Probabilistic & Unsupervised Learning

Expectation Propagation

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Term 1, Autumn 2016
Intractabilities and approximations

- Inference – computational intractability
  - Factored variational approx
  - Loopy BP/EP/Power EP
  - Gibbs sampling, other MCMC

- Inference – analytic intractability
  - Laplace approximation (global)
  - Parametric variational approx (for special cases).
  - Message approximations (linearised, sigma-point, Laplace)
  - Assumed-density methods and Expectation-Propagation
  - (Sequential) Monte-Carlo

- Learning – intractable partition function
  - Contrastive divergence
  - Sampling parameters
  - Score-matching

- Posterior estimation and model selection
  - Laplace approximation / BIC
  - Variational Bayes
  - Monte-Carlo
  - (Annealed) importance sampling
  - Reversible jump MCMC

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Nonlinear state-space model (NLSSM)

\[
y_{t+1} = f(y_t, u_t) + w_t \\
x_t = g(y_t, u_t) + v_t
\]

\(w_t, v_t\) usually still Gaussian.
Nonlinear state-space model (NLSSM)

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Extended Kalman Filter (EKF): linearise nonlinear functions about current estimate, \( \hat{y}_t \):

\[ y_{t+1} \approx f(\hat{y}_t, u_t) + \frac{\partial f}{\partial y_t} \bigg|_{\hat{y}_t} (y_t - \hat{y}_t) + w_t \]
\[ x_t \approx g(\hat{y}_{t-1}, u_t) + \frac{\partial g}{\partial y_t} \bigg|_{\hat{y}_{t-1}} (y_t - \hat{y}_{t-1}) + v_t \]
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$$

$$
x_t \approx g(\hat{y}_{t-1}^t, u_t) + \frac{\partial g}{\partial y_t} \bigg|_{\hat{y}_{t-1}^t} (y_t - \hat{y}_{t-1}^t) + v_t
$$

Run the Kalman filter (smoother) on non-stationary linearised system ($\tilde{A}_t, \tilde{B}_t, \tilde{C}_t, \tilde{D}_t$):

$w_t, v_t$ usually still Gaussian.
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y_{t+1} = f(y_t, u_t) + w_t \\
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Run the Kalman filter (smoother) on non-stationary linearised system \((\tilde{A}_t, \tilde{B}_t, \tilde{C}_t, \tilde{D}_t)\):

- Adaptively approximates non-Gaussian messages by Gaussians.
Nonlinear state-space model (NLSSM)

\[
\begin{align*}
    \mathbf{y}_{t+1} &= f(\mathbf{y}_t, \mathbf{u}_t) + \mathbf{w}_t \\
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\end{align*}
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Extended Kalman Filter (EKF): linearise nonlinear functions about current estimate, \(\hat{\mathbf{y}}_t^t\):

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    \mathbf{y}_{t+1} &\approx f(\hat{\mathbf{y}}_t^t, \mathbf{u}_t) + \frac{\partial f}{\partial \mathbf{y}_t} \bigg|_{\hat{\mathbf{y}}_t^t} (\mathbf{y}_t - \hat{\mathbf{y}}_t^t) + \mathbf{w}_t \\
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- Adaptively approximates non-Gaussian messages by Gaussians.
- Local linearisation depends on central point of distribution \(\Rightarrow\) approximation degrades with increased state uncertainty.
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- Local linearisation depends on central point of distribution ⇒ approximation degrades with increased state uncertainty. May work acceptably for close-to-linear systems.
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Can base EM-like algorithm on EKF/EKS (or alternatives).
Other message approximations

Consider the forward messages on a latent chain:

\[ P(y_t|_{x_1:t}) = \frac{1}{Z} P(x_t|y_t) \int dy_{t-1} P(y_t|y_{t-1}) P(y_{t-1}|_{x_1:t-1}) \]

We want to approximate the messages to retain a tractable form (i.e. Gaussian).

\[ \tilde{P}(y_t|_{x_1:t}) \approx \frac{1}{Z} P(x_t|y_t) \int dy_{t-1} P(y_t|y_{t-1}) \underbrace{\mathcal{N}(f(y_{t-1}), Q)} \underbrace{\mathcal{N}(\hat{y}_{t-1}, V_{t-1})} \tilde{P}(y_{t-1}|_{x_1:t-1}) \]
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- Sigma-point (“unscented”) filter:
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- Parametric variational: \( \arg\min_{\mathcal{N}(\hat{y}_t, \hat{V}_t)} \mathbb{E} [\int dy_{t-1} \ldots] \). Requires Gaussian expectations of log \( \int \Rightarrow \) may be challenging.
Other message approximations

Consider the forward messages on a latent chain:

\[
P(y_t | x_{1:t}) = \frac{1}{Z} P(x_t | y_t) \int dy_{t-1} \ P(y_t | y_{t-1}) P(y_{t-1} | x_{1:t-1})
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\tilde{P}(y_t | x_{1:t}) \approx \frac{1}{Z} P(x_t | y_t) \int dy_{t-1} \ P(y_t | y_{t-1}) \ \mathcal{N}(f(y_{t-1}), Q) \ \mathcal{N}(\hat{y}_{t-1}, V_{t-1})
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  - “Fit” Gaussian to these \( 2K + 1 \) points.
  - Equivalent to numerical evaluation of mean and covariance by Gaussian quadrature.
  - One form of “Assumed Density Filtering” and EP.
- Parametric variational: \( \text{argmin} \ KL[\mathcal{N}(\hat{y}_t, \hat{V}_t) \parallel \int dy_{t-1} \ldots] \). Requires Gaussian expectations of log \( \int \Rightarrow \) may be challenging.
- The other KL: \( \text{argmin} \ KL[\int dy_{t-1} \parallel \mathcal{N}(\hat{y}_t, \hat{V}_t)] \) needs only first and second moments of nonlinear message \( \Rightarrow \) EP.
Variational learning

Free energy:

\[ F(q, \theta) = \langle \log P(X, Y | \theta) \rangle_{q(Y|X)} + H[q] = \log P(X | \theta) - \text{KL}[q(Y) || P(Y | X, \theta)] \leq \ell(\theta) \]
Variational learning

Free energy:

$$\mathcal{F}(q, \theta) = \langle \log P(\mathcal{X}, \mathcal{Y}|\theta) \rangle_{q(\mathcal{Y}|\mathcal{X})} + H[q] = \log P(\mathcal{X}|\theta) - \text{KL}[q(\mathcal{Y})||P(\mathcal{Y}|\mathcal{X}, \theta)] \leq \ell(\theta)$$

E-steps:

- Exact EM: $q(\mathcal{Y}) = \arg\max_q \mathcal{F} = P(\mathcal{Y}|\mathcal{X}, \theta)$
Variational learning

Free energy:

\[ \mathcal{F}(q, \theta) = \langle \log P(X, Y|\theta) \rangle_{q(Y|X)} + H[q] = \log P(X|\theta) - \text{KL}[q(Y)||P(Y|X, \theta)] \leq \ell(\theta) \]

E-steps:

- **Exact EM:** \( q(Y) = \text{argmax}_q \mathcal{F} = P(Y|X, \theta) \)
  - Saturates bound: converges to local maximum of likelihood.

- **(Factored) variational approximation:**
  \( q(Y) = \text{argmax}_q \mathcal{F} = \text{argmin}_q \text{KL}[q_1(Y_1)q_2(Y_2)||P(Y|X, \theta)] \)

- **Increases bound:** converges, but not necessarily to ML.

- **Other approximations:**
  \( q(Y) \approx P(Y|X, \theta) \)
  - Usually no guarantees, but if learning converges it may be more accurate than the factored approximation.
Variational learning

Free energy:

\[
F(q, \theta) = \langle \log P(\mathcal{X}, \mathcal{Y}|\theta) \rangle_{q(\mathcal{Y}|\mathcal{X})} + H[q] = \log P(\mathcal{X}|\theta) - \text{KL}[q(\mathcal{Y})||P(\mathcal{Y}|
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  \[
  q(\mathcal{Y}) = \text{argmax}_{q_1(\mathcal{Y}_1)q_2(\mathcal{Y}_2)} F = \text{argmin}_{q_1(\mathcal{Y}_1)q_2(\mathcal{Y}_2)} \text{KL}[q_1(\mathcal{Y}_1)q_2(\mathcal{Y}_2)||P(\mathcal{Y}|
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Free energy:

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  \[ q(\mathcal{Y}) = \text{argmax} \mathcal{F} = \text{argmin} \text{KL}[q_1(\mathcal{Y}_1)q_2(\mathcal{Y}_2)||P(\mathcal{Y}|\mathcal{X}, \theta)] \]
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Variational learning

Free energy:

\[ \mathcal{F}(q, \theta) = \langle \log P(\mathcal{X}, \mathcal{Y} | \theta) \rangle_{q(\mathcal{Y} | \mathcal{X})} + H[q] = \log P(\mathcal{X} | \theta) - KL[q(\mathcal{Y}) \| P(\mathcal{Y} | \mathcal{X}, \theta)] \leq \ell(\theta) \]

E-steps:

▸ Exact EM: \( q(\mathcal{Y}) = \arg\max_q \mathcal{F} = P(\mathcal{Y} | \mathcal{X}, \theta) \)
  ▸ Saturates bound: converges to local maximum of likelihood.

▸ (Factored) variational approximation:

\[ q(\mathcal{Y}) = \arg\max_{q_1(\mathcal{Y}_1)q_2(\mathcal{Y}_2)} \mathcal{F} = \arg\min_{q_1(\mathcal{Y}_1)q_2(\mathcal{Y}_2)} KL[q_1(\mathcal{Y}_1)q_2(\mathcal{Y}_2) \| P(\mathcal{Y} | \mathcal{X}, \theta)] \]
  ▸ Increases bound: converges, but not necessarily to ML.

▸ Other approximations: \( q(\mathcal{Y}) \approx P(\mathcal{Y} | \mathcal{X}, \theta) \)
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  \[ q(\mathcal{Y}) = \arg\max_{q_1(\mathcal{Y}_1)q_2(\mathcal{Y}_2)} \mathcal{F} = \arg\min_{q_1(\mathcal{Y}_1)q_2(\mathcal{Y}_2)} \text{KL}[q_1(\mathcal{Y}_1)q_2(\mathcal{Y}_2)||P(\mathcal{Y}|\mathcal{X}, \theta)] \]
  - Increases bound: converges, but not necessarily to ML.

- **Other approximations:** \( q(\mathcal{Y}) \approx P(\mathcal{Y}|\mathcal{X}, \theta) \)
  - Usually no guarantees, but if learning converges it may be more accurate than the factored approximation.
Approximating the posterior

Linearisation (or local Laplace, sigma-point and other such approaches) seem *ad hoc*. A more principled approach might look for an approximate $q$ that is closest to $P$ in some sense.

$$q = \arg\min_{q \in \mathcal{Q}} D(P \leftrightarrow q)$$
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What about the ‘other’ KL \(q = \text{argmin} \text{KL}[P||q]\)?
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$$\arg\min_{q_i} \text{KL}\left[ P(Y|X) \left\| \prod q_j(Y_j|X) \right. \right] = \arg\min_{q_i} \left. - \int dY \; P(Y|X) \log \prod q_j(Y_j|X) \right.$$

and the marginals are what we need for learning (although if factored over disjoint sets as in the variational approximation some cliques will be missing).
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&= \text{argmin}_{q_i} - \sum_j \int dY \ P(Y|X) \log q_j(Y_j|X) \\
&= \text{argmin}_{q_i} - \int dY_i \ P(Y_i|X) \log q_i(Y_i|X)
\end{align*}
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Perversely, this means finding the best \( q \) for this KL is intractable!

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Approximate optimisation

The posterior distribution in a graphical model is a (normalised) product of factors:

\[
P(Y|X) = \frac{P(Y, X)}{P(X)} = \frac{1}{Z} \prod_i P(Y_i | \text{pa}(Y_i)) \propto \prod_{i=1}^{N} f_i(Y_i)
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where the \(Y_i\) are not necessarily disjoint. In the language of EP the \(f_i\) are called sites.
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Consider \(q\) with the same factorisation, but potentially approximated sites: \(q(Y) \overset{\text{def}}{=} \prod_{i=1}^{N} f_i(Y_i)\).

We would like to minimise (at least in some sense) \(\text{KL}[P||q]\).
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\begin{align*}
\min_{\{\tilde{f}_i\}} \text{KL} & \left[ \prod_{i=1}^{N} f_i(\mathcal{Y}_i) \left\| \prod_{i=1}^{N} \tilde{f}_i(\mathcal{Y}_i) \right\] \quad \text{(global: intractable)} \\
\min_{\tilde{f}_i} \text{KL} & \left[ f_i(\mathcal{Y}_i) \left\| \tilde{f}_i(\mathcal{Y}_i) \right\] \quad \text{(local, fixed: simple, inaccurate)}
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Consider \(q\) with the same factorisation, but potentially approximated sites:

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q(Y) \overset{\text{def}}{=} N \prod_{i=1}^{N} \tilde{f}_i(Y_i).
\]

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\[
\min_{\{\tilde{f}_i\}} \text{KL} \left[ \prod_{i=1}^{N} f_i(Y_i) \middle\| \prod_{i=1}^{N} \tilde{f}_i(Y_i) \right] \quad \text{(global: intractable)}
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\]

\[
\min_{\tilde{f}_i} \text{KL} \left[ f_i(Y_i) \prod_{j \neq i} \tilde{f}_j(Y_j) \middle\| \tilde{f}_i(Y_i) \prod_{j \neq i} \tilde{f}_j(Y_j) \right] \quad \text{(local, contextual: iterative, accurate)}
\]
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\min_{\tilde{f}_i} \text{KL} \left[ f_i(Y_i) \left| \tilde{f}_i(Y_i) \right. \right] & \quad \text{(local, fixed: simple, inaccurate)} \\
\min_{\tilde{f}_i} \text{KL} \left[ f_i(Y_i) \prod_{j \neq i} \tilde{f}_j(Y_j) \left| \tilde{f}_i(Y_i) \prod_{j \neq i} \tilde{f}_j(Y_j) \right. \right] & \quad \text{(local, contextual: iterative, accurate)} \leftarrow \text{EP}
\end{align*}
\]
Expectation? Propagation?

EP is really two ideas:

- Approximation of factors.
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Expectation? Propagation?

EP is really two ideas:

▶ **Approximation** of factors.
  ▶ Usually by “projection” to exponential families.
  ▶ This involves finding expected sufficient statistics, hence **expectation**.

▶ **Local** divergence minimization in the context of other factors.
  ▶ This leads to a message passing approach, hence **propagation**.
Local updates

Each EP update involves a KL minimisation:

$$\tilde{f}_{i}^{\text{new}}(\mathcal{Y}) \leftarrow \arg\min_{f \in \tilde{f}} \text{KL}[f(\mathcal{Y}_{i})q_{-i}(\mathcal{Y})||f(\mathcal{Y}_{i})q_{-i}(\mathcal{Y})]$$

$$[q_{-i}(\mathcal{Y}) \overset{\text{def}}{=} \prod_{j \neq i} \tilde{f}_{j}(\mathcal{Y}_{j})]$$

Write $q_{-i}(\mathcal{Y}) = q_{-i}(\mathcal{Y}_{i})q_{-i}(\mathcal{Y}_{-i}|\mathcal{Y}_{i})$. Then:

$$\min_{f} \text{KL}[f(\mathcal{Y}_{i})q_{-i}(\mathcal{Y})||f(\mathcal{Y}_{i})q_{-i}(\mathcal{Y})]$$

$$= \max_{f} \int d\mathcal{Y}_{i} d\mathcal{Y}_{-i} f(\mathcal{Y}_{i})q_{-i}(\mathcal{Y}_{i}) \log f(\mathcal{Y}_{i})q_{-i}(\mathcal{Y})$$

$$= \max_{f} \int d\mathcal{Y}_{i} d\mathcal{Y}_{-i} f(\mathcal{Y}_{i})q_{-i}(\mathcal{Y}_{i})q_{-i}(\mathcal{Y}_{-i}|\mathcal{Y}_{i})( \log f(\mathcal{Y}_{i})q_{-i}(\mathcal{Y}_{i}) + \log q_{-i}(\mathcal{Y}_{-i}|\mathcal{Y}_{i}))$$

$$= \max_{f} \int d\mathcal{Y}_{i} f(\mathcal{Y}_{i})q_{-i}(\mathcal{Y}_{i})( \log f(\mathcal{Y}_{i})q_{-i}(\mathcal{Y}_{i})) \int d\mathcal{Y}_{-i} q_{-i}(\mathcal{Y}_{-i}|\mathcal{Y}_{i})$$

$$= \min_{f} \text{KL}[f(\mathcal{Y}_{i})q_{-i}(\mathcal{Y}_{i})||f(\mathcal{Y}_{i})q_{-i}(\mathcal{Y}_{i})]$$

$q_{-i}(\mathcal{Y}_{i})$ is sometimes called the cavity distribution.
Expectation Propagation (EP)

Input $f_1(Y_1) \ldots f_N(Y_N)$

Initialize $\tilde{f}_1(Y_1) = \text{argmin}_{f \in \{\tilde{f}_1\}} \text{KL}[f_1(Y_1) \parallel f_1(Y_1)]$, $\tilde{f}_i(Y_i) = 1$ for $i > 1$, $q(Y) \propto \prod_i \tilde{f}_i(Y_i)$

repeat

for $i = 1 \ldots N$ do

   Delete: $q_{-i}(Y) \leftarrow \frac{q(Y)}{\tilde{f}_i(Y_i)} = \prod_{j \neq i} \tilde{f}_j(Y_j)$

   Project: $\tilde{f}_{i}^{\text{new}}(Y) \leftarrow \text{argmin}_{f \in \{\tilde{f}_i\}} \text{KL}[f_i(Y_i)q_{-i}(Y_i) \parallel f(Y_i)q_{-i}(Y_i)]$

   Include: $q(Y) \leftarrow \tilde{f}_{i}^{\text{new}}(Y_i) q_{-i}(Y)$

end for

until convergence
Message Passing

- The cavity distribution (in a tree) can be further broken down into a product of terms from each neighbouring clique:

\[ q_{\neg i}(\mathcal{V}_i) = \prod_{j \in \text{ne}(i)} M_{j \rightarrow i}(\mathcal{V}_j \cap \mathcal{V}_i) \]
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\[ q_{-i}(\mathcal{V}_i) = \prod_{j \in \text{ne}(i)} M_{j \to i}(\mathcal{V}_j \cap \mathcal{V}_i) \]

- Once the \( i \)th site has been approximated, the messages can be passed on to neighbouring cliques by marginalising to the shared variables (SSM example follows). ⇒ belief propagation.

- In loopy graphs, we can use loopy belief propagation. In that case becomes an approximation to the true cavity distribution (or we can recast the approximation directly in terms of messages ⇒ later lecture).

- For some approximations (e.g. Gaussian) may be able to compute true loopy cavity using approximate sites, even if computing exact message would have been intractable.

- In either case, message updates can be scheduled in any order.

- No guarantee of convergence (but see “power-EP” methods).
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- No guarantee of convergence (but see “power-EP” methods).
$P(y_i|y_{i-1}) = \phi_i(y_i, y_{i-1})$

$P(x_i|y_i) = \psi_i(y_i)$

e.g. $\exp(-\|y_i - h_s(y_{i-1})\|^2/2\sigma^2)$

e.g. $\exp(-\|x_i - h_o(y_i)\|^2/2\sigma^2)$
EP for a NLSSM

\[
P(y_i | y_{i-1}) = \phi_i(y_i, y_{i-1}) \\
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\text{e.g.} \ \exp(-\|x_i - h_o(y_i)\|^2/2\sigma^2)

Then \( f_i(y_i, y_{i-1}) = \phi_i(y_i, y_{i-1})\psi_i(y_i) \). As \( \phi_i \) and \( \psi_i \) are non-linear, inference is not generally tractable.
EP for a NLSSM

\[ P(y_i|y_{i-1}) = \phi_i(y_i, y_{i-1}) \quad \text{e.g. } \exp(-\|y_i - h_s(y_{i-1})\|^2/2\sigma^2) \]

\[ P(x_i|y_i) = \psi_i(y_i) \quad \text{e.g. } \exp(-\|x_i - h_o(y_i)\|^2/2\sigma^2) \]

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Assume \( \tilde{f}_i(y_i, y_{i-1}) \) is Gaussian. Then,

\[
q_{-i}(y_i, y_{i-1}) = \int \prod_{y_{i-2}, y_{i-1}, x_i x_{i-2}, x_{i-1}} \tilde{f}_{i'}(y_{i'}, y_{i'-1}) = \int \prod_{y_{i-2}, y_{i-1}, x_i x_{i-2}, x_{i-1}} \tilde{f}_{i'}(y_{i'}, y_{i'-1}) \int \prod_{y_{i+1}, y_{i+2}, \ldots, y_n, \alpha_{i-1}(y_{i-1}), \beta_i(y_i)} \tilde{f}_{i'}(y_{i'}, y_{i'-1})
\]

with both \( \alpha \) and \( \beta \) Gaussian.
EP for a NLSSM

\[
P(y_i|y_{i-1}) = \phi_i(y_i, y_{i-1})
\]

\[
P(x_i|y_i) = \psi_i(y_i)
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Assume \( \tilde{f}_i(y_i, y_{i-1}) \) is Gaussian. Then,

\[
q_{-i}(y_i, y_{i-1}) = \int \prod_{y_1 \cdots y_{i-2} \atop y_{i+1} \cdots y_i} \tilde{f}_{i'}(y_{i'}, y_{i'-1}) = \int \prod_{y_1 \cdots y_{i-2} \atop y_{i+1} \cdots y_i} \tilde{f}_{i'}(y_{i'}, y_{i'-1}) \Bigg\| \int \prod_{\alpha_{i-1}(y_{i-1})}^{y_i \cdots y_{i+1} \cdots y_n} \tilde{f}_{i'}(y_{i'}, y_{i'-1}) \Bigg\| \beta_i(y_i)
\]

with both \( \alpha \) and \( \beta \) Gaussian.

\[
\tilde{f}_i(y_i, y_{i-1}) = \arg\min_{f \in \mathcal{N}} \text{KL} \left[ \phi_i(y_i, y_{i-1})\psi_i(y_i)\alpha_{i-1}(y_{i-1})\beta_i(y_i) || f(y_i, y_{i-1})\alpha_{i-1}(y_{i-1})\beta_i(y_i) \right]
\]
NLSSM EP message updates

\[ \tilde{f}_i(y_i, y_{i-1}) = \arg\min_{f \in \mathcal{N}} \text{KL} \left[ f(y_i, y_{i-1}) \mid \tilde{q}_i(y_i, y_{i-1}) \right] \]
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\]

\[
\tilde{P}(y_{i-1}, y_i) = \arg\min_{P \in \mathcal{N}} \text{KL} \left[ \tilde{P}(y_{i-1}, y_i) \right] P(y_{i-1}, y_i)
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\[ \tilde{f}_i(y_i, y_{i-1}) = \arg\min_{f \in \mathcal{N}} \text{KL} \left[ \phi_i(y_i, y_{i-1}) \psi(y_i) \alpha_{i-1}(y_{i-1}) \beta_i(y_i) \vert \frac{f(y_i, y_{i-1}) \alpha_{i-1}(y_{i-1}) \beta_i(y_i)}{P(y_{i-1}, y_i)} \right] \]

\[ \tilde{P}(y_{i-1}, y_i) = \arg\min_{P \in \mathcal{N}} \text{KL} \left[ \tilde{P}(y_{i-1}, y_i) \vert P(y_{i-1}, y_i) \right] \]

\[ \tilde{f}_i(y_i, y_{i-1}) = \frac{\tilde{P}(y_{i-1}, y_i)}{\alpha_{i-1}(y_{i-1}) \beta_i(y_i)} \]
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\[
\alpha_i(y_i) = \int \prod_{y_1 \cdots y_{i-1} < i+1} \tilde{f}_{i'}(y_{i'}, y_{i'-1}) = \int \alpha_{i-1}(y_{i-1})\tilde{f}_i(y_i, y_{i-1}) = \frac{1}{\beta_i(y_i)} \int \tilde{P}(y_{i-1}, y_i)
\]

\[
\beta_{i-1}(y_{i-1}) = \int \prod_{y_{i+1} \cdots y_{i'} > i} \tilde{f}_{i'}(y_{i'}, y_{i'-1}) = \int \beta_i(y_i)\tilde{f}_i(y_i, y_{i-1}) = \frac{1}{\alpha_{i-1}(y_{i-1})} \int \tilde{P}(y_{i-1}, y_i)
\]
Moment Matching

Each EP update involves a KL minimisation:

\[
\tilde{f}_i^{\text{new}}(\mathcal{Y}) \leftarrow \arg\min_{f \in \{\tilde{f}\}} \mathbf{KL}[f_i(\mathcal{Y})q_{-i}(\mathcal{Y})\|f(\mathcal{Y})q_{-i}(\mathcal{Y})]
\]

Usually, both \(q_{-i}(\mathcal{Y})\) and \(\tilde{f}\) are in the same exponential family. Let \(q(x) = \frac{1}{Z(\theta)} e^{T(x) \cdot \theta}\). Then

\[
\arg\min_{q} \mathbf{KL}[p(x)\|q(x)] = \arg\min_{\theta} \mathbf{KL}\left[p(x)\left\|\frac{1}{Z(\theta)} e^{T(x) \cdot \theta}\right\|ight]
\]

\[
= \arg\min_{\theta} - \int dx \ p(x) \log \frac{1}{Z(\theta)} e^{T(x) \cdot \theta}
\]

\[
= \arg\min_{\theta} - \int dx \ p(x) T(x) \cdot \theta + \log Z(\theta)
\]

\[
\frac{\partial}{\partial \theta} = - \int dx \ p(x) T(x) + \frac{1}{Z(\theta)} \frac{\partial}{\partial \theta} \int dx \ e^{T(x) \cdot \theta}
\]

\[
= -\langle T(x) \rangle_p + \frac{1}{Z(\theta)} \int dx \ e^{T(x) \cdot \theta} T(x)
\]

\[
= -\langle T(x) \rangle_p + \langle T(x) \rangle_q
\]

So minimum is found by matching sufficient stats. This is usually moment matching.
Numerical issues

How do we calculate $\langle T(x) \rangle_p$?
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- **Laplace approximation.**
  - Equivalent to Laplace propagation.
  - As long as messages remain positive definite will converge to global Laplace approximation.
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EP for Gaussian process classification

EP provides a successful framework for Gaussian-process modelling of non-Gaussian observations (e.g. for classification).
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![Diagram of x and g variables](image)

Recall:
- A GP defines a **multivariate Gaussian** distribution on any finite subset of random vars \( \{g_1 \ldots g_n\} \) drawn from a (usually uncountable) potential set indexed by “inputs” \( x_i \).
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$\begin{align*}
\mathbf{x}_1 & \quad \mathbf{x}_2 \quad \mathbf{x}_3 \quad \ldots \quad \mathbf{x}_n \\
\mathbf{g}_1 & \quad \mathbf{g}_2 \quad \mathbf{g}_3 \quad \ldots \quad \mathbf{g}_n \\
y_1 & \quad y_2 \quad y_3 \quad \ldots \quad y_n
\end{align*}$

$\begin{align*}
\mathbf{x'} & \quad \mathbf{g'} \\
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- The Gaussian parameters depend on the inputs: $(\mu = [\mu(\mathbf{x}_i)], \Sigma = [K(\mathbf{x}_i, \mathbf{x}_j)])$.
- If we think of the $g$s as function values, a GP provides a prior over functions.
- In a GP regression model, noisy observations $y_i$ are conditionally independent given $g_i$.
- No parameters to learn (though often hyperparameters); instead, we make predictions on test data directly: [assuming $\mu = 0$, and matrix $\Sigma$ incorporates diagonal noise]

$$P(y' | \mathbf{x'}, D) = \mathcal{N} \left( \Sigma_{x',x}^{-1} \Sigma_{X,x} y, \Sigma_{x',x'} - \Sigma_{x',x} \Sigma_{X,x} \Sigma_{X,x'} \right)$$
We can write the GP joint on $g_i$ and $y_i$ as a factor graph:

$$P(g_1 \ldots g_n, y_1, \ldots y_n) = \mathcal{N}(g_1 \ldots g_n|\mathbf{0}, K) \prod_i \mathcal{N}(y_i|g_i, \sigma^2_i)$$
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The same factorisation applies to non-Gaussian $P(y_i | g_i)$ (e.g. $P(y_i=1) = 1/(1 + e^{-g_i})$).
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![Factor graph diagram]
GP EP updates

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$q_{-i}(g_i)$ can be constructed by the usual GP marginalisation. If $\Sigma = K + \text{diag} \begin{bmatrix} \tilde{\psi}_1^2 \ldots \tilde{\psi}_n^2 \end{bmatrix}$

$$q_{-i}(g_i) = \mathcal{N}(\Sigma_{-i,-i}^{-1} \Sigma_{-i,-i}^{-1} \tilde{\mu}_{-i}, K_{i,i} - \Sigma_{i,-i} \Sigma_{-i,-i}^{-1} \Sigma_{-i,i})$$
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- The EP updates thus require calculating Gaussian expectations of $f_i(g)g_{\{1,2\}}$:

$$\tilde{f}_i^{\text{new}}(g_i) = \mathcal{N} \left( \int dg q_{-i}(g) f_i(g)g, \int dg q_{-i}(g) f_i(g)g^2 - (\tilde{\mu}_i^{\text{new}})^2 \right) / q_{-i}(g_i)$$
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- Thus no change is needed to the approximating potentials $\tilde{f}_i$. 

\[ P(y' | x', D) = \int dg' P(y' | g') N(g' | Kx', X(Kx', X + \tilde{\Psi})^{-1} \tilde{\mu}, Kx', x' - Kx', X(Kx', X + \tilde{\Psi})^{-1} Kx', x') \]
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Predictions are obtained by marginalising the approximation: [let $\tilde{\Psi} = \text{diag} [\tilde{\psi}_1^2 \ldots \tilde{\psi}_n^2]]$

$$P(y'|x', D) = \int dg' P(y'|g') \mathcal{N}(g' | K_{x',x}(K_{x,x} + \tilde{\Psi})^{-1} \tilde{\mu},$$

$$K_{x',x'} - K_{x',x}(K_{x,x} + \tilde{\Psi})^{-1} K_{x,x'}$$
Approximate sites determined by moment matching are naturally normalised.
Normalisers

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- To compute likelihood need to keep track of site integrals:

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\text{KL}[p \parallel q] = \int dx \, p(x) \log p(x) q(x) + \int dx \, (q(x) - p(x))
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incorporates normaliser into each \( \tilde{f}(\text{match zeroth moment, along with suff stats}) \) as well as the overall normaliser of \( \prod_i \tilde{f}_i(Y_i) \).
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Alpha divergences and Power EP

- Alpha divergences $D_\alpha[p\|q] = \frac{1}{\alpha(1 - \alpha)} \int dx \alpha p(x) + (1 - \alpha)q(x) - p(x)^\alpha q(x)^{1-\alpha}$

Local (EP) minimisation gives fixed-point updates that blend messages (to power $\alpha$) with previous site approximations.

$\tilde{f}_{\text{new}}^i = \text{argmin}_{f \in \{\tilde{f}^i\}} KL[f_i(Y^i) \alpha \tilde{f}^i(Y^i)]^{1-\alpha}$

Small changes (for $\alpha < 1$) lead to more stable updates, and more reliable convergence.
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$$D_{-1}[p\|q] = \frac{1}{2} \int dx \frac{(p(x) - q(x))^2}{p(x)}$$

$$\lim_{\alpha \to 0} D_\alpha[p\|q] = KL[q\|p]$$

Note: $\lim_{\alpha \to 0} \frac{(p(x)/q(x))^\alpha}{\alpha} = \log \frac{p(x)}{q(x)}$

$$D_1[p\|q] = 2 \int dx (p(x)^{\frac{1}{2}} - q(x)^{\frac{1}{2}})^2$$

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$\lim_{\alpha \to 0} D_\alpha[p\|q] = KL[q\|p]$

$D_{\frac{1}{2}}[p\|q] = 2 \int dx (p(x)^{\frac{1}{2}} - q(x)^{\frac{1}{2}})^2$

$\lim_{\alpha \to 1} D_\alpha[p\|q] = KL[p\|q]$

$D_2[p\|q] = \frac{1}{2} \int dx \frac{(p(x) - q(x))^2}{q(x)}$

Local (EP) minimisation gives fixed-point updates that blend messages (to power $\alpha$) with previous site approximations.

$\tilde{f}_i^{\text{new}} = \operatorname{argmin}_{f \in \{\tilde{f}\}} KL[f_i(Y_i)^\alpha \tilde{f}_i(Y_i)^{1-\alpha} q_{-i}(Y) \| f(Y_i) q_{-i}(Y)]$

Small changes (for $\alpha < 1$) lead to more stable updates, and more reliable convergence.