Lecture 13: Message passing on Factor Graphs

4F13: Machine Learning

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http://mlg.eng.cam.ac.uk/teaching/4f13/

Factor Graphs

Factor graphs allow to represent the product structure of a function.

They are bipartite graphs with two types of nodes:

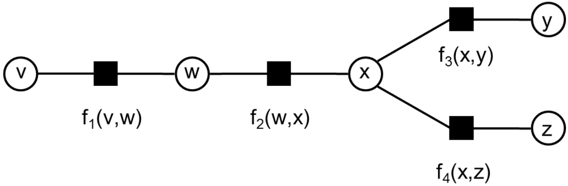
- Factor node: ■ Variable node: ◯
- Edges represent the dependency of factors on variables.

Example: consider the factorising probability density function

$$p(v, w, x, y, z) = f_1(v, w) f_2(w, x) f_3(x, y) f_4(x, z)$$

- What are the marginal distributions of the individual variables?
- What is $p(w)$?

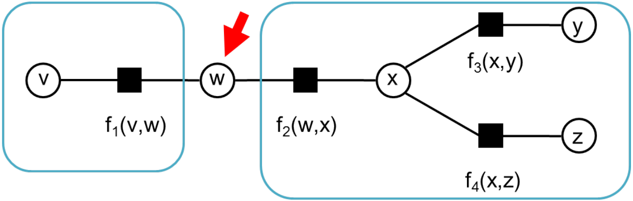
Factor trees: separation (1)



$$p(w) = \sum_{v} \sum_{x} \sum_{y} \sum_{z} f_1(v, w) f_2(w, x) f_3(x, y) f_4(x, z)$$

- If v, x, y and z take K values each, we have $\approx 3K^4$ products and $\approx K^4$ sums.
- Multiplication is distributive: $c(a + b) = ca + cb$.
  The left hand is more efficient!

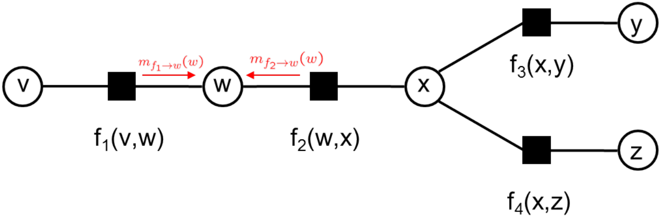
Factor trees: separation (2)



$$p(w) = \Big[\sum_v f_1(v,w)\Big] \cdot \Big[\sum_x \sum_y \sum_z f_2(w,x) f_3(x,y) f_4(x,z)\Big]$$

- From sums of products to products of sums.
- The complexity is now $\approx 2K^3$.

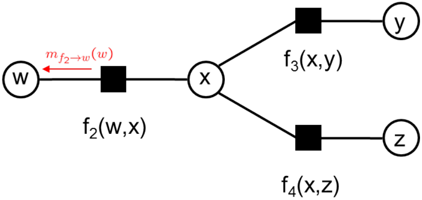
Factor trees: separation (3)



$$p(w) = \underbrace{\Big[\sum_{v} f_1(v,w)\Big]}_{m_{f_1 \to w}(w)} \cdot \underbrace{\Big[\sum_{x}\sum_{y}\sum_{z} f_2(w,x) f_3(x,y) f_4(x,z)\Big]}_{m_{f_2 \to w}(w)}$$

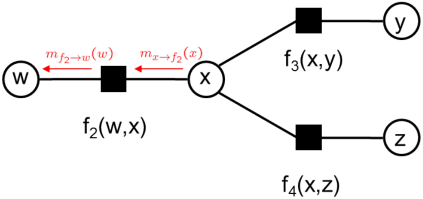
- Sums of products becomes products of sums of all messages from neighbouring factors to variable.

Messages: from factors to variables (1)



$$m_{f_2 \to w}(w) = \sum_{x} \sum_{y} \sum_{z} f_2(w, x) f_3(x, y) f_4(x, z)$$

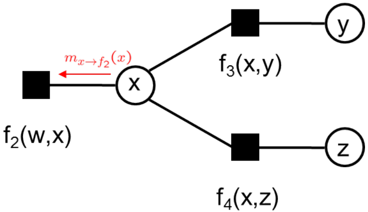
Messages: from factors to variables (2)



$$m_{f_2 \to w}(w) = \sum_x f_2(w,x) \cdot \underbrace{\Big[\sum_y \sum_z f_3(x,y) f_4(x,z)\Big]}_{m_{x \to f_2}(x)}$$

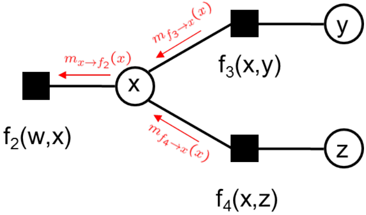
- Factors only need to sum out all their local variables.

Messages: from variables to factors (1)



$$\color{red}{m_{x \to f_2}(x)} = \sum_y \sum_z f_3(x, y) f_4(x, z)$$

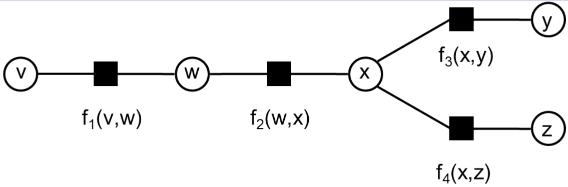
Messages: from variables to factors (2)



$$m_{x\to f_2}(x) = \underbrace{\Big[\sum_y f_3(x,y)\Big]}_{m_{f_3\to x}(x)} \cdot \underbrace{\Big[\sum_z f_4(x,z)\Big]}_{m_{f_4\to x}(x)}$$

- Variables pass on the product of all incoming messages.

Factor graph marginalisation: summary



$$p(w) = \sum_v \sum_x \sum_y \sum_z f_1(v,w) f_2(w,x) f_3(x,y) f_4(x,z)$$

$$= \underbrace{\Big[\sum_v f_1(v,w)\Big]}_{m_{f_1 \to w}(w)} \cdot \underbrace{\Big[\sum_x f_2(w,x) \cdot \underbrace{\Big[\underbrace{\Big[\sum_y f_3(x,y)\Big]}_{m_{f_3 \to x}(x)} \cdot \underbrace{\Big[\sum_z f_4(x,z)\Big]}_{m_{f_4 \to x}(x)}\Big]}_{m_{x \to f_2}(x)}\Big]}_{m_{f_2 \to w}(w)}$$

- The complexity is now reduced to $\approx K$.

The sum-product algorithm

Three update equations:

- Marginals are the product of all incoming messages from neighbour factors

$$p(t) = \prod_{f \in F_t} m_{f \to t}(t)$$

- Messages from factors sum out all variables except the receiving one

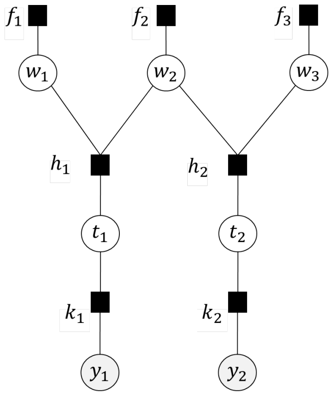
$$m_{f \to t}(t_1) = \sum_{t_2} \sum_{t_3} \ldots \sum_{t_n} f(t_1, t_2, \ldots, t_n) \prod_{i>1} m_{t_i \to f}(t)$$

- Messages from variables are the product of all incoming messages except that from the receiving factor

$$m_{t \to f}(t) = \prod_{f_j \in F_t \setminus \{f\}} m_{f_j \to t}(t)$$

Messages are results of partial computations. Computations are localised.

The full TrueSkill graph



Prior: $f_i(w_i) = \mathcal{N}(w_i; \mu_0, \sigma_0^2)$

"Game" factor:

$$h_g(w_{I_g}, w_{J_g}, t_g) = \mathcal{N}(t_g; w_{I_g} - w_{J_g}, 1)$$

(I_g and J_g are the players in game g)

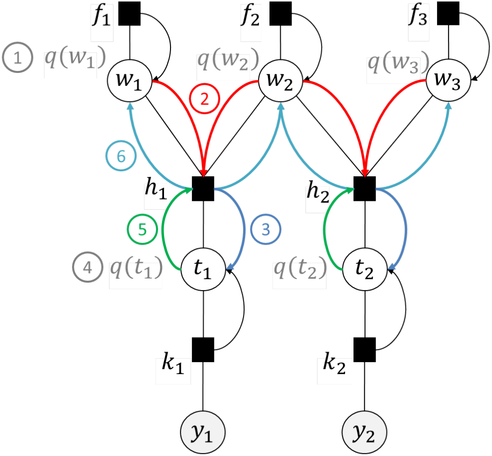
Outcome factor:

$$k_g(t_g, y_g) = \delta\big(y_g - \text{sign}(t_g)\big)$$

We are interested in the marginal distributions of the skills w_i.

- What shape do these distributions have?
- We need to make some approximations.
- We will also pretend the structure is a tree (ignore loops).

Expectation Propagation in the full TrueSkill graph



Iterate

(1) Update skill marginals.

(2) Compute skill to game messages.

(3) Compute game to performance messages.

(4) Approximate performance marginals.

(5) Compute performance to game messages.

(6) Compute game to skill messages.

Message passing for TrueSkill

$$
\begin{aligned}
m^{\tau=0}_{h_g \to w_{I_g}}(w_{I_g}) &= 1, \quad m^{\tau=0}_{h_g \to w_{J_g}}(w_{J_g}) = 1, \quad \forall\, g, \\
q^{\tau}(w_i) &= f(w_i) \prod_{g=1}^{N} m^{\tau}_{h_g \to w_i}(w_i) \;\sim\; \mathcal{N}(\mu_i, \sigma_i^2), \\
m^{\tau}_{w_{I_g} \to h_g}(w_{I_g}) &= \frac{q^{\tau}(w_{I_g})}{m^{\tau}_{h_g \to w_{I_g}}(w_{I_g})}, \quad m^{\tau}_{w_{J_g} \to h_g}(w_{J_g}) = \frac{q^{\tau}(w_{J_g})}{m^{\tau}_{h_g \to w_{J_g}}(w_{J_g})}, \\
m^{\tau}_{h_g \to t_g}(t_g) &= \iint h_g(t_g, w_{I_g}, w_{J_g})\, m^{\tau}_{w_{I_g} \to h_g}(w_{I_g})\, m^{\tau}_{w_{J_g} \to h_g}(w_{J_g})\, dw_{I_g}\, dw_{J_g}, \\
q^{\tau+1}(t_g) &= \mathrm{Approx}\big(m^{\tau}_{h_g \to t_g}(t_g)\, m_{k_g \to t_g}(t_g)\big), \\
m^{\tau+1}_{t_g \to h_g}(t_g) &= \frac{q^{\tau+1}(t_g)}{m^{\tau}_{h_g \to t_g}(t_g)}, \\
m^{\tau+1}_{h_g \to w_{I_g}}(w_{I_g}) &= \iint h_g(t_g, w_{I_g}, w_{J_g})\, m^{\tau+1}_{t_g \to h_g}(t_g)\, m^{\tau}_{w_{J_g} \to h_g}(w_{J_g})\, dt_g\, dw_{J_g}, \\
m^{\tau+1}_{h_g \to w_{J_g}}(w_{J_g}) &= \iint h_g(t_g, w_{J_g}, w_{J_g})\, m^{\tau+1}_{t_g \to h_g}(t_g)\, m^{\tau}_{w_{I_g} \to h_g}(w_{I_g})\, dt_g\, dw_{I_g}.
\end{aligned}
$$

In a little more detail

At iteration τ messages m and marginals q are Gaussian, with *means* μ, *standard deviations* σ, *variances* $v = \sigma^2$, *precisions* $r = v^{-1}$ and *natural means* $\lambda = r\mu$.

Step 0 Initialise incoming skill messages:

$$\left.\begin{aligned} r^{\tau=0}_{h_g \to w_i} &= 0 \\ \mu^{\tau=0}_{h_g \to w_i} &= 0 \end{aligned}\right\} m^{\tau=0}_{h_g \to w_i}(w_i)$$

Step 1 Compute marginal skills:

$$\left.\begin{aligned} r^{\tau}_{i} &= r_0 + \textstyle\sum_g r^{\tau}_{h_g \to w_i} \\ \lambda^{\tau}_{i} &= \lambda_0 + \textstyle\sum_g \lambda^{\tau}_{h_g \to w_i} \end{aligned}\right\} q^{\tau}(w_i)$$

Step 2 Compute skill to game messages:

$$\left.\begin{aligned} r^{\tau}_{w_i \to h_g} &= r^{\tau}_{i} - r^{\tau}_{h_g \to w_i} \\ \lambda^{\tau}_{w_i \to h_g} &= \lambda^{\tau}_{i} - \lambda^{\tau}_{h_g \to w_i} \end{aligned}\right\} m^{\tau}_{w_i \to h_g}(w_i)$$

Step 3 Game to performance messages:

$$\left.\begin{aligned} v^{\tau}_{h_g \to t_g} &= 1 + v^{\tau}_{w_{I_g} \to h_g} + v^{\tau}_{w_{J_g} \to h_g} \\ \mu^{\tau}_{h_g \to t_g} &= \mu^{\tau}_{I_g \to h_g} - \mu^{\tau}_{J_g \to h_g} \end{aligned}\right\} m^{\tau}_{h_g \to t_g}(t_g)$$

Step 4 Compute marginal performances:

$$\begin{aligned} p(t_g) &\propto \mathcal{N}(\mu^{\tau}_{h_g \to t_g}, v^{\tau}_{h_g \to t_g})\mathbb{I}\big(y - \mathrm{sign}(t)\big) \\ &\simeq \mathcal{N}(\tilde{\mu}^{\tau+1}_g, \tilde{v}^{\tau+1}_g) \;=\; q^{\tau+1}(t_g) \end{aligned}$$

We find the parameters of q by *moment matching*

$$\left.\begin{aligned} \tilde{v}^{\tau+1}_g &= v^{\tau}_{h_g \to t_g}\Big(1 - \Lambda\big(\tfrac{\mu^{\tau}_{h_g \to t_g}}{\sigma^{\tau}_{h_g \to t_g}}\big)\Big) \\ \tilde{\mu}^{\tau+1}_g &= \mu^{\tau}_{h_g \to t_g} + \sigma^{\tau}_{h_g \to t_g}\Psi\big(\tfrac{\mu^{\tau}_{h_g \to t_g}}{\sigma^{\tau}_{h_g \to t_g}}\big) \end{aligned}\right\} q^{\tau+1}(t_g)$$

where we have defined $\Psi(x) = \mathcal{N}(x)/\Phi(x)$ and $\Lambda(x) = \Psi(x)(\Psi(x) + x)$.

Step 5 Performance to game message:

$$\left.\begin{array}{rcl} r_{t_g \to h_g}^{\tau+1} & = & \tilde{r}_g^{\tau+1} - r_{h_g \to t_g}^{\tau} \\ \lambda_{t_g \to h_g}^{\tau+1} & = & \tilde{\lambda}_g^{\tau+1} - \lambda_{h_g \to t_g}^{\tau} \end{array}\right\} m_{t_g \to h_g}^{\tau+1}(t_g)$$

Step 6 Game to skill message:
For player 1 (the winner):

$$\left.\begin{array}{rcl} \nu_{h_g \to w_{I_g}}^{\tau+1} & = & 1 + \nu_{t_g \to h_g}^{\tau+1} + \nu_{w_{J_g} \to h_g}^{\tau} \\ \mu_{h_g \to w_{I_g}}^{\tau+1} & = & \mu_{w_{J_g} \to h_g}^{\tau} + \mu_{t_g \to h_g}^{\tau+1} \end{array}\right\} m_{h_g \to w_{I_g}}^{\tau+1}(w_{I_g})$$

and for player 2 (the looser):

$$\left.\begin{array}{rcl} \nu_{h_g \to w_{J_g}}^{\tau+1} & = & 1 + \nu_{t_g \to h_g}^{\tau+1} + \nu_{w_{I_g} \to h_g}^{\tau} \\ \mu_{h_g \to w_{J_g}}^{\tau+1} & = & \mu_{w_{I_g} \to h_g}^{\tau} - \mu_{t_g \to h_g}^{\tau+1} \end{array}\right\} m_{h_g \to w_{J_g}}^{\tau+1}(w_{J_g})$$

Go back to **Step 1** with $\tau := \tau + 1$ (or stop).

Moments of a truncated Gaussian density (1)

Consider the truncated Gaussian density function

$$p(t) = \frac{1}{Z_t}\delta\big(y - \text{sign}(t)\big)\mathcal{N}(t; \mu, \sigma^2)$$

where $y \in \{-1, 1\}$ and $\delta(x) = 1$ only if $x = 0$ ($\delta(x) = 0$ if $x \neq 0$).

We have seen that the normalisation constant is $Z_t = \Phi\big(\frac{y\mu}{\sigma}\big)$.

We want to approximate $p(t)$ by a Gaussian density function $q(t)$ with mean and variance equal to the first and second central moments of $p(t)$.

This means we need to compute:

- First moment: $\mathbb{E}[t] = \langle t \rangle_{p(t)}$
- Second central moment: $\mathbb{V}[t] = \langle t^2 \rangle_{p(t)} - \langle t \rangle^2_{p(t)}$

Moments of a truncated Gaussian density (2)

First moment. We take the derivative of Z_t wrt. μ:

$$\begin{aligned}\frac{\partial Z_t}{\partial \mu} &= \frac{\partial}{\partial \mu}\int_0^{+\infty} N(t; y\mu, \sigma^2)dt = \int_0^{+\infty}\frac{\partial}{\partial \mu} N(t; y\mu, \sigma^2)dt \\ &= \int_0^{+\infty} y\sigma^{-2}(t - y\mu)N(t; y\mu, \sigma^2)dt = yZ_t\sigma^{-2}\int_{-\infty}^{+\infty}(t - y\mu)p(t)dt \\ &= yZ_t\sigma^{-2}\langle t - y\mu\rangle_{p(t)} = yZ_t\sigma^{-2}\langle t\rangle_{p(t)} - \mu Z_t\sigma^{-2}\end{aligned}$$

where $\langle t\rangle_{p(t)}$ is the expectation of t under $p(t)$. We can also write:

$$\frac{\partial Z_t}{\partial \mu} = \frac{\partial}{\partial \mu}\Phi\big(\frac{y\mu}{\sigma}\big) = y\mathcal{N}(y\mu; 0, \sigma^2)$$

Combining both expressions for $\frac{\partial Z_t}{\partial \mu}$ we obtain

$$\langle t\rangle_{p(t)} = y\mu + \sigma^2\frac{\mathcal{N}(y\mu; 0, \sigma^2)}{\Phi(\frac{y\mu}{\sigma})} = y\mu + \sigma\frac{\mathcal{N}(\frac{y\mu}{\sigma}; 0, 1)}{\Phi(\frac{y\mu}{\sigma})} = y\mu + \sigma\Psi\big(\frac{y\mu}{\sigma}\big)$$

where use $\mathcal{N}(y\mu; 0, \sigma^2) = \sigma^{-1}\mathcal{N}(\frac{y\mu}{\sigma}; 0, 1)$ and define $\Psi(z) = \frac{N(z;0,1)}{\Phi(z)}$.

Moments of a truncated Gaussian density (3)

Second moment. We take the second derivative of Z_t wrt. μ:

$$\frac{\partial^2 Z_t}{\partial \mu^2} = \frac{\partial}{\partial \mu}\int_0^{+\infty} y\sigma^{-2}(t - y\mu)N(t; y\mu, \sigma^2)dt$$
$$= \Phi\big(\frac{y\mu}{\sigma}\big)\langle -\sigma^{-2} + \sigma^{-4}(t - y\mu)^2\rangle_{p(t)}$$

We can also write

$$\frac{\partial^2 Z_t}{\partial \mu^2} = \frac{\partial}{\partial \mu} y\mathcal{N}(y\mu; 0, \sigma^2) = -\sigma^{-2} y\mu\mathcal{N}(y\mu; 0, \sigma^2)$$

Combining both we obtain

$$\mathbb{V}[t] = \sigma^2\big(1 - \Lambda(\frac{y\mu}{\sigma})\big)$$

where we define $\Lambda(z) = \Psi(z)\big(\Psi(z) + z\big)$.