x_{i-1}} \sum_{x_{i+1}} \cdots \sum_{x_n} \left(b(x_1,x_2,\ldots x_n) \times ln(\phi_{i}(x_i)) \right) \right) - \\ &- \left(\sum_{j} \sum_{x_1} \sum_{x_1} \cdots \sum_{x_{i-1}} \sum_{x_{i+1}} \cdots \sum_{x_n} \left(b(x_1,x_2,\ldots x_n) \times ln(\phi_{i}(x_i)) \right) \right) - \\ &- \left(\sum_{j} \sum_{x_1} \sum_{x_1} \cdots \sum_{x_{i-1}} \sum_{x_{i+1}} \cdots \sum_{x_n} \left(b(x_1,x_2,\ldots x_n) \times ln(\phi_{i}(x_i)) \right) \right) - \\ &- \left(\sum_{j} \sum_{x_1} \sum_{x_1} \cdots \sum_{x_{i-1}} \sum_{x_{i+1}} \cdots \sum_{x_n} \left(b(x_1,x_2,\ldots x_n) \times ln(\phi_{i}(x_i)) \right) \right) - \\ &- \left(\sum_{j} \sum_{x_1} \sum_{x_1} \cdots \sum_{x_{i-1}} \sum_{x_{i+1}} \cdots \sum_{x_n} \left(b(x_1,x_2,\ldots x_n) \times ln(\phi_{i}(x_i,x_i) \right) \right) \right) - \\ &- \left(\sum_{j} \sum_{x_1} \sum_{x_1} \cdots \sum_{x_n} \sum_{x_{i+1}} \cdots \sum_{x_n} \left(b(x_1,x_2,\ldots x_n) \times ln(\phi_{i}(x_i,x_i) \right) \right) \right) - \\ &- \left(\sum_{j} \sum_{x_1} \sum_{x_1} \cdots \sum_{x_n} \sum_{x_{i+1}} \cdots \sum_{x_n} \sum_{x_{i+1}} \cdots \sum_{x_n} \left(b(x_1,x_2,\ldots x_n) \times ln($$

As far, as $\psi_{ij}(x_i, x_j)$ – depends only on x_i and x_j , and $\phi_i(x_i)$ – depends only on x_i , and $\phi_j(x_j)$ – depends only on x_j – we could rewrite sums as:

(24)

$$\begin{split} &U(b(x_1,x_2,\ldots x_n)) = -\left(\sum_{(i,j)}\sum_{x_i}\sum_{x_j}\ln(\psi_{ij}(x_i,x_j))\times\left(\sum_{x_1}\cdots\sum_{x_{i-1}}\sum_{x_{i+1}}\cdots\sum_{x_j}\sum_{x_{j+1}}\cdots\sum_{x_n}b(x_1,x_2,\ldots x_n)\right)\right) - \\ &-\left(\sum_{i}\sum_{x_i}\ln(\phi_i(x_i))\times\left(\sum_{x_1}\cdots\sum_{x_{i-1}}\sum_{x_{i+1}}\cdots\sum_{x_n}b(x_1,x_2,\ldots x_n)\right)\right) - \\ &-\left(\sum_{j}\sum_{x_j}\ln(\phi_j(x_j))\times\left(\sum_{x_1}\cdots\sum_{x_{j-1}}\sum_{x_{j+1}}\cdots\sum_{x_n}b(x_1,x_2,\ldots x_n)\right)\right) \end{split}$$

Taking into account Equations (12) and (13): we can substitute summations of probability density function – to marginal probabilities:

(25)
$$U(b(x_1, x_2, \dots x_n)) = -\left(\sum_{(i,j)} \sum_{x_i} \sum_{x_j} ln(\psi_{ij}(x_i, x_j)) \times b_{ij}(x_i, x_j)\right) - \left(\sum_{i} \sum_{x_i} ln(\phi_i(x_i)) \times b_i(x_i)\right) - \left(\sum_{j} \sum_{x_j} ln(\phi_j(x_j)) \times b_j(x_j)\right)$$

Lets introduce following variables ("local energies"):

$$E_i(x_i) = -ln(\phi_i(x_i))$$

(26)
$$E_j(x_j) = -ln(\phi_j(x_j))$$

 $E_{ij}(x_i, x_j) = -ln(\psi_{ij}(x_i, x_j)) - ln(\phi_i(x_i)) - ln(\phi_j(x_j))$

So, now we can express $ln(\phi_i(x_i))$, $ln(\phi_j(x_j))$ and $ln(\psi_{ij}(x_i,x_j))$ – using "local energies" (26):

$$ln(\phi_i(x_i)) = -E_i(x_i)$$

(27)
$$ln(\phi_j(x_j)) = -E_j(x_j)$$

 $ln(\psi_{ij}(x_i, x_j)) = -E_{ij}(x_i, x_j) + E_i(x_i) + E_j(x_j)$

Lets transform $U(b(x_1, x_2, \dots x_n))$ using Equations (27):

$$U(b(x_{1}, x_{2}, \dots x_{n})) = -\left(\sum_{(i,j)} \sum_{x_{i}} \sum_{x_{j}} b_{ij}(x_{i}, x_{j}) \times (-E_{ij}(x_{i}, x_{j}) + E_{i}(x_{i}) + E_{j}(x_{j}))\right) - \left(\sum_{i} \sum_{x_{i}} b_{i}(x_{i}) \times (-E_{i}(x_{i}))\right) - \left(\sum_{j} \sum_{x_{j}} b_{j}(x_{j}) \times (-E_{j}(x_{j}))\right) =$$

$$= \left(\sum_{(i,j)} \sum_{x_{i}} \sum_{x_{j}} b_{ij}(x_{i}, x_{j}) \times E_{ij}(x_{i}, x_{j})\right) - \left(\sum_{(i,j)} \sum_{x_{i}} \sum_{x_{j}} b_{ij}(x_{i}, x_{j}) \times E_{i}(x_{i})\right) - \left(\sum_{(i,j)} \sum_{x_{j}} \sum_{x_{i}} b_{ij}(x_{i}, x_{j}) \times E_{j}(x_{j})\right) + \left(\sum_{i} \sum_{x_{i}} b_{i}(x_{i}) \times E_{i}(x_{i})\right) + \left(\sum_{j} \sum_{x_{j}} b_{j}(x_{j}) \times E_{j}(x_{j})\right)$$

Taking into account that $E_i(x_i)$ is not depends on x_j , and $E_j(x_j)$ is not depends on x_i - we can move these multipliers out of corresponding summations:

$$U(b(x_1, x_2, \dots x_n)) = \left(\sum_{(i,j)} \sum_{x_i} \sum_{x_j} b_{ij}(x_i, x_j) \times E_{ij}(x_i, x_j)\right) - \left(\sum_{(i,j)} \sum_{x_i} E_i(x_i) \times \sum_{x_j} b_{ij}(x_i, x_j)\right) - \left(\sum_{(i,j)} \sum_{x_j} E_i(x_j) \times \sum_{x_j} b_{ij}(x_i, x_j)\right) - \left(\sum_{(i,j)} \sum_{x_j} E_i(x_j) \times \sum_{x_j} b_{ij}(x_i, x_j)\right) + \left(\sum_{i} \sum_{x_j} b_i(x_i) \times E_i(x_i)\right) + \left(\sum_{j} \sum_{x_j} b_j(x_j) \times E_j(x_j)\right)$$

Taking into account (16) – we can substitute summations over two-node marginal probabilities – to single-node marginal probabilities:

$$(30) \quad U(b(x_1, x_2, \dots x_n)) = \left(\sum_{(i,j)} \sum_{x_i} \sum_{x_j} b_{ij}(x_i, x_j) \times E_{ij}(x_i, x_j)\right) - \left(\sum_{(i,j)} \sum_{x_i} E_i(x_i) \times b_i(x_i)\right) - \left(\sum_{(i,j)} \sum_{x_j} E_j(x_j) \times b_j(x_j)\right) + \left(\sum_{i} \sum_{x_i} b_i(x_i) \times E_i(x_i)\right) + \left(\sum_{j} \sum_{x_j} b_j(x_j) \times E_j(x_j)\right)$$

Finally, we can substitute summations over edges – to summation over nodes, as described by Equation (7):

$$U(b(x_1, x_2, \dots x_n)) = \left(\sum_{(i,j)} \sum_{x_i} \sum_{x_j} b_{ij}(x_i, x_j) \times E_{ij}(x_i, x_j)\right) - \left(\sum_{x_i} \sum_{(i,j)} E_i(x_i) \times b_i(x_i)\right) - \left(\sum_{x_j} \sum_{(i,j)} E_j(x_j) \times b_j(x_j)\right) + \left(\sum_{i} \sum_{x_i} b_i(x_i) \times E_i(x_i)\right) + \left(\sum_{j} \sum_{x_j} b_j(x_j) \times E_j(x_j)\right) =$$

$$= \left(\sum_{(i,j)} \sum_{x_i} \sum_{x_j} b_{ij}(x_i, x_j) \times E_{ij}(x_i, x_j)\right) - \left(\sum_{x_i} \sum_{i} q_i \times E_i(x_i) \times b_i(x_i)\right) -$$

$$- \left(\sum_{x_j} \sum_{i} \sum_{x_j} b_{ij}(x_i, x_j) \times E_{ij}(x_i, x_j)\right) + \left(\sum_{i} \sum_{x_i} b_i(x_i) \times E_i(x_i)\right) + \left(\sum_{j} \sum_{x_j} b_j(x_j) \times E_j(x_j)\right) =$$

$$= \left(\sum_{(i,j)} \sum_{x_i} \sum_{x_j} b_{ij}(x_i, x_j) \times E_{ij}(x_i, x_j)\right) - \left(\sum_{i} \sum_{x_j} (q_i - 1) \times E_i(x_i) \times b_i(x_i)\right) - \left(\sum_{i} \sum_{x_j} (q_i - 1) \times E_i(x_i) \times b_i(x_i)\right) - \left(\sum_{i} \sum_{x_j} (q_i - 1) \times E_i(x_i) \times b_i(x_i)\right) - \left(\sum_{i} \sum_{x_j} (q_i - 1) \times E_i(x_i) \times b_i(x_i)\right) - \left(\sum_{i} \sum_{x_j} (q_i - 1) \times E_i(x_i) \times b_i(x_i)\right) - \left(\sum_{i} \sum_{x_j} (q_i - 1) \times E_i(x_i) \times b_i(x_i)\right) - \left(\sum_{i} \sum_{x_j} (q_i - 1) \times E_i(x_i) \times b_i(x_i)\right) - \left(\sum_{i} \sum_{x_j} (q_i - 1) \times E_i(x_i) \times b_i(x_i)\right) - \left(\sum_{i} \sum_{x_j} (q_i - 1) \times E_i(x_i) \times b_i(x_i)\right) - \left(\sum_{i} \sum_{x_j} (q_i - 1) \times E_i(x_i) \times b_i(x_i)\right) - \left(\sum_{i} \sum_{x_j} (q_i - 1) \times E_i(x_i) \times b_i(x_i)\right) - \left(\sum_{i} \sum_{x_j} (q_i - 1) \times E_i(x_i) \times b_i(x_i)\right) - \left(\sum_{i} \sum_{x_j} (q_i - 1) \times E_i(x_i) \times b_i(x_i)\right) - \left(\sum_{i} \sum_{x_j} (q_i - 1) \times E_i(x_i) \times b_i(x_i)\right) - \left(\sum_{i} \sum_{x_j} (q_i - 1) \times E_i(x_i) \times b_i(x_i)\right) - \left(\sum_{i} \sum_{x_j} (q_i - 1) \times E_i(x_j) \times b_i(x_i)\right) - \left(\sum_{i} \sum_{x_j} (q_i - 1) \times E_i(x_i) \times b_i(x_i)\right) - \left(\sum_{i} \sum_{x_j} (q_i - 1) \times E_i(x_i) \times b_i(x_i)\right) - \left(\sum_{i} \sum_{x_j} (q_i - 1) \times E_i(x_i) \times b_i(x_i)\right) - \left(\sum_{i} \sum_{x_j} (q_i - 1) \times E_i(x_j) \times b_i(x_i)\right)$$

So, finally, we derived representation of $U(b(x_1, x_2, \dots x_n))$ in terms of marginal probabilities and "local

energies":

(32)
$$U(b(x_1, x_2, \dots x_n)) = \left(\sum_{(i,j)} \sum_{x_i} \sum_{x_j} b_{ij}(x_i, x_j) \times E_{ij}(x_i, x_j) \right) - \left(\sum_{i} \sum_{x_i} (q_i - 1) \times E_i(x_i) \times b_i(x_i) \right) - \left(\sum_{j} \sum_{x_j} (q_j - 1) \times E_j(x_j) \times b_j(x_j) \right)$$

Now, lets transform $-H(b(x_1, x_2, \dots x_n))$ from Equations (21):

(33)
$$-H(b(x_1, x_2, \dots x_n)) = \sum_{x_1} \sum_{x_2} \dots \sum_{x_n} (b(x_1, x_2, \dots x_n) \times ln(b(x_1, x_2, \dots x_n)))$$

Lets introduce additional statement [5] (which can be proven by induction [6]) – probability distribution can be expressed via marginal probabilities (over max-cliques and single nodes), and node-degrees of graph. For Pairwise Markov Random Field this statement can be formalised as:

(34)
$$b(x_1, x_2, \dots x_n) = \frac{\prod_{(i,j)} b_{ij}(x_i, x_j)}{\prod_i b_i(x_i)^{q_i - 1} \times \prod_j b_j(x_j)^{q_j - 1}}$$

So, lets rewrite Equation (33), keeping in mind Equation (34):

$$\begin{split} &-H(b(x_{1},x_{2},\ldots x_{n})) = \sum_{x_{1}} \sum_{x_{2}} \cdots \sum_{x_{n}} \left(b(x_{1},x_{2},\ldots x_{n}) \times \ln\left(b(x_{1},x_{2},\ldots x_{n})\right)\right) = \\ &= \sum_{x_{1}} \sum_{x_{2}} \cdots \sum_{x_{n}} \left(b(x_{1},x_{2},\ldots x_{n}) \times \ln\left(\frac{\prod_{(i,j)} b_{ij}(x_{i},x_{j})}{\prod_{i} b_{i}(x_{i})^{q_{i}-1}} \times \prod_{j} b_{j}(x_{j})^{q_{j}-1}}\right)\right) = \\ &= \sum_{x_{1}} \sum_{x_{2}} \cdots \sum_{x_{n}} \left(b(x_{1},x_{2},\ldots x_{n}) \times \left(\ln\left(\prod_{(i,j)} b_{ij}(x_{i},x_{j})\right) - \ln\left(\prod_{i} b_{i}(x_{i})^{q_{i}-1}\right) - \ln\left(\prod_{j} b_{j}(x_{j})^{q_{j}-1}\right)\right)\right) = \\ &= \sum_{x_{1}} \sum_{x_{2}} \cdots \sum_{x_{n}} \left(b(x_{1},x_{2},\ldots x_{n}) \times \left(\left(\sum_{(i,j)} \ln\left(b_{ij}(x_{i},x_{j})\right)\right) - \left(\sum_{i} \ln\left(b_{i}(x_{i})^{q_{i}-1}\right)\right) - \left(\sum_{j} \ln\left(b_{j}(x_{j})^{q_{j}-1}\right)\right)\right)\right) = \\ &= \left(\sum_{x_{1}} \sum_{x_{2}} \cdots \sum_{x_{n}} b(x_{1},x_{2},\ldots x_{n}) \times \sum_{(i,j)} \ln\left(b_{ij}(x_{i},x_{j})\right)\right) - \\ &- \left(\sum_{x_{1}} \sum_{x_{2}} \cdots \sum_{x_{n}} b(x_{1},x_{2},\ldots x_{n}) \times \ln\left(b_{i}(x_{i})^{q_{i}-1}\right)\right) - \left(\sum_{x_{1}} \sum_{x_{2}} \cdots \sum_{x_{n}} b(x_{1},x_{2},\ldots x_{n}) \times \ln\left(b_{j}(x_{j})^{q_{j}-1}\right)\right) - \\ &- \left(\sum_{i} \sum_{x_{1}} \sum_{x_{2}} \cdots \sum_{x_{n}} b(x_{1},x_{2},\ldots x_{n}) \times \ln\left(b_{i}(x_{i})^{q_{i}-1}\right)\right) - \left(\sum_{j} \sum_{x_{1}} \sum_{x_{2}} \cdots \sum_{x_{n}} b(x_{1},x_{2},\ldots x_{n}) \times \ln\left(b_{j}(x_{j})^{q_{i}-1}\right)\right) - \\ &- \left(\sum_{i} \sum_{x_{1}} \sum_{x_{2}} \cdots \sum_{x_{n}} b(x_{1},x_{2},\ldots x_{n}) \times \ln\left(b_{i}(x_{i})^{q_{i}-1}\right)\right) - \left(\sum_{j} \sum_{x_{1}} \sum_{x_{2}} \cdots \sum_{x_{n}} b(x_{1},x_{2},\ldots x_{n}) \times \ln\left(b_{j}(x_{j})^{q_{i}-1}\right)\right) - \left(\sum_{j} \sum_{x_{1}} \sum_{x_{2}} \cdots \sum_{x_{n}} b(x_{1},x_{2},\ldots x_{n}) \times \ln\left(b_{j}(x_{i})^{q_{i}-1}\right)\right) - \left(\sum_{j} \sum_{x_{1}} \sum_{x_{2}} \cdots \sum_{x_{n}} b(x_{1},x_{2},\ldots x_{n}) \times \ln\left(b_{j}(x_{i})^{q_{i}-1}\right)\right) - \left(\sum_{j} \sum_{x_{1}} \sum_{x_{2}} \cdots \sum_{x_{n}} b(x_{1},x_{2},\ldots x_{n}) \times \ln\left(b_{j}(x_{i})^{q_{i}-1}\right)\right) - \left(\sum_{j} \sum_{x_{1}} \sum_{x_{2}} \cdots \sum_{x_{n}} b(x_{1},x_{2},\ldots x_{n}) \times \ln\left(b_{j}(x_{i})^{q_{i}-1}\right)\right) - \left(\sum_{j} \sum_{x_{1}} \sum_{x_{2}} \cdots \sum_{x_{n}} b(x_{1},x_{2},\ldots x_{n}) \times \ln\left(b_{i}(x_{i})^{q_{i}-1}\right)\right) - \left(\sum_{j} \sum_{x_{1}} \sum_{x_{2}} \cdots \sum_{x_{n}} b(x_{1},x_{2},\ldots x_{n}) \times \ln\left(b_{i}(x_{i})^{q_{i}-1}\right)\right) - \left(\sum_{j} \sum_{x_{1}} \sum_{x_{2}} \cdots \sum_{x_{n}} b(x_{1},x_{2},\ldots x_{n}) \times \ln\left(b_{i}(x_{1})^{q_{i}-1}\right)\right) - \left(\sum_{j} \sum_{x_{1}$$

Lets rearrange sums, according to dependance of marginal probabilities:

(36)

$$-H(b(x_{1},x_{2},\ldots x_{n})) = \left(\sum_{(i,j)}\sum_{x_{i}}\sum_{x_{j}}\sum_{x_{1}}\cdots\sum_{x_{i-1}}\sum_{x_{i+1}}\cdots\sum_{x_{j-1}}\sum_{x_{j+1}}\cdots\sum_{x_{n}}b(x_{1},x_{2},\ldots x_{n})\times \ln(b_{ij}(x_{i},x_{j}))\right) - \left(\sum_{i}\sum_{x_{i}}\sum_{x_{1}}\cdots\sum_{x_{i-1}}\sum_{x_{i+1}}\cdots\sum_{x_{n}}b(x_{1},x_{2},\ldots x_{n})\times \ln\left(b_{i}(x_{i})^{q_{i}-1}\right)\right) - \left(\sum_{j}\sum_{x_{j}}\sum_{x_{1}}\cdots\sum_{x_{j-1}}\sum_{x_{j+1}}\cdots\sum_{x_{n}}b(x_{1},x_{2},\ldots x_{n})\times \ln\left(b_{j}(x_{j})^{q_{j}-1}\right)\right) = \left(\sum_{(i,j)}\sum_{x_{i}}\sum_{x_{j}}\ln(b_{ij}(x_{i},x_{j}))\times \left(\sum_{x_{1}}\cdots\sum_{x_{i-1}}\sum_{x_{i+1}}\cdots\sum_{x_{j}}\sum_{x_{j+1}}\cdots\sum_{x_{n}}b(x_{1},x_{2},\ldots x_{n})\right)\right) - \left(\sum_{i}\sum_{x_{i}}\ln\left(b_{i}(x_{i})^{q_{i}-1}\right)\times \left(\sum_{x_{1}}\cdots\sum_{x_{i-1}}\sum_{x_{i+1}}\cdots\sum_{x_{n}}b(x_{1},x_{2},\ldots x_{n})\right)\right) - \left(\sum_{j}\sum_{x_{j}}\ln\left(b_{j}(x_{j})^{q_{j}-1}\right)\times \left(\sum_{x_{1}}\cdots\sum_{x_{j-1}}\sum_{x_{j+1}}\cdots\sum_{x_{n}}b(x_{1},x_{2},\ldots x_{n})\right)\right)\right) - \left(\sum_{j}\sum_{x_{j}}\ln\left(b_{j}(x_{j})^{q_{j}-1}\right)\times \left(\sum_{x_{1}}\cdots\sum_{x_{j-1}}\sum_{x_{j+1}}\cdots\sum_{x_{n}}b(x_{1},x_{2},\ldots x_{n})\right)\right)\right)$$

Again, taking into account Equations (12) and (13): we can substitute summations of probability density function – to marginal probabilities:

$$-H(b(x_{1}, x_{2}, \dots x_{n})) = \left(\sum_{(i,j)} \sum_{x_{i}} \sum_{x_{j}} \ln (b_{ij}(x_{i}, x_{j})) \times \left(\sum_{x_{1}} \dots \sum_{x_{i-1}} \sum_{x_{i+1}} \dots \sum_{x_{j-1}} \sum_{x_{j+1}} \dots \sum_{x_{n}} b(x_{1}, x_{2}, \dots x_{n})\right)\right) - \left(\sum_{i} \sum_{x_{i}} \ln \left(b_{i}(x_{i})^{q_{i}-1}\right) \times \left(\sum_{x_{1}} \dots \sum_{x_{i-1}} \sum_{x_{i+1}} \dots \sum_{x_{n}} b(x_{1}, x_{2}, \dots x_{n})\right)\right) - \left(\sum_{j} \sum_{x_{j}} \ln \left(b_{j}(x_{j})^{q_{j}-1}\right) \times \left(\sum_{x_{1}} \dots \sum_{x_{j-1}} \sum_{x_{j+1}} \dots \sum_{x_{n}} b(x_{1}, x_{2}, \dots x_{n})\right)\right) = \left(\sum_{i} \sum_{x_{j}} \sum_{x_{j}} \ln \left(b_{ij}(x_{i}, x_{j})\right) \times b_{ij}(x_{i}, x_{j})\right) - \left(\sum_{i} \sum_{x_{i}} \ln \left(b_{i}(x_{i})^{q_{i}-1}\right) \times b_{i}(x_{i})\right) - \left(\sum_{j} \sum_{x_{j}} \ln \left(b_{j}(x_{j})^{q_{j}-1}\right) \times b_{j}(x_{j})\right)\right)$$

So, finally, we can represent $-H(b(x_1, x_2, \dots x_n))$ only in terms of marginal probabilities:

$$(38) - H(b(x_1, x_2, \dots x_n)) = \left(\sum_{(i,j)} \sum_{x_i} \sum_{x_j} \ln(b_{ij}(x_i, x_j)) \times b_{ij}(x_i, x_j) \right) - \left(\sum_{i} \sum_{x_i} (q_i - 1) \times \ln(b_i(x_i)) \times b_i(x_i) \right) - \left(\sum_{j} \sum_{x_j} (q_j - 1) \times \ln(b_j(x_j)) \times b_j(x_j) \right)$$

Lets represent Kullback-Leibler divergence (22) – in terms of marginal probabilities and local energies (keeping in mind Equations (32) and (38)):

$$\begin{split} &D_{KL}(b||p) = U(b(x_1, x_2, \dots x_n)) - H(b(x_1, x_2, \dots x_n)) + ln(Z) = \\ &= \left(\sum_{(i,j)} \sum_{x_i} \sum_{x_j} b_{ij}(x_i, x_j) \times E_{ij}(x_i, x_j)\right) - \\ &- \left(\sum_{i} \sum_{x_i} (q_i - 1) \times E_i(x_i) \times b_i(x_i)\right) - \left(\sum_{j} \sum_{x_j} (q_j - 1) \times E_j(x_j) \times b_j(x_j)\right) + \\ &+ \left(\sum_{(i,j)} \sum_{x_i} \sum_{x_j} ln\left(b_{ij}(x_i, x_j)\right) \times b_{ij}(x_i, x_j)\right) - \\ &- \left(\sum_{i} \sum_{x_i} (q_i - 1) \times ln(b_i(x_i)) \times b_i(x_i)\right) - \left(\sum_{j} \sum_{x_j} (q_j - 1) \times ln(b_j(x_j)) \times b_j(x_j)\right) + ln(Z) = \\ &= \left(\sum_{(i,j)} \sum_{x_i} \sum_{x_j} b_{ij}(x_i, x_j) \times (E_{ij}(x_i, x_j) + ln\left(b_{ij}(x_i, x_j)\right))\right) - \\ &- \left(\sum_{i} \sum_{x} (q_i - 1) \times b_i(x_i) \times (E_i(x_i) + ln(b_i(x_i)))\right) - \left(\sum_{j} \sum_{x} (q_j - 1) \times b_j(x_j) \times (E_j(x_j) + ln(b_j(x_j)))\right) + ln(Z) \end{split}$$

So, again, I would like to pay attention on the fact – that we avoided potentially exponential amount of operations, during calculation of Kullback-Leibler divergence:

$$\begin{aligned} &(40) \\ &D_{KL}(b||p) = \sum_{x_1} \sum_{x_2} \cdots \sum_{x_n} \left(b(x_1, x_2, \dots x_n) \times ln \left(\frac{b(x_1, x_2, \dots x_n)}{p(x_1, x_2, \dots x_n)} \right) \right) = \\ &= \left(\sum_{(i,j)} \sum_{x_i} \sum_{x_j} b_{ij}(x_i, x_j) \times \left(E_{ij}(x_i, x_j) + ln \left(b_{ij}(x_i, x_j) \right) \right) \right) - \\ &- \left(\sum_{i} \sum_{x_i} (q_i - 1) \times b_i(x_i) \times \left(E_{i}(x_i) + ln(b_i(x_i)) \right) \right) - \left(\sum_{j} \sum_{x_j} (q_j - 1) \times b_j(x_j) \times \left(E_{j}(x_j) + ln(b_j(x_j)) \right) \right) + ln(Z) \end{aligned}$$

So, our goal is to find such values of $b_i(x_i)$, $b_j(x_j)$ and $b_{ij}(x_i, x_j)$ – which leads to minimal value of $D_{KL}(b||p)$, with respect to conditions, defined by Equations (14)–(16).

Lets use Lagrange multipliers method [8] for this purpose. Lets construct lagrangian, according to restrictions from Equations (14)–(16):

$$\mathcal{L} = D_{KL}(b||p) + \left(\sum_{i} \gamma_{i} \times \left(1 - \sum_{x_{i}} b_{i}(x_{i})\right)\right) + \left(\sum_{j} \gamma_{j} \times \left(1 - \sum_{x_{j}} b_{j}(x_{j})\right)\right) + \left(\sum_{i} \sum_{x_{i}} \sum_{j \in N(i)} \lambda_{ji}(x_{i}) \times \left(b_{i}(x_{i}) - \sum_{x_{j}} b_{ij}(x_{i}, x_{j})\right)\right) + \left(\sum_{j} \sum_{x_{j}} \sum_{i \in N(j)} \lambda_{ij}(x_{j}) \times \left(b_{j}(x_{j}) - \sum_{x_{i}} b_{ij}(x_{i}, x_{j})\right)\right) + \left(\sum_{j} \sum_{x_{j}} \sum_{i \in N(j)} \lambda_{ij}(x_{j}) \times \left(b_{j}(x_{j}) - \sum_{x_{i}} b_{ij}(x_{i}, x_{j})\right)\right)$$

Where:

- $\gamma_i, \gamma_j, \gamma_{ij}, \lambda_{ji}(x_i)$ and $\lambda_{ij}(x_j)$ lagrange multipliers (just some constants)
- $\sum_{j \in N(i)}$ sum over node-indices j, which are adjacent to node i ("neighbours") Which means, that $\forall j \in N(i)$ exists edge (which represented by tuple (i,j))
- $\sum_{i \in N(j)}$ sum over node-indices i, which are adjacent to node j

So, \mathcal{L} – is a function, which depends on variables:

- $b_i(x_i)$ defined $\forall i \in OddNodes$, and $\forall x_i \in StatesOfNode(i)$
- $b_j(x_j)$ defined $\forall j \in EvenNodes$, and $\forall x_j \in StatesOfNode(j)$
- $b_{ij}(x_i, x_j)$ defined $\forall (i, j) \in Edges$, and $\forall x_i \in StatesOfNode(i)$, and $\forall x_j \in StatesOfNode(j)$

By definition of Lagrange multipliers method, we are interested in stationary points of \mathcal{L} :

$$(42) \quad \frac{\partial \mathcal{L}}{\partial b_{ij}(x_i, x_j)} = 0, \ (\forall (i, j) \in Edges, \ \forall x_i \in StatesOfNode(i), \ \forall x_j \in StatesOfNode(j))$$

(43)
$$\frac{\partial \mathcal{L}}{\partial b_i(x_i)} = 0$$
, $(\forall i \in OddNodes, \ \forall x_i \in StatesOfNode(i))$

(44)
$$\frac{\partial \mathcal{L}}{\partial b_i(x_i)} = 0$$
, $(\forall j \in EvenNodes, \ \forall x_j \in StatesOfNode(j))$

Lets transform Equation (42), using Equation (41):

$$\frac{\partial \mathcal{L}}{\partial b_{ij}(x_i, x_j)} = \frac{\partial \left(D_{KL}(b||p)\right)}{\partial b_{ij}(x_i, x_j)} + \frac{\partial \left(-\gamma_{ij} \times b_{ij}(x_i, x_j)\right)}{\partial b_{ij}(x_i, x_j)} +$$

$$(45) + \frac{\partial \left(-\frac{\lambda_{ji}(x_i)}{\partial b_{ij}(x_i, x_j)} \times b_{ij}(x_i, x_j)\right)}{\partial b_{ij}(x_i, x_j)} + \frac{\partial \left(-\frac{\lambda_{ij}(x_j)}{\partial b_{ij}(x_i, x_j)} \times b_{ij}(x_i, x_j)\right)}{\partial b_{ij}(x_i, x_j)} =$$

$$= \frac{\partial \left(D_{KL}(b||p)\right)}{\partial b_{ij}(x_i, x_j)} - \frac{\lambda_{ji}(x_i)}{\lambda_{ji}(x_i)} - \frac{\lambda_{ij}(x_j)}{\lambda_{ij}(x_j)} = 0$$

For the further transformation of partial derivative – lets use expression for $D_{KL}(b||p)$ from Equation (40):

$$\frac{\partial \mathcal{L}}{\partial b_{ij}(x_i, x_j)} = \frac{\partial \left(D_{KL}(b||p)\right)}{\partial b_{ij}(x_i, x_j)} - \gamma_{ij} - \lambda_{ji}(x_i) - \lambda_{ij}(x_j) =$$

$$= \frac{\partial \left(b_{ij}(x_i, x_j) \times \left(E_{ij}(x_i, x_j) + \ln\left(b_{ij}(x_i, x_j)\right)\right)\right)}{\partial b_{ij}(x_i, x_j)} - \gamma_{ij} - \lambda_{ji}(x_i) - \lambda_{ij}(x_j) =$$

$$= E_{ij}(x_i, x_j) + \frac{\partial \left(b_{ij}(x_i, x_j) \times \ln\left(b_{ij}(x_i, x_j)\right)\right)}{\partial b_{ij}(x_i, x_j)} - \gamma_{ij} - \lambda_{ji}(x_i) - \lambda_{ij}(x_j) =$$

$$= E_{ij}(x_i, x_j) + \ln\left(b_{ij}(x_i, x_j)\right) + 1 - \gamma_{ij} - \lambda_{ji}(x_i) - \lambda_{ij}(x_j) = 0$$

So, finally, from Equation (46) – we can derive expression for $\ln(b_{ij}(x_i, x_j))$:

(47)
$$ln(b_{ij}(x_i, x_j)) = \gamma_{ij} + \lambda_{ji}(x_i) + \lambda_{ij}(x_j) - E_{ij}(x_i, x_j) - 1$$

Now, lets transform Equation (43), using Equation (41):

$$\frac{\partial \mathcal{L}}{\partial b_{i}(x_{i})} = \frac{\partial \left(D_{KL}(b||p)\right)}{\partial b_{i}(x_{i})} + \frac{\partial \left(-\gamma_{i} \times b_{i}(x_{i})\right)}{\partial b_{i}(x_{i})} + \frac{\partial \left(\sum_{j \in N(i)} \lambda_{ji}(x_{i}) \times b_{i}(x_{i})\right)}{\partial b_{i}(x_{i})} =$$

$$= \frac{\partial \left(D_{KL}(b||p)\right)}{\partial b_{i}(x_{i})} - \gamma_{i} + \sum_{j \in N(i)} \left(\frac{\partial \left(\lambda_{ji}(x_{i}) \times b_{i}(x_{i})\right)}{\partial b_{i}(x_{i})}\right) =$$

$$= \frac{\partial \left(D_{KL}(b||p)\right)}{\partial b_{i}(x_{i})} - \gamma_{i} + \sum_{j \in N(i)} \lambda_{ji}(x_{i}) = 0$$

Again, for the further transformation of partial derivative – lets use expression for $D_{KL}(b||p)$ from Equation (40):

$$\frac{\partial \mathcal{L}}{\partial b_i(x_i)} = \frac{\partial \left(-(q_i - 1) \times b_i(x_i) \times \left(E_i(x_i) + \ln(b_i(x_i)) \right) \right)}{\partial b_i(x_i)} - \gamma_i + \sum_{j \in N(i)} \lambda_{ji}(x_i) =$$

$$(49) = -(q_i - 1) \times E_i(x_i) - (q_i - 1) \times \frac{\partial (b_i(x_i) \times ln(b_i(x_i)))}{\partial b_i(x_i)} - \gamma_i + \sum_{j \in N(i)} \lambda_{ji}(x_i) =$$

$$= -(q_i - 1) \times E_i(x_i) - (q_i - 1) \times (1 + ln(b_i(x_i))) - \gamma_i + \sum_{j \in N(i)} \lambda_{ji}(x_i) = 0$$

So, finally, from Equation (49) – we can derive expression for $ln(b_i(x_i))$:

$$(q_i - 1) \times (1 + ln(b_i(x_i))) = -(q_i - 1) \times E_i(x_i) - \gamma_i + \sum_{j \in N(i)} \lambda_{ji}(x_i)$$

(50)
$$(1 + \ln(b_i(x_i))) = -E_i(x_i) - \frac{\gamma_i}{q_i - 1} + \frac{\sum_{j \in N(i)} \lambda_{ji}(x_i)}{q_i - 1}$$
$$\ln(b_i(x_i)) = -E_i(x_i) - \frac{\gamma_i}{q_i - 1} - 1 + \frac{1}{q_i - 1} \times \sum_{j \in N(i)} \lambda_{ji}(x_i)$$

In the identical way – we can derive expression for $ln(b_i(x_i))$:

$$(51) ln(b_j(x_j)) = -E_j(x_j) - \frac{\gamma_j}{q_j - 1} - 1 + \frac{1}{q_j - 1} \times \sum_{i \in N(j)} \lambda_{ij}(x_j)$$

So, finally, we derived expressions for logarithms of marginal probabilities, which corresponds to stationary points of lagrangian:

(52)
$$\begin{cases} ln(b_{ij}(x_i, x_j)) = \gamma_{ij} + \lambda_{ji}(x_i) + \lambda_{ij}(x_j) - E_{ij}(x_i, x_j) - 1 \\ ln(b_i(x_i)) = -E_i(x_i) - \frac{\gamma_i}{q_i - 1} - 1 + \frac{1}{q_i - 1} \times \sum_{j \in N(i)} \lambda_{ji}(x_i) \\ ln(b_j(x_j)) = -E_j(x_j) - \frac{\gamma_j}{q_j - 1} - 1 + \frac{1}{q_j - 1} \times \sum_{i \in N(j)} \lambda_{ij}(x_j) \end{cases}$$

As you remember (from Equation (41)): γ_i , γ_j , γ_{ij} , $\lambda_{ji}(x_i)$ and $\lambda_{ij}(x_j)$ – are just some constants. So, if we find a way to compute these constants we will be able to compute marginal probabilities.

Lets represent $\lambda_{ji}(x_i)$ – as a sum of $(q_i - 1)$ constants:

(53)
$$\lambda_{ji}(x_i) = \sum_{k \in N(i) \setminus j} ln(m_{k \to i}(x_i))$$

As far as node i has q_i neighbours, we can imagine, that each constant $ln(m_{k\to i}(x_i))$ – belongs to edge (k,i) (except edge (j,i)).

The same is applied to $\lambda_{ij}(x_i)$:

(54)
$$\lambda_{ij}(x_j) = \sum_{k \in N(j) \setminus i} \ln(m_{k \to j}(x_j))$$

Lets rewrite Equations (52), using Equations (53) and (54):

$$\begin{cases}
ln\left(b_{ij}(x_{i}, x_{j})\right) = -E_{ij}(x_{i}, x_{j}) + \gamma_{ij} - 1 + \left(\sum_{k \in N(i) \setminus j} ln\left(m_{k \to i}(x_{i})\right)\right) + \left(\sum_{k \in N(j) \setminus i} ln\left(m_{k \to j}(x_{j})\right)\right) \\
ln(b_{i}(x_{i})) = -E_{i}(x_{i}) - \frac{\gamma_{i}}{q_{i} - 1} - 1 + \frac{1}{q_{i} - 1} \times \sum_{j \in N(i)} \left(\sum_{k \in N(i) \setminus j} ln\left(m_{k \to i}(x_{i})\right)\right) \\
ln(b_{j}(x_{j})) = -E_{j}(x_{j}) - \frac{\gamma_{j}}{q_{j} - 1} - 1 + \frac{1}{q_{j} - 1} \times \sum_{i \in N(j)} \left(\sum_{k \in N(j) \setminus i} ln\left(m_{k \to j}(x_{j})\right)\right)
\end{cases}$$

Also, it can be easy shown that:

(56)
$$\frac{1}{q_i - 1} \times \sum_{j \in N(i)} \sum_{k \in N(i) \setminus j} f(k) \equiv \sum_{k \in N(i)} f(k)$$
$$\frac{1}{q_j - 1} \times \sum_{i \in N(j)} \sum_{k \in N(j) \setminus i} f(k) \equiv \sum_{k \in N(j)} f(k)$$

So, finally we can represent logarithms of marginal probabilities as:

$$\begin{cases}
ln\left(b_{ij}(x_{i}, x_{j})\right) = -E_{ij}(x_{i}, x_{j}) + \gamma_{ij} - 1 + \left(\sum_{k \in N(i) \setminus j} ln\left(m_{k \to i}(x_{i})\right)\right) + \left(\sum_{k \in N(j) \setminus i} ln\left(m_{k \to j}(x_{j})\right)\right) \\
ln(b_{i}(x_{i})) = -E_{i}(x_{i}) - \frac{\gamma_{i}}{q_{i} - 1} - 1 + \sum_{k \in N(i)} ln\left(m_{k \to i}(x_{i})\right) \\
ln(b_{j}(x_{j})) = -E_{j}(x_{j}) - \frac{\gamma_{j}}{q_{j} - 1} - 1 + \sum_{k \in N(j)} ln\left(m_{k \to j}(x_{j})\right)
\end{cases}$$

Lets substitute local energies $(E_i(x_i), E_j(x_j))$ and $E_{ij}(x_i, x_j)$ – using Equations (26):

$$\begin{cases}
ln\left(b_{ij}(x_{i}, x_{j})\right) = ln(\psi_{ij}(x_{i}, x_{j})) + ln(\phi_{i}(x_{i})) + ln(\phi_{j}(x_{j})) + \gamma_{ij} - 1 + \\
+ \left(\sum_{k \in N(i) \setminus j} ln\left(m_{k \to i}(x_{i})\right)\right) + \left(\sum_{k \in N(j) \setminus i} ln\left(m_{k \to j}(x_{j})\right)\right) \\
ln(b_{i}(x_{i})) = ln(\phi_{i}(x_{i})) - \frac{\gamma_{i}}{q_{i} - 1} - 1 + \sum_{k \in N(i)} ln\left(m_{k \to i}(x_{i})\right) \\
ln(b_{j}(x_{j})) = ln(\phi_{j}(x_{j})) - \frac{\gamma_{j}}{q_{j} - 1} - 1 + \sum_{k \in N(j)} ln\left(m_{k \to j}(x_{j})\right)
\end{cases}$$

Now, lets exponentiate Equations (58) – to get expressions for marginal probabilities:

Now, lets exponentiate Equations (58) – to get expressions for marginal probabilities:
$$\begin{pmatrix}
b_{ij}(x_i, x_j) = \exp(\gamma_{ij} - 1) \times \left(\prod_{k \in N(i) \setminus j} m_{k \to i}(x_i)\right) \times \phi_i(x_i) \times \psi_{ij}(x_i, x_j) \times \phi_j(x_j) \times \left(\prod_{k \in N(j) \setminus i} m_{k \to j}(x_j)\right) \\
b_i(x_i) = \exp\left(-\frac{\gamma_i}{q_i - 1} - 1\right) \times \phi_i(x_i) \times \left(\prod_{k \in N(i)} m_{k \to i}(x_i)\right) \\
b_j(x_j) = \exp\left(-\frac{\gamma_j}{q_j - 1} - 1\right) \times \phi_j(x_j) \times \left(\prod_{k \in N(j)} m_{k \to j}(x_j)\right)$$
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If we look at Equations (59) - we can notice, that following multipliers does not depend on states of graph nodes $(x_i \text{ and } x_i)$:

(60)
$$\begin{cases} \exp(\gamma_{ij} - 1) \neq f(x_i, x_j) \\ \exp\left(-\frac{\gamma_i}{q_i - 1} - 1\right) \neq f(x_i) \\ \exp\left(-\frac{\gamma_j}{q_j - 1} - 1\right) \neq f(x_j) \end{cases}$$

Lets denote:

(61)
$$\begin{cases} Z_{ij} = \exp(\gamma_{ij} - 1) \\ Z_i = \exp\left(-\frac{\gamma_i}{q_i - 1} - 1\right) \\ Z_j = \exp\left(-\frac{\gamma_j}{q_j - 1} - 1\right) \end{cases}$$

So, actually, it means, that given multipliers just corresponds to normalization coefficients (with respect to Equations (14) and (15)):

$$\begin{cases} b_{ij}(x_i, x_j) = Z_{ij} \times \left(\prod_{k \in N(i) \setminus j} m_{k \to i}(x_i) \right) \times \phi_i(x_i) \times \psi_{ij}(x_i, x_j) \times \phi_j(x_j) \times \left(\prod_{k \in N(j) \setminus i} m_{k \to j}(x_j) \right), \\ \text{where } Z_{ij} \text{ is such that } \sum_{x_i} \sum_{x_j} b_{ij}(x_i, x_j) = 1 \end{cases}$$

$$b_i(x_i) = Z_i \times \phi_i(x_i) \times \left(\prod_{k \in N(i)} m_{k \to i}(x_i) \right),$$

$$\text{where } Z_i \text{ is such that } \sum_{x_i} b_i(x_i) = 1$$

$$b_j(x_j) = Z_j \times \phi_j(x_j) \times \left(\prod_{k \in N(j)} m_{k \to j}(x_j) \right),$$

$$\text{where } Z_j \text{ is such that } \sum_{x_j} b_j(x_j) = 1$$

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