

Factor graphs, belief propagation and variational inference

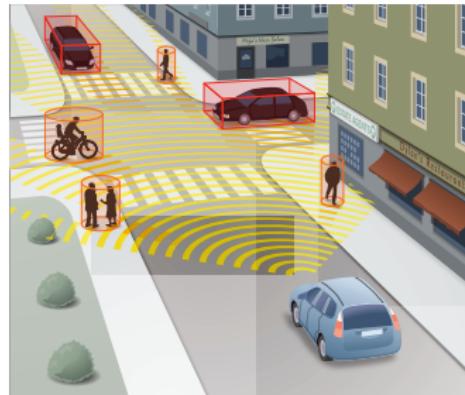
Lennart Svensson

Signal Processing Group
Department of Signals and Systems
Chalmers University of Technology, Sweden



Probabilistic graphical models (PGMs)

- PGMs are important in a wide range of applications:
- Self-driving vehicles.
- Cooperative localisation.
- Speech processing.
- Communication systems.
- Image segmentation.
- etc.



- **Purpose with PGMs:**
 - illustrate problem structure (conditional independencies),
 - exploit structure to design tractable inference algorithms.
- **Today's focus:** factor graphs, belief propagation and variational inference.

Why factor graphs?

Factor graphs are important/useful because:

- they provide new perspectives on “old” algorithms,
 ~> filtering, smoothing, dynamic programming, Viterbi decoding, . . .
are all **instances of factor graph algorithms!**
- they **visualize the structure of the problem**:
clarify “dependencies” and how we can split one complicated function of many variables into simple functions.
- there are **efficient standard algorithms** that we can use,
once we have defined the factor graph!

Learning objectives

After this lecture you should be able to

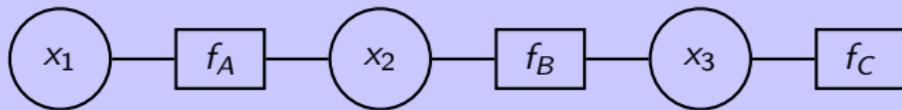
- formulate a factor graph (FG) given a factorization of a function,
- explain why it is important to make use of the structure/sparseness of a problem,
- describe how the sum-product algorithm works on a factor graph (without loops),
- summarize the basic ideas behind variational Bayes.

What is a factor graph?

- **Example 1:** given a factorization

$$g(x_1, x_2, x_3) = f_A(x_1, x_2)f_B(x_2, x_3)f_C(x_3)$$

we obtain the factor graph:



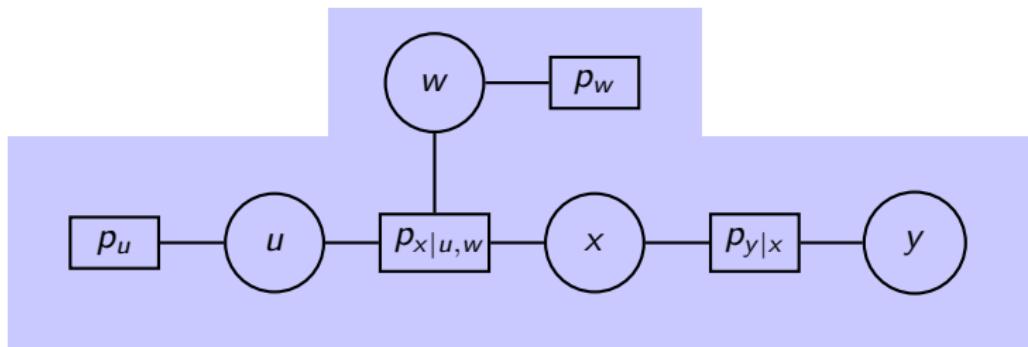
- A factor graph contains:
 - one **variable node** for each variable,
 - one **factor node** for each function,
 - one **edge** between x_i and f_j if x_i is a variable in f_j .

What is a factor graph?

- **Example 2:** given a factorization

$$p(u, w, x, y) = p_u(u)p_w(w)p_{x|u,w}(x|u, w)p_{y|x}(y|x)$$

we obtain the factor graph:



- A FG is a **bipartite** graph:
 - it contains two types of nodes,
 - edges always connect nodes of different types.
- Functions do not have to be probability densities.

What is a factor graph?

- **A DIY example:** given a probability density function

$$p(x, y, z) = p_x(x)p_{y|x}(y|x)p_{z|x,y}(z|x, y),$$

we obtain the factor graph:

Optional: for comparison you can also draw the corresponding Bayesian network.

Two important problems

Marginal distributions

- Find

$$p(x_i | y) = \sum_{\sim x_i} p(x | y)$$

where $\sim x_i$ means “over all variables but x_i ”.

- **Example:** find $p(x_k | y_{1:k})$ from $p(x_{1:k} | y_{1:k})$, i.e., perform filtering.

Maximization

- Find

$$\hat{x}_i = \arg \max_{x_i} \max_{\sim x_i} p(x | y)$$

- **Example:** find the most probable symbol in a communication message. Often closely related to dynamic programming.

Efficient marginalization

- **Example:** consider a function

$$g(x_1, x_2, x_3) = f_A(x_1)f_B(x_1, x_2)f_C(x_2, x_3)$$

where $x_1, x_2, x_3 \in \{1, 2, \dots, N\}$. Describe how to compute

$$g_1(x_1) = \sum_{x_2, x_3} g(x_1, x_2, x_3)$$

efficiently.

Solution: the trick is to “push in the summations”:

$$\begin{aligned} \sum_{x_2, x_3} g(x_1, x_2, x_3) &= f_A(x_1) \underbrace{\sum_{x_2} f_B(x_1, x_2)}_{\mu_{f_C \rightarrow x_2}(x_2)} \underbrace{\sum_{x_3} f_C(x_2, x_3)}_{\mu_{f_C \rightarrow x_2}(x_2)} \\ &= f_A(x_1) \underbrace{\sum_{x_2} f_B(x_1, x_2) \mu_{f_C \rightarrow x_2}(x_2)}_{\mu_{f_B \rightarrow x_1}(x_1)} \end{aligned}$$

$$\begin{aligned} &\implies g_1(x_1) = f_A(x_1) \mu_{f_B \rightarrow x_1}(x_1) \end{aligned}$$

Efficient marginalization

- **Example, DIY:** describe how to compute

$$g_2(x_2) = \sum_{x_1, x_3} f_A(x_1) f_B(x_1, x_2) f_C(x_2, x_3)$$

efficiently! (Remember to “push in” the summations.)

Why is structure important?

- Suppose

$$g(x_1, x_2, \dots, x_k) = f_2(x_1, x_2)f_3(x_2, x_3)\dots f_k(x_{k-1}, x_k),$$

where $x_1, x_2, \dots, x_k \in \{1, 2, \dots, N\}$.

- How many calculations are needed to compute

$$g_1(x_1) = \sum_{\sim x_1} g(x_1, x_2, \dots, x_k)?$$

- **Without using structure:** one summation over $k - 1$ variables
 $\Rightarrow N^{k-1}$ terms for each value of x_1 , i.e., $O(N^k)$ calculations.
- **Pushing in summations:** $k - 1$ summations over 1 variable
 $\Rightarrow O(k \times N^2)$ calculations.
- **Example:** $k = 100$ and $N = 2 \Rightarrow N^k \approx 1.3 \times 10^{30}$ and
 $k \times N^2 = 400$,
 \rightsquigarrow using the structure makes a **massive difference!**

The sum-product algorithm

The sum-product algorithm

- is also known as belief propagation,
- computes marginal distributions by “pushing in summations”,
- performs message passing on a graph,
- is exact for linear graphs and trees, but often performs remarkably well on general graphs (with loops),

The sum-product algorithm

The sum-product update rule

The message sent from a node v on an edge e is the product of the local function at v (or the unit function if v is a variable node) with all messages received at v on edges *other* than e , summarized for the variables not associated with e .

The sum-product algorithm

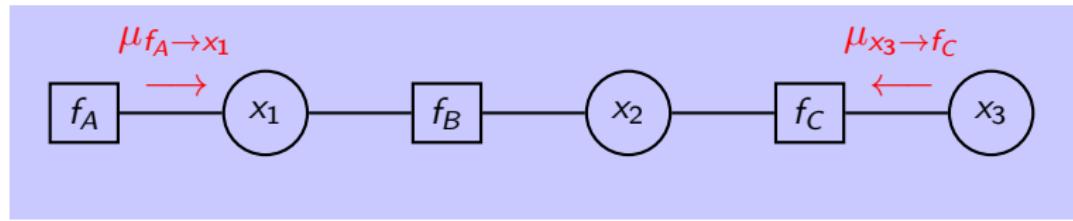
- Calculating marginal distributions of

$$g(x_1, x_2, x_3) = f_A(x_1)f_B(x_1, x_2)f_C(x_2, x_3)$$

- The sum-product algorithm operates in **three phases**:

Phase 1: initialization

- Send messages from the edges of the graph
 - messages from factor to variable: $\mu_{f_A \rightarrow x_1}(x_1) = f_A(x_1)$,
 - messages from variable to factor: $\mu_{x_3 \rightarrow f_C}(x_3) = 1$.



The sum-product algorithm

- Calculating marginal distributions of

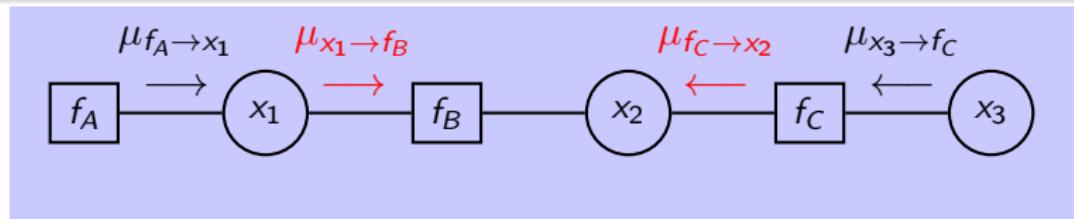
$$g(x_1, x_2, x_3) = f_A(x_1)f_B(x_1, x_2)f_C(x_2, x_3)$$

Phase 2: message passing

- Compute outgoing messages when incoming message(s) are available:

- messages from variable to factor: product of all incoming messages, $\mu_{x_1 \rightarrow f_B}(x_1) = \mu_{f_A \rightarrow x_1}(x_1)$,
- messages from factor to variable: product of incoming messages and factor, sum out previous variables:

$$\mu_{f_C \rightarrow x_2}(x_2) = \sum_{x_3} \mu_{x_3 \rightarrow f_C}(x_3)f_C(x_2, x_3).$$



The sum-product algorithm

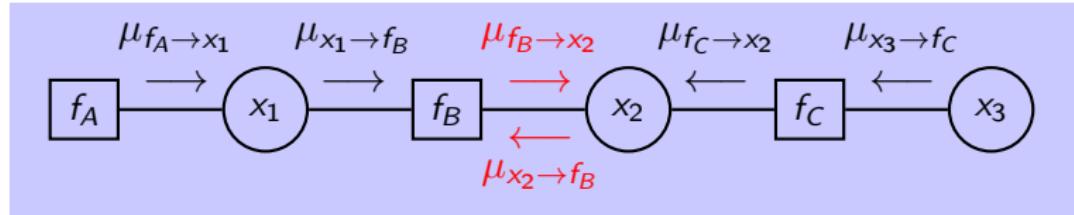
- Calculating marginal distributions of

$$g(x_1, x_2, x_3) = f_A(x_1)f_B(x_1, x_2)f_C(x_2, x_3)$$

Phase 2: message passing

- Compute outgoing messages when incoming message(s) are available:

- $\mu_{f_B \rightarrow x_2}(x_2) = \sum_{x_1} \mu_{x_1 \rightarrow f_B}(x_1) f_B(x_1, x_2)$
- $\mu_{x_2 \rightarrow f_B}(x_2) = \mu_{f_C \rightarrow x_2}(x_2)$



The sum-product algorithm

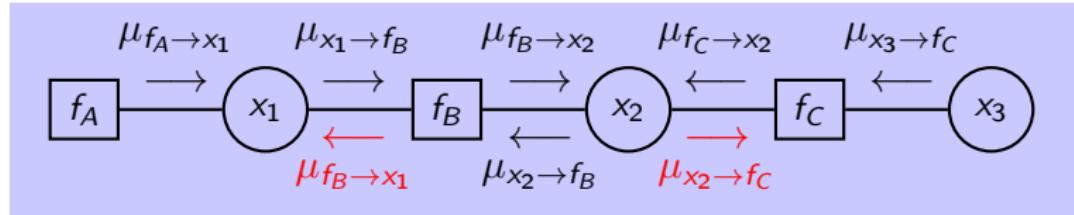
- Calculating marginal distributions of

$$g(x_1, x_2, x_3) = f_A(x_1)f_B(x_1, x_2)f_C(x_2, x_3)$$

Phase 2: message passing

- Compute outgoing messages when incoming message(s) are available:

- $\mu_{f_B \rightarrow x_1}(x_1) = \sum_{x_2} \mu_{x_2 \rightarrow f_B}(x_2) f_B(x_1, x_2)$
- $\mu_{x_2 \rightarrow f_C}(x_2) = \mu_{f_B \rightarrow x_2}(x_2)$



The sum-product algorithm

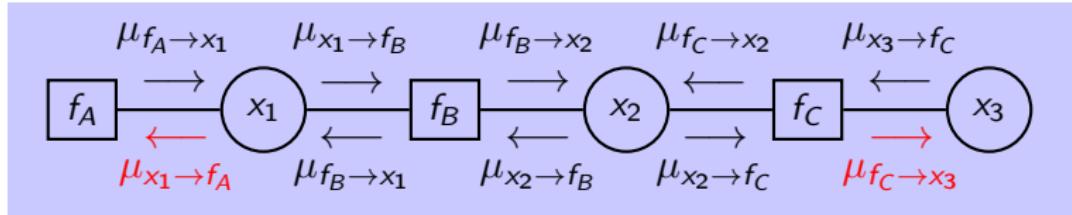
- Calculating marginal distributions of

$$g(x_1, x_2, x_3) = f_A(x_1)f_B(x_1, x_2)f_C(x_2, x_3)$$

Phase 2: message passing

- Compute outgoing messages when incoming message(s) are available:

- $\mu_{x_1 \rightarrow f_A}(x_1) = \mu_{f_B \rightarrow x_1}(x_1)$
- $\mu_{f_C \rightarrow x_3}(x_3) = \sum_{x_2} \mu_{x_2 \rightarrow f_C}(x_2)f_C(x_2, x_3)$



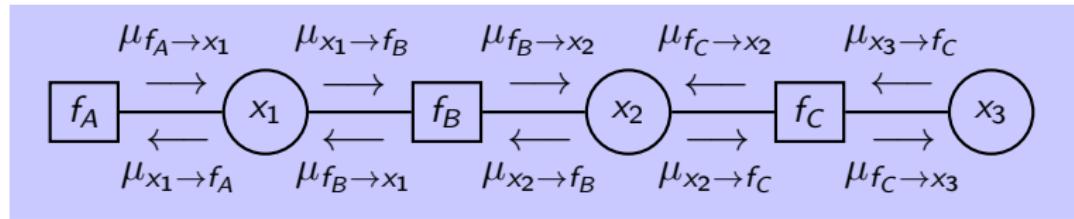
The sum-product algorithm

- Calculating marginal distributions of

$$g(x_1, x_2, x_3) = f_A(x_1)f_B(x_1, x_2)f_C(x_2, x_3)$$

Phase 3: termination

- A marginal distribution is the product of the incoming messages to the variable node:
 - $g_1(x_1) = \sum_{x_2, x_3} g(x_1, x_2, x_3) = \mu_{f_A \rightarrow x_1}(x_1)\mu_{f_B \rightarrow x_1}(x_1)$
 - $g_2(x_2) = \sum_{x_1, x_3} g(x_1, x_2, x_3) = \mu_{f_B \rightarrow x_2}(x_2)\mu_{f_C \rightarrow x_2}(x_2)$
 - $g_3(x_3) = \sum_{x_1, x_2} g(x_1, x_2, x_3) = \mu_{f_C \rightarrow x_3}(x_3).$

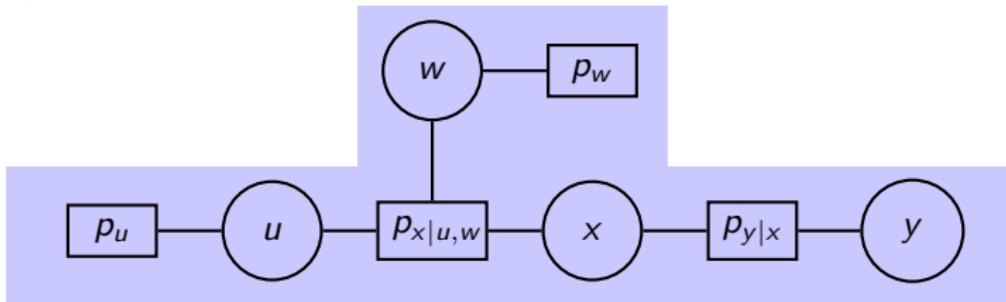


The sum-product algorithm

- **DIY:** verify that the sum-product algorithm computes $g_2(x_2)$ correctly.

Remarks on the sum-product algorithm

- We considered a linear graph, but the sum-product algorithm (SPA) is exact also for trees, like



- You get, e.g.,

$$\mu_{p_{x|u,w} \rightarrow x}(x) = \sum_{u,w} \mu_{w \rightarrow p_{x|u,w}}(w) \mu_{u \rightarrow p_{x|u,w}}(u) p_{x|u,w}(x|u, w)$$

- If the variables are continuous you replace summations with integrals.

Factor graphs and maximization

- We can find

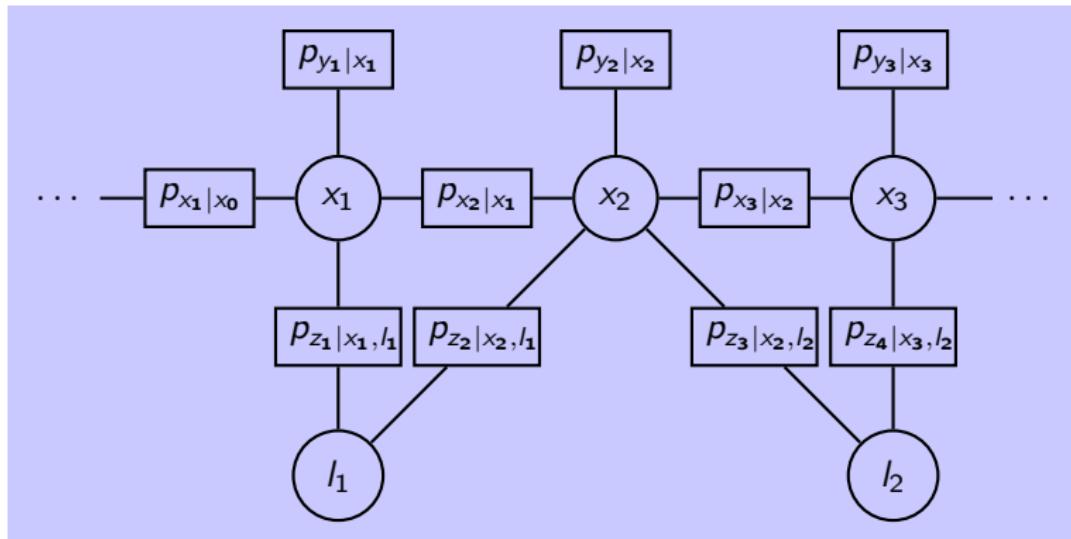
$$\max_{\sim x_i} p(x|y)$$

using the **max-product algorithm**.

- The max-product algorithm is identical to the sum-product algorithm, but summations are “replaced by maximisations”.
- For linear graphs, the max-product algorithm gives a version of **dynamic programming and Viterbi decoding**.

Factor graphs for SLAM

- For many problems, the factor graph contains loops.
- Simultaneous localization and mapping (SLAM)**: position both a moving vehicle, x_1, x_2, \dots , and different stationary landmarks, l_1, l_2, \dots .



Graphs with loops

- Two important strategies for graphs with loops:
 - ➊ **Use belief propagation** (the sum-product algorithm). The algorithm is no longer exact and needs to be iterated, but often yields remarkably good performance in practice.
 - ➋ **Exact marginalization.** Often still a feasible alternative, but it is important to marginalize the variables in the correct order. We can still use the structure of the problem!

A variational perspective on BP, and more

- How can we approximate $p(x)$ when exact inference is intractable?

The variational idea

Find a tractable distribution $q(x) \in \mathbf{Q}$ which is close to $p(x)$:

$$q(x) = \arg \min_{\tilde{q}(x) \in \mathbf{Q}} D(\tilde{q}(x) \| p(x)),$$

where $D(\tilde{q}(x) \| p(x))$ is small when $\tilde{q} \approx p$.

- By modifying \mathbf{Q} and/or D we can derive belief propagation (BP), expectation propagation (EP), variational Bayes (VB), TRW-BP, GBP, Power-EP, etc.

Motivating examples – estimation in SSMs

Let us study VB using a toy example:

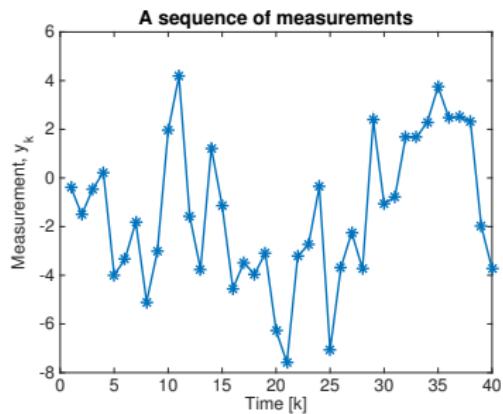
- Consider a state space model

$$x_k = x_{k-1} + q_k, \quad q_k \sim \mathcal{N}(0, \tau_q^{-1})$$

$$y_k = x_k + r_k, \quad r_k \sim \mathcal{N}(0, \tau_r^{-1}).$$
- Can we estimate τ_q and τ_r from y_1, \dots, y_T ?
- Difficulty:** the state sequence x_1, \dots, x_T is unknown!

Relevant?

- Enables us to estimate parameters without knowing the true state sequence.
- In practice, models tend to be nonlinear and high-dimensional which makes the problem less trivial.



Intractable problems?

- Let θ denote parameters of interest, y be our observations and x represent the hidden variables.
 - In **toy example**: θ contains mean and covariances, y are the samples and x denotes assignments: measurements \leftrightarrow Gaussian components.
- Can we compute** $p(\theta|y)$?
- An **important complication** is that we need x to express the relation between y and θ :

$$p(y|\theta) = \sum_x p(y, x|\theta),$$

which is often intractable.

Variational Bayesian theory

- **Idea 1:** find a distribution $q(\theta, x)$ that approximates $p(\theta, x|y)$ well, in the sense that the Kullback-Leibler divergence (KLD)

$$\int q(\theta, x) \log \frac{q(\theta, x)}{p(\theta, x|y)} d\theta dx$$

is small.

- If $q(\theta, x)$ has suitable properties, we can then easily find an approximation to $p(\theta|y)$.
- **Note:** the optimal approximation in the KLD sense is $q(\theta, x) = p(\theta, x|y)$, but this is not tractable.
 \rightsquigarrow We need to restrict $q(\theta, x)$ to obtain a tractable solution!

Variational Bayesian theory

- **Idea 2:** seek the best approximation $q(\theta, \mathbf{x}) \approx p(\theta, \mathbf{x}|\mathbf{y})$ among all distributions that factorise $q(\theta, \mathbf{x}) = q_\theta(\theta)q_x(\mathbf{x})$.

Variational Bayesian – main results

Given $q_\theta(\theta)$, the optimal distribution $q_x(\mathbf{x})$ is

$$q_x(\mathbf{x}) \propto \exp \left(\mathbb{E}_{q_\theta(\theta)} [\log [p(\theta, \mathbf{y}, \mathbf{x})]] \right).$$

Given $q_x(\mathbf{x})$, the optimal distribution $q_\theta(\theta)$ is

$$q_\theta(\theta) \propto \exp \left(\mathbb{E}_{q_x(\mathbf{x})} [\log [p(\theta, \mathbf{y}, \mathbf{x})]] \right).$$

- A few remarks:
 - We use these results to iteratively minimize the KLD.
 - We handle the distribution of the parameters of interests θ and the hidden variables \mathbf{x} in the same way.
 - We take expected values of $\log [p(\theta, \mathbf{y}, \mathbf{x})]$ instead of $p(\theta, \mathbf{y}, \mathbf{x})$, which **simplifies things considerably**.

Example – VB solution (1)

Let us use VB to estimate parameters in a state space model.

- We have a state space model

$$x_k = x_{k-1} + q_k, \quad q_k \sim \mathcal{N}(0, \tau_q^{-1})$$

$$y_k = x_k + r_k, \quad r_k \sim \mathcal{N}(0, \tau_r^{-1}).$$

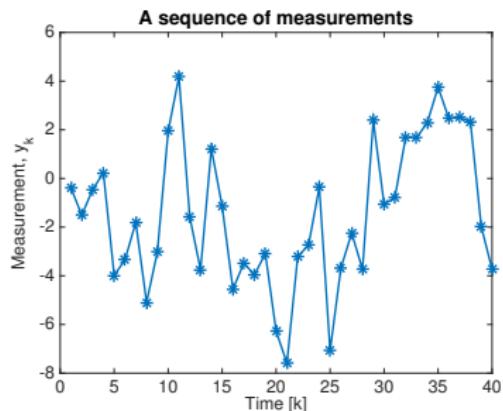
- Parameters of interest are $\theta = [\tau_q \quad \tau_r]^T$. For simplicity, we assume $p(\theta) \propto 1$.

- y denotes the meas. sequence and x the state sequence.

- We get

$$p(x|\theta) = p(x_0) \prod_{k=1}^T p(x_k|x_{k-1}) = \mathcal{N}(x_0; \bar{x}_0, P_0) \prod_{k=1}^T \mathcal{N}(x_k; x_{k-1}, \tau_q^{-1})$$

$$p(y|x, \theta) = \mathcal{N}(y; x, \tau_r^{-1} I)$$



Example – VB solution (2)

- An important part of VB is:

$$\begin{aligned}\log p(\theta, \mathbf{y}, \mathbf{x}) &= \log p(\mathbf{y}|\mathbf{x}, \theta)p(\mathbf{x}|\theta)p(\theta) \\ &= \log p(\mathbf{y}|\mathbf{x}, \theta) + \log p(\mathbf{x}|\theta) + \log p(\theta)\end{aligned}$$

- Plugging in expressions from the previous slide yields:

$$\log p(\mathbf{y}|\mathbf{x}, \theta) = \log \mathcal{N}(\mathbf{y}; \mathbf{x}, \tau_r^{-1} \mathbf{I}) = \frac{T}{2} \log(\tau_r / (2\pi)) - \frac{\tau_r}{2} \sum_{k=1}^T (y_k - x_k)^2$$

$$\begin{aligned}\log p(\mathbf{x}|\theta) &= \log \mathcal{N}(x_0; \bar{x}_0, P_0) + \sum_{k=1}^T \log \mathcal{N}(x_k; x_{k-1}, \tau_q^{-1}) \\ &= \log p(x_0) + \frac{T}{2} \log(\tau_q / (2\pi)) - \frac{\tau_q}{2} \sum_{k=1}^T (x_k - x_{k-1})^2\end{aligned}$$

- Bottom line:** the logarithm turns $p(\theta, \mathbf{y}, \mathbf{x})$ into a simple sum!

Example – VB solution (3)

- According to the **VB algorithm**, we should set

$$q_x(\mathbf{x}) \propto \exp \left(\mathbb{E}_{q_\theta(\boldsymbol{\theta})} [\log [p(\boldsymbol{\theta}, \mathbf{y}, \mathbf{x})]] \right).$$

- We can rewrite this as

$$\begin{aligned} q_x(\mathbf{x}) &\propto p(x_0) \exp \left(-\mathbb{E}_{q_\theta(\boldsymbol{\theta})} \left[\frac{\tau_q}{2} \sum_{k=1}^T (x_k - x_{k-1})^2 \right] \right) \\ &\quad \exp \left(\mathbb{E}_{q_\theta(\boldsymbol{\theta})} \left[-\frac{\tau_r}{2} \sum_{k=1}^T (y_k - x_k)^2 \right] \right) \\ &\propto p(x_0) \exp \left(-\frac{\mathbb{E}_{q_\theta(\boldsymbol{\theta})}[\tau_q]}{2} \sum_{k=1}^T (x_k - x_{k-1})^2 \right) \\ &\quad \exp \left(-\frac{\mathbb{E}_{q_\theta(\boldsymbol{\theta})}[\tau_r]}{2} \sum_{k=1}^T (y_k - x_k)^2 \right) \end{aligned}$$

- Do you recognize this as **something tractable?**

Example – VB solution (4)

- Let us introduce the notations $\bar{\tau}_q = \mathbb{E}_{q_\theta(\theta)}[\tau_q]$ and $\bar{\tau}_r = \mathbb{E}_{q_\theta(\theta)}[\tau_r]$.
- The previous equation can then be simplified to

$$q_x(\mathbf{x}) \propto p(x_0) \prod_{k=1}^T \mathcal{N}(x_k; x_{k-1}, \bar{\tau}_q^{-1}) \mathcal{N}(\mathbf{y}; \mathbf{x}, \bar{\tau}_r^{-1} \mathbf{I})$$

- Conclusion:** to compute $q_x(\mathbf{x})$ we simply perform conventional (RTS) smoothing under the assumptions that $\tau_q = \bar{\tau}_q$ and $\tau_r = \bar{\tau}_r$.

Example – VB solution (5)

- According to the **VB algorithm**, we should set

$$q_{\theta}(\theta) \propto \exp \left(\mathbb{E}_{q_x(x)} [\log [p(\theta, y, x)]] \right).$$

- This simplifies to $q_{\theta}(\theta) = q_{\tau_r}(\tau_r)q_{\tau_q}(\tau_q)$, where

$$\begin{aligned} q_{\tau_r}(\tau_r) &\propto \exp \left(\mathbb{E}_{q_x(x)} \left[\frac{T}{2} \log(\tau_r) - \frac{\tau_r}{2} \sum_{k=1}^T (y_k - x_k)^2 \right] \right) \\ &\propto \tau_r^{T/2} \exp \left(-\frac{\tau_r}{2} \mathbb{E}_{q_x(x)} \left[\sum_{k=1}^T (y_k - x_k)^2 \right] \right) \\ &\propto \text{Gam} \left(\tau_r; \frac{T+2}{2}, \frac{1}{2} \mathbb{E}_{q_x(x)} \left[\sum_{k=1}^T (y_k - x_k)^2 \right] \right) \end{aligned}$$

Example – VB solution (6)

- According to the **VB algorithm**, we should set

$$q_{\theta}(\theta) \propto \exp \left(\mathbb{E}_{q_x(x)} [\log [p(\theta, y, x)]] \right).$$

- Using the above derivations, we can show that

$$q_{\theta}(\theta) = \text{Gam} \left(\tau_r; \frac{T+2}{2}, \frac{1}{2} b_r \right) \text{Gam} \left(\tau_q; \frac{T+2}{2}, \frac{1}{2} b_q \right)$$

where

$$b_r = \mathbb{E}_{q_x(x)} \left[\sum_{k=1}^T (y_k - x_k)^2 \right] \quad \text{and} \quad b_q = \mathbb{E}_{q_x(x)} \left[\sum_{k=1}^T (x_k - x_{k-1})^2 \right]$$

- It follows that $\mathbb{E}_{q_{\theta}}[\theta] = (T+2) \begin{bmatrix} b_r^{-1} \\ b_q^{-1} \end{bmatrix}$. Is this reasonable?

Example – illustration of VB solution

- We can now study how the algorithm performs on an example.
- The true precisions were $\theta = \begin{bmatrix} \tau_r \\ \tau_q \end{bmatrix} = \begin{bmatrix} 1/4 \\ 1 \end{bmatrix}$ and we initiated the algorithm with $\theta = \begin{bmatrix} 1/10 \\ 10 \end{bmatrix}$. That is, with very little motion noise.

• Our θ estimates:

$$\text{Iter. 1: } \bar{\theta} = [0.14 \quad 2.07]^T$$

$$\text{Iter. 2: } \bar{\theta} = [0.18 \quad 1.32]^T$$

$$\text{Iter. 3: } \bar{\theta} = [0.21 \quad 1.24]^T$$

$$\text{Iter. 4: } \bar{\theta} = [0.23 \quad 1.26]^T$$

$$\text{Iter. 5: } \bar{\theta} = [0.23 \quad 1.30]^T$$

⋮

$$\text{Iter. 10: } \bar{\theta} = [0.23 \quad 1.34]^T$$

Final remarks on VB

Pros:

- VB is simple to employ in a wide range of contexts and often yields efficient algorithms.
- It decreases the KL-divergence in every iteration and is thus guaranteed to converge (to a certain KLD).
- There is an alternative perspective on VB, as a maximizer of a lower bound on $p(\mathbf{y})$. That bound is useful for model selection.

Cons:

- It is a relatively crude approximation for at least two reasons:
1) the assumed factorisation breaks existing dependencies
2) it minimises the “wrong” KLD.
- For many problems, it is sensitive to initialization and may get stuck in a local minima.

Learning objectives

After this lecture you should be able to

- formulate a factor graph (FG) given a factorization of a function,
- explain why it is important to make use of the structure/sparseness of a problem,
- describe how the sum-product algorithm works on a factor graph (without loops),
- summarize the basic ideas behind variational Bayes.

A selection of references

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