Probabilistic & Unsupervised Learning
Approximate Inference

Expectation Propagation

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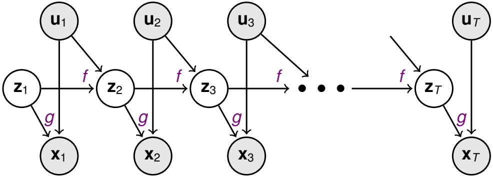
Term 1, Autumn 2021

Intractabilities and approximations

- Inference – computational intractability
  - Gibbs sampling, other MCMC
  - Factored variational approx
  - Loopy BP/EP/Power EP
  - Recognition models
- Inference – analytic intractability
  - Laplace approximation (global)
  - (Sequential) Monte-Carlo
  - Message approximations (linearised, sigma-point, Laplace)
  - Assumed-density methods and Expectation-Propagation
  - Parametric variational approx
  - Recognition models
- Learning – intractable partition function
  - Sampling parameters
  - Constrastive divergence
  - Score-matching
- Posterior estimation and model selection
  - Laplace approximation / BIC
  - Monte-Carlo
  - (Annealed) importance sampling
  - Reversible jump MCMC
  - Variational Bayes

Not a complete list!

Nonlinear state-space model (NLSSM)



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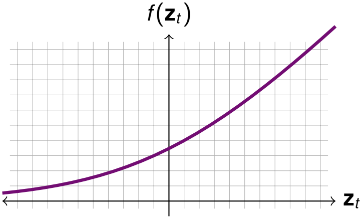

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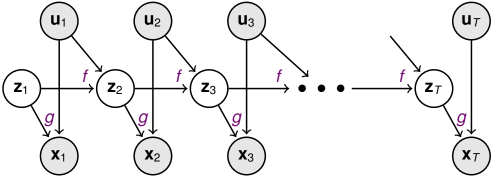

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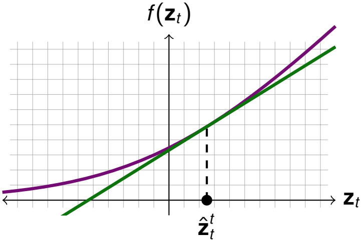

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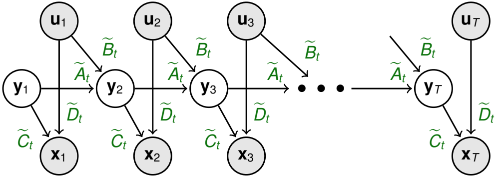

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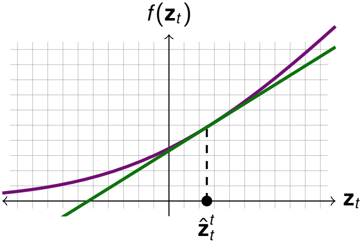

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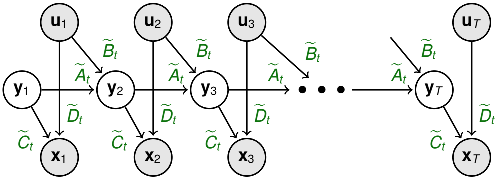

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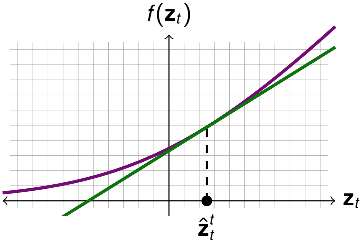

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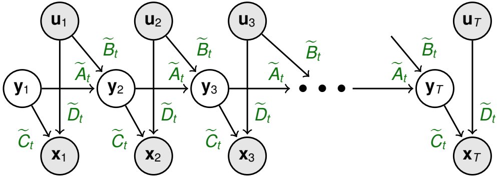

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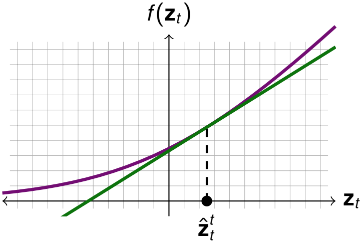

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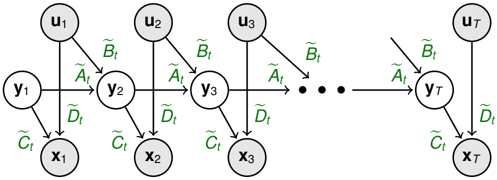

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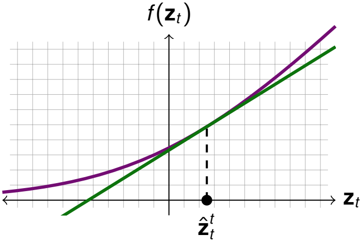

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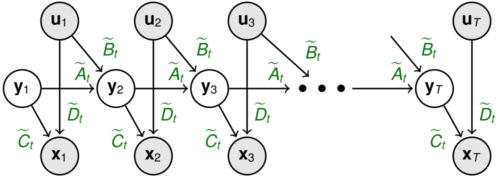

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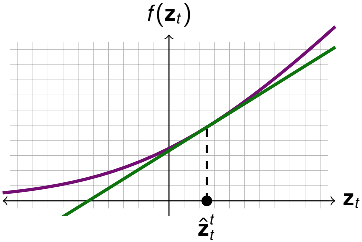

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Can base EM-like algorithm on EKF/EKS (or alternatives).

Other message approximations

Consider the forward messages on a latent chain:

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- The other KL: $\operatorname{argmin} \mathbf{KL}\left[\int d\mathbf{z}_{t-1} \,\middle\|\, \mathcal{N}(\hat{\mathbf{z}}_t, \hat{V}_t)\right]$ needs only first and second moments of nonlinear message $\Rightarrow$ EP.

Variational learning

Free energy:

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  - 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.

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- Can we use other divergences?

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But it raises the hope that approximate minimisation might still yield useful results.

Approximate optimisation

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

$$P(\mathcal{Z}|\mathcal{X}) = \frac{P(\mathcal{Z},\mathcal{X})}{P(\mathcal{X})} = \frac{1}{Z}\prod_i P(Z_i|\,\mathrm{pa}(Z_i)) \propto \prod_{i=1}^{N} f_i(\mathcal{Z}_i)$$

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Consider q with the same factorisation, but potentially approximated sites:
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  - This leads to a message passing approach, hence propagation.

Local updates

Each EP update involves a KL minimisation:

$$\tilde{f}_i^{\mathrm{new}}(\mathcal{Z}) \leftarrow \operatorname*{argmin}_{f \in \{\tilde{f}\}} \mathbf{KL}[f_i(\mathcal{Z}_i) q_{\neg i}(\mathcal{Z}) \| f(\mathcal{Z}_i) q_{\neg i}(\mathcal{Z})] \qquad \left[q_{\neg i}(\mathcal{Z}) \stackrel{\mathrm{def}}{=} \prod_{j \neq i} \tilde{f}_j(\mathcal{Z}_j) \right]$$

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\end{aligned}$$

Local updates

Each EP update involves a KL minimisation:

$$\tilde{f}_i^{\text{new}}(\mathcal{Z}) \leftarrow \underset{f \in \{\tilde{f}\}}{\operatorname{argmin}} \, \mathbf{KL}[f_i(\mathcal{Z}_i) q_{\neg i}(\mathcal{Z}) \| f(\mathcal{Z}_i) q_{\neg i}(\mathcal{Z})] \qquad \left[q_{\neg i}(\mathcal{Z}) \stackrel{\text{def}}{=} \prod_{j \neq i} \tilde{f}_j(\mathcal{Z}_j) \right]$$

Separate the contextual factor: $q_{\neg i}(\mathcal{Z}) = q_{\neg i}(\mathcal{Z}_i) q_{\neg i}(\mathcal{Z}_{\neg i} | \mathcal{Z}_i)$ $\qquad [\mathcal{Z}_{\neg i} \stackrel{\text{def}}{=} \mathcal{Z} \backslash \mathcal{Z}_i]$

Then:

$$\begin{aligned}
&\min_f \mathbf{KL}[f_i(\mathcal{Z}_i) q_{\neg i}(\mathcal{Z}) \| f(\mathcal{Z}_i) q_{\neg i}(\mathcal{Z})] \\
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\end{aligned}$$

$q_{\neg i}(\mathcal{Z}_i)$ is sometimes called the cavity distribution.

Expectation Propagation (EP)

Input $f_1(\mathcal{Z}_1) \ldots f_N(\mathcal{Z}_N)$

Initialize $\tilde{f}_1(\mathcal{Z}_1) = \underset{f \in \{\tilde{f}\}}{\operatorname{argmin}} \, \mathbf{KL}[f_1(\mathcal{Z}_1) \| f_1(\mathcal{Z}_1)]$, $\tilde{f}_i(\mathcal{Z}_i) = 1$ for $i > 1$, $q(\mathcal{Z}) \propto \prod_i \tilde{f}_i(\mathcal{Z}_i)$

repeat

for $i = 1 \ldots N$ **do**

Delete: $q_{\neg i}(\mathcal{Z}) \leftarrow \dfrac{q(\mathcal{Z})}{\tilde{f}_i(\mathcal{Z}_i)} = \prod_{j \neq i} \tilde{f}_j(\mathcal{Z}_j)$

Project: $\tilde{f}_i^{\mathrm{new}}(\mathcal{Z}) \leftarrow \underset{f \in \{\tilde{f}\}}{\operatorname{argmin}} \, \mathbf{KL}[f_i(\mathcal{Z}_i) q_{\neg i}(\mathcal{Z}_i) \| f(\mathcal{Z}_i) q_{\neg i}(\mathcal{Z}_i)]$

Include: $q(\mathcal{Z}) \leftarrow \tilde{f}_i^{\mathrm{new}}(\mathcal{Z}_i) \, q_{\neg i}(\mathcal{Z})$

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:

$$q_{\neg i}(\mathcal{Z}_i) = \prod_{j \in \mathrm{ne}(i)} M_{j \to i}(\mathcal{Z}_j \cap \mathcal{Z}_i)$$

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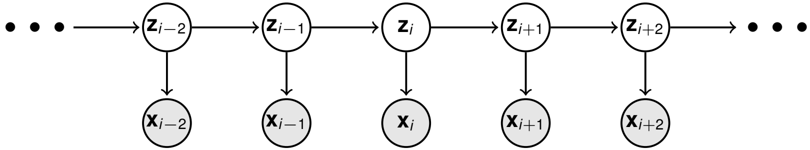
- For some approximations (e.g. Gaussian) may be able to compute true loopy cavity using approximate sites, even if computing exact message would have been intractable.
- In either case, message updates can be scheduled in any order.
- No guarantee of convergence (but see “power-EP” methods).

EP for a NLSSM



$$P(\mathbf{z}_i|\mathbf{z}_{i-1}) = \phi_i(\mathbf{z}_i, \mathbf{z}_{i-1}) \qquad \textit{e.g.}\ \exp(-\|\mathbf{z}_i - h_s(\mathbf{z}_{i-1})\|^2/2\sigma^2)$$

$$P(\mathbf{x}_i|\mathbf{z}_i) = \psi_i(\mathbf{z}_i) \qquad \textit{e.g.}\ \exp(-\|\mathbf{x}_i - h_o(\mathbf{z}_i)\|^2/2\sigma^2)$$

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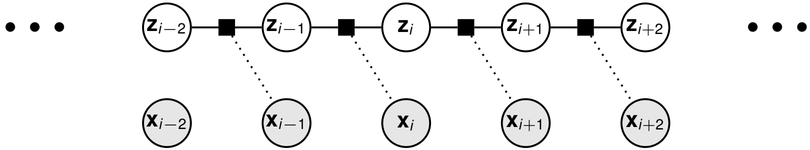

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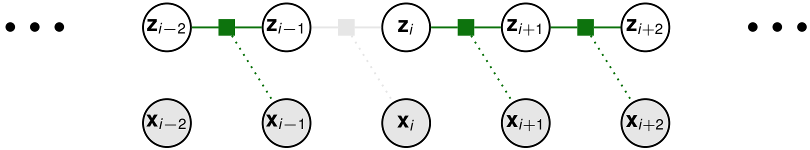
Then $f_i(\mathbf{z}_i, \mathbf{z}_{i-1}) = \phi_i(\mathbf{z}_i, \mathbf{z}_{i-1})\psi_i(\mathbf{z}_i)$. As ϕ_i and ψ_i are non-linear, inference is not generally tractable.

EP for a NLSSM



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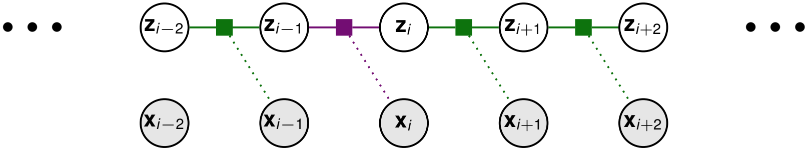
Assume $\tilde{f}_i(\mathbf{z}_i, \mathbf{z}_{i-1})$ is Gaussian. Then,

$$q_{\neg i}(\mathbf{z}_i, \mathbf{z}_{i-1}) = \int\limits_{\substack{\mathbf{z}_1 \ldots \mathbf{z}_{i-2} \\ \mathbf{z}_{i+1} \ldots \mathbf{z}_i}} \prod_{i' \neq i} \tilde{f}_{i'}(\mathbf{z}_{i'}, \mathbf{z}_{i'-1}) = \underbrace{\int\limits_{\mathbf{z}_1 \ldots \mathbf{z}_{i-2}} \prod_{i' < i} \tilde{f}_{i'}(\mathbf{z}_{i'}, \mathbf{z}_{i'-1})}_{\alpha_{i-1}(\mathbf{z}_{i-1})} \underbrace{\int\limits_{\mathbf{z}_{i+1} \ldots \mathbf{z}_n} \prod_{i' > i} \tilde{f}_{i'}(\mathbf{z}_{i'}, \mathbf{z}_{i'-1})}_{\beta_i(\mathbf{z}_i)}$$

with both α and β Gaussian.

EP for a NLSSM



$$P(\mathbf{z}_i|\mathbf{z}_{i-1}) = \phi_i(\mathbf{z}_i, \mathbf{z}_{i-1}) \qquad \textit{e.g.}\ \exp(-\|\mathbf{z}_i - h_s(\mathbf{z}_{i-1})\|^2/2\sigma^2)$$

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with both α and β Gaussian.

$$\tilde{f}_i(\mathbf{z}_i, \mathbf{z}_{i-1}) = \underset{f \in \mathcal{N}}{\operatorname{argmin}}\, \mathbf{KL}\left[\phi_i(\mathbf{z}_i, \mathbf{z}_{i-1})\psi_i(\mathbf{z}_i)\alpha_{i-1}(\mathbf{z}_{i-1})\beta_i(\mathbf{z}_i) \middle\| f(\mathbf{z}_i, \mathbf{z}_{i-1})\alpha_{i-1}(\mathbf{z}_{i-1})\beta_i(\mathbf{z}_i)\right]$$

NLSSM EP message updates

$$\tilde{f}_i(\mathbf{z}_i, \mathbf{z}_{i-1}) = \operatorname*{argmin}_{f \in \mathcal{N}} \mathbf{KL}\left[f(\mathbf{z}_i, \mathbf{z}_{i-1}) q_{\neg i}(\mathbf{z}_i, \mathbf{z}_{i-1}) \middle\| f(\mathbf{z}_i, \mathbf{z}_{i-1}) q_{\neg i}(\mathbf{z}_i, \mathbf{z}_{i-1}) \right]$$

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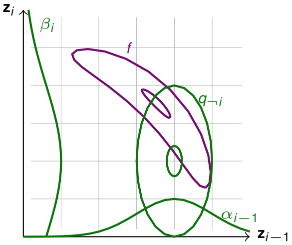
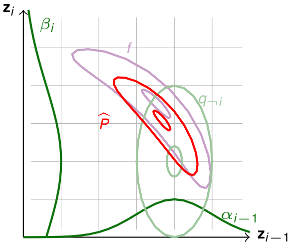


NLSSM EP message updates

$$\tilde{f}_i(\mathbf{z}_i, \mathbf{z}_{i-1}) = \underset{f \in \mathcal{N}}{\operatorname{argmin}} \, \mathbf{KL}\Big[\underbrace{\phi_i(\mathbf{z}_i, \mathbf{z}_{i-1})\psi_i(\mathbf{z}_i)\alpha_{i-1}(\mathbf{z}_{i-1})\beta_i(\mathbf{z}_i)}_{\widehat{P}(\mathbf{z}_{i-1}, \mathbf{z}_i)} \Big\| \underbrace{f(\mathbf{z}_i, \mathbf{z}_{i-1})\alpha_{i-1}(\mathbf{z}_{i-1})\beta_i(\mathbf{z}_i)}_{P(\mathbf{z}_{i-1}, \mathbf{z}_i)}\Big]$$



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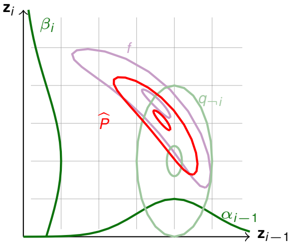
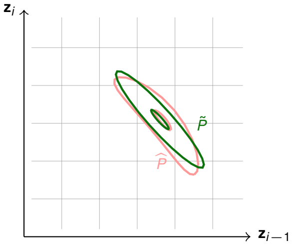
$$\tilde{P}(\mathbf{z}_{i-1}, \mathbf{z}_i) = \underset{P \in \mathcal{N}}{\operatorname{argmin}} \, \mathbf{KL}\Big[\widehat{P}(\mathbf{z}_{i-1}, \mathbf{z}_i) \Big\| P(\mathbf{z}_{i-1}, \mathbf{z}_i)\Big]$$





NLSSM EP message updates

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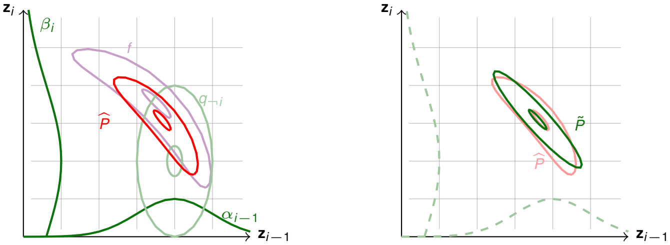

NLSSM EP message updates

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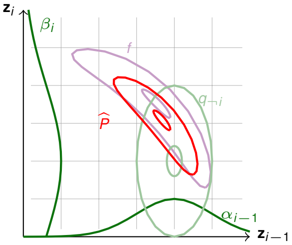
$$\alpha_i(\mathbf{z}_i) = \int_{\mathbf{z}_1 \ldots \mathbf{z}_{i-1}} \prod_{i' < i+1} \tilde{f}_{i'}(\mathbf{z}_{i'}, \mathbf{z}_{i'-1}) = \int_{\mathbf{z}_{i-1}} \alpha_{i-1}(\mathbf{z}_{i-1})\tilde{f}_i(\mathbf{z}_i, \mathbf{z}_{i-1}) = \frac{1}{\beta_i(\mathbf{z}_i)} \int_{\mathbf{z}_{i-1}} \tilde{P}(\mathbf{z}_{i-1}, \mathbf{z}_i)$$

$$\beta_{i-1}(\mathbf{z}_{i-1}) = \int_{\mathbf{z}_{i+1} \ldots \mathbf{z}_i} \prod_{i' > i} \tilde{f}_{i'}(\mathbf{z}_{i'}, \mathbf{z}_{i'-1}) = \int_{\mathbf{z}_i} \beta_i(\mathbf{z}_i)\tilde{f}_i(\mathbf{z}_i, \mathbf{z}_{i-1}) = \frac{1}{\alpha_{i-1}(\mathbf{z}_{i-1})} \int_{\mathbf{z}_i} \tilde{P}(\mathbf{z}_{i-1}, \mathbf{z}_i)$$



Moment Matching

Each EP update involves a KL minimisation:

$$\tilde{f}_i^{\text{new}}(\mathcal{Z}) \leftarrow \underset{f \in \{\tilde{f}\}}{\operatorname{argmin}} \ \mathbf{KL}[f_i(\mathcal{Z}_i) q_{\neg i}(\mathcal{Z}) \| f(\mathcal{Z}_i) q_{\neg i}(\mathcal{Z})]$$

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

$$\begin{aligned}
\underset{q}{\operatorname{argmin}} \, \mathbf{KL}\big[p(x) \big\| q(x)\big] &= \underset{\boldsymbol{\theta}}{\operatorname{argmin}} \, \mathbf{KL}\left[p(x) \middle\| \frac{1}{Z(\boldsymbol{\theta})} e^{\mathsf{T}(x) \cdot \boldsymbol{\theta}}\right] \\
&= \underset{\boldsymbol{\theta}}{\operatorname{argmin}} - \int dx \; p(x) \log \frac{1}{Z(\boldsymbol{\theta})} e^{\mathsf{T}(x) \cdot \boldsymbol{\theta}} \\
&= \underset{\boldsymbol{\theta}}{\operatorname{argmin}} - \int dx \; p(x) \mathsf{T}(x) \cdot \boldsymbol{\theta} + \log Z(\boldsymbol{\theta}) \\
\frac{\partial}{\partial \boldsymbol{\theta}} &= - \int dx \; p(x) \mathsf{T}(x) + \frac{1}{Z(\boldsymbol{\theta})} \frac{\partial}{\partial \boldsymbol{\theta}} \int dx \; e^{\mathsf{T}(x) \cdot \boldsymbol{\theta}} \\
&= -\langle \mathsf{T}(x) \rangle_p + \frac{1}{Z(\boldsymbol{\theta})} \int dx \; e^{\mathsf{T}(x) \cdot \boldsymbol{\theta}} \mathsf{T}(x) \\
&= -\langle \mathsf{T}(x) \rangle_p + \langle \mathsf{T}(x) \rangle_q
\end{aligned}$$

So minimum is found by matching sufficient stats or moment matching.

Numerical issues

How do we calculate $\langle \mathrm{T}(x) \rangle_p$?

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Often analytically tractable, but even if not requires a (relatively) low-dimensional integral:

- Quadrature methods.

Numerical issues

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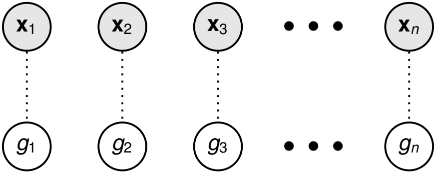

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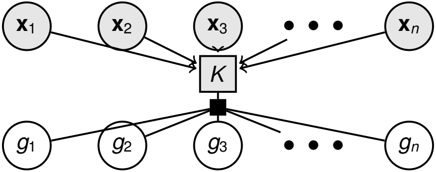

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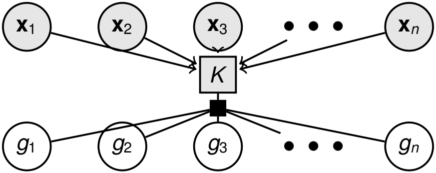

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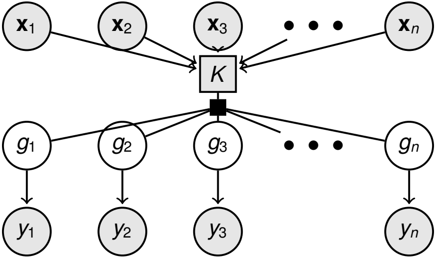

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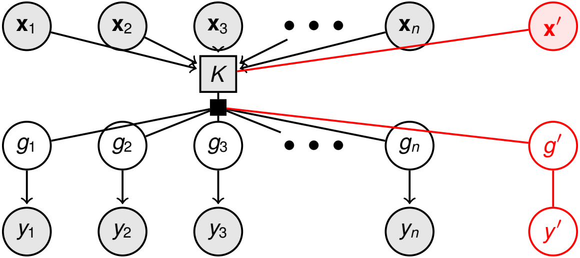

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- No parameters to learn (though often hyperparameters); instead, we make predictions on test data directly: [assuming $\mu = 0$, and matrix Σ incorporates diagonal noise]

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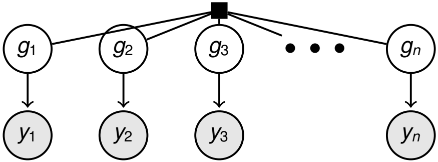

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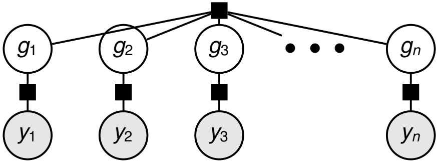

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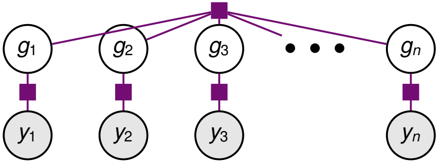

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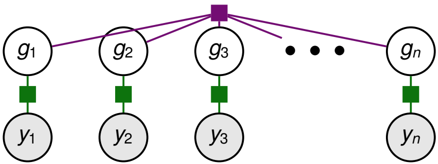

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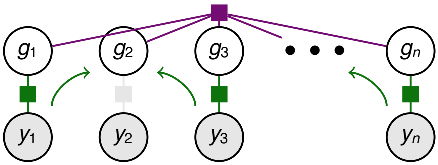

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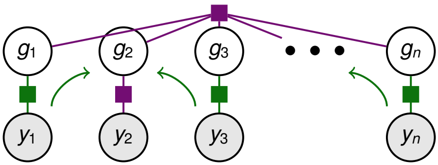

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- The EP updates thus require calculating Gaussian expectations of $f_i(g)g^{\{1,2\}}$:

$$\tilde{f}_i^{\text{new}}(g_i) = \mathcal{N}\left(\int dg\, q_{\neg i}(g) f_i(g) g,\ \int dg\, q_{\neg i}(g) f_i(g) g^2 - (\tilde{\mu}_i^{\text{new}})^2\right) / q_{\neg i}(g_i)$$

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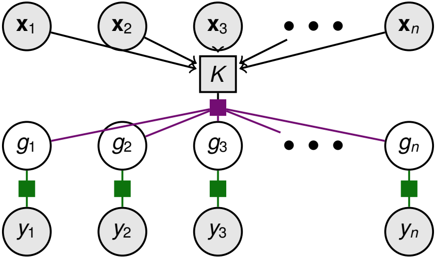

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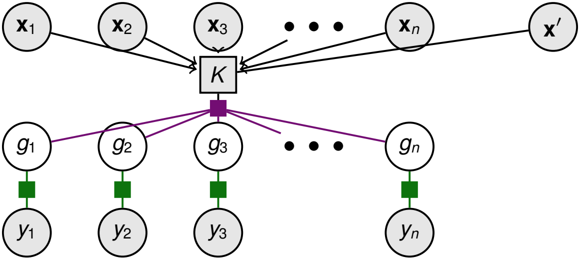

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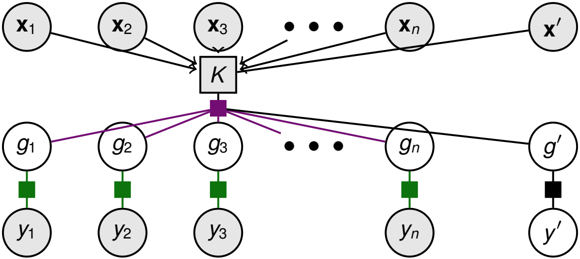

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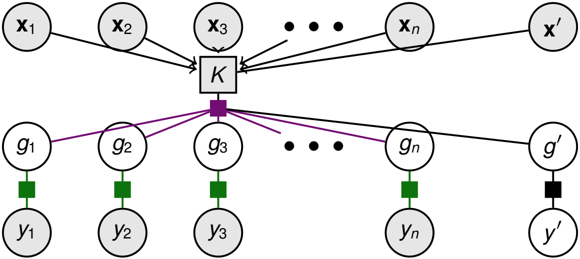

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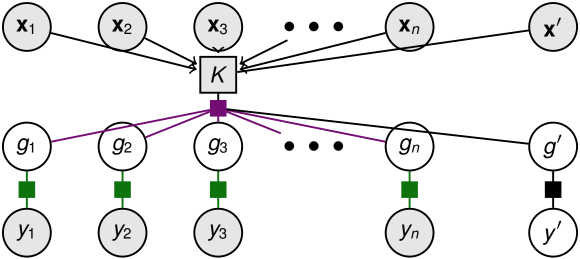

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- Thus no change is needed to the approximating potentials $\tilde{f}_i$.
- Predictions are obtained by marginalising the approximation: [let $\tilde{\Psi} = \text{diag}[\tilde{\psi}_1^2 \dots \tilde{\psi}_n^2]$]

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

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- However, to compute an approximation to the likelihood $\prod_i f_i(\mathcal{Z}_i)$ we need to keep track of the site integrals.

Computing likelihoods – keeping track of normalisers

- Define unnormalised ExpFam approximating sites $\tilde{f}_i = \tilde{C}_i e^{\mathsf{T}(\mathcal{Z})\cdot\boldsymbol{\theta}_i}$.

  Write $\boldsymbol{\theta} = \sum \boldsymbol{\theta}_j$ for the natural parameters of $q(\mathcal{Z})$ and $\boldsymbol{\theta}_{\neg i} = \sum_{j \neq i} \boldsymbol{\theta}_j$ for the natural parameters of $q_{\neg i}(\mathcal{Z})$.

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- Now, at each EP step minimise the "unnormalised KL":

$$\mathbf{KL}[p\|q] = \int dx\, p(x) \log \frac{p(x)}{q(x)} + \int dx\, \big(q(x) - p(x)\big)$$

  This matches the zeroth moment of $f_i(\mathcal{Z}_i) q_{\neg i}(\mathcal{Z})$ as well as the expected sufficient statistics as before. That is:

$$\int \tilde{C}_i e^{\mathbf{T}(\mathcal{Z})\cdot\boldsymbol{\theta}_i} \prod_{\neg i} \tilde{C}_j e^{\mathbf{T}(\mathcal{Z})\cdot\boldsymbol{\theta}_j} = \int f_i(\mathcal{Z}_i) \prod_{\neg i} \tilde{C}_j e^{\mathbf{T}(\mathcal{Z})\cdot\boldsymbol{\theta}_j} \quad \Rightarrow \quad \tilde{C}_i = e^{\Phi_i(\boldsymbol{\theta}_{\neg i}) - \Phi(\boldsymbol{\theta})}$$

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- The likelihood approximation is then:

$$\log \int \prod_{i=1}^{N} f_i(\mathcal{Z}_i) \approx \log \int \prod_{i=1}^{N} \tilde{f}_i(\mathcal{Z}_i) = \Phi(\boldsymbol{\theta}) + \sum \log \tilde{C}_i \stackrel{\text{def}}{=} \tilde{\ell}$$

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  - However, proves to be simpler than it sounds.

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&= \langle T(\mathcal{Z}) \rangle_{\widehat{P}_i} \cdot \nabla_\eta \boldsymbol{\theta}_{\neg i} + \int \nabla_\eta \log f_i(\mathcal{Z}_i) f_i(\mathcal{Z}_i) e^{\mathsf{T}(\mathcal{Z}) \cdot \boldsymbol{\theta}_{\neg i} - \Phi_i(\boldsymbol{\theta}_{\neg i})}
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\end{aligned}$$

by EP moment matching at convergence!

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So putting it all together:

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and the gradient can be computed provided EP converges.

A final generalisation: alpha divergences and Power EP

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

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