

Probabilistic & Unsupervised Learning

Approximate Inference

Expectation Propagation

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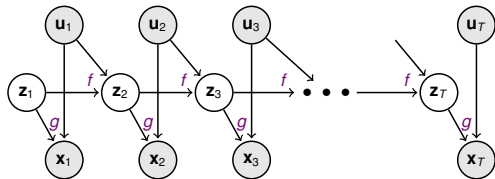
Term 1, Autumn 2020

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
 - ▶ Contrastive 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!

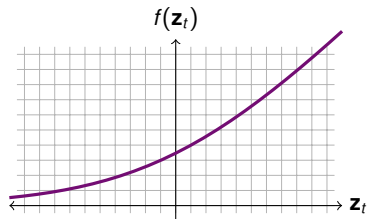
Nonlinear state-space model (NLSSM)



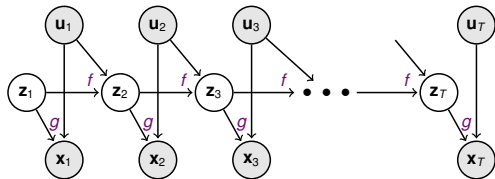
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$$\mathbf{x}_t = g(\mathbf{z}_t, \mathbf{u}_t) + \mathbf{v}_t$$

$\mathbf{w}_t, \mathbf{v}_t$ usually still Gaussian.



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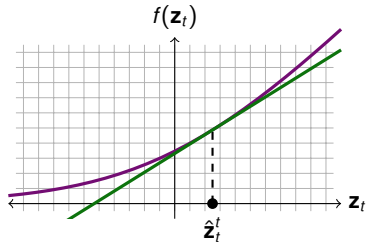
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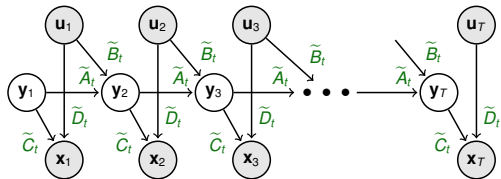
Extended Kalman Filter (EKF): linearise nonlinear functions about current estimate, $\hat{\mathbf{z}}_t^t$:

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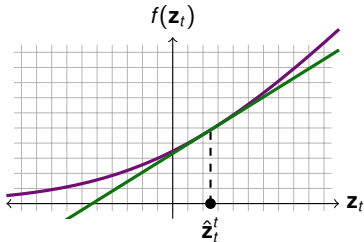
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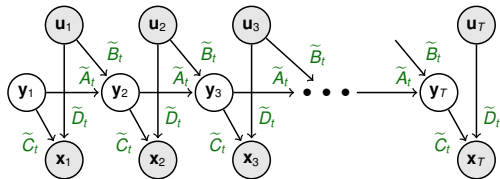
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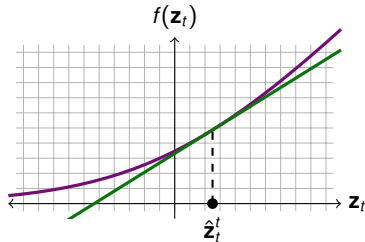
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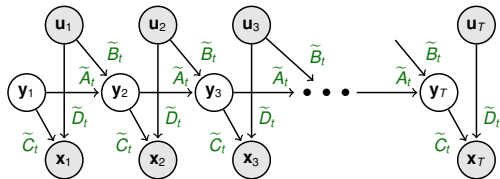
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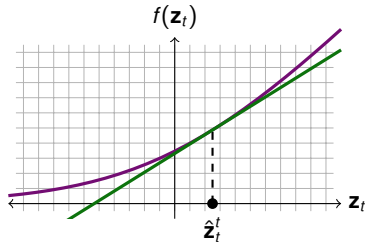
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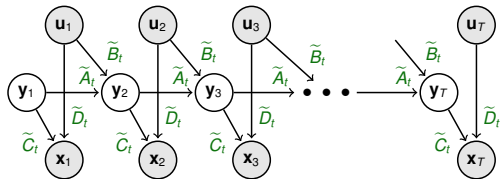
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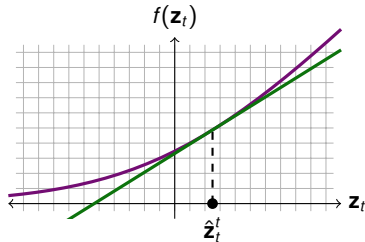
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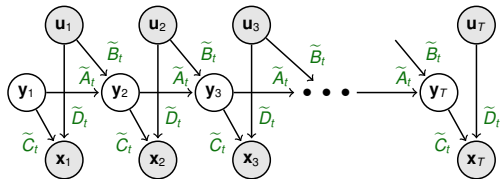
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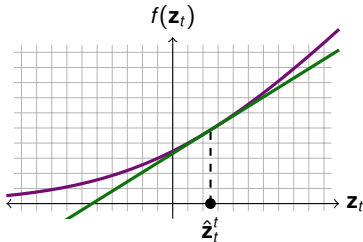
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Can base EM-like algorithm on EKF/EKS (or alternatives).

Other message approximations

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- ▶ Parametric variational: $\operatorname{argmin} \mathbf{KL}[\mathcal{N}(\hat{\mathbf{z}}_t, \hat{V}_t) || \int d\mathbf{z}_{t-1} \dots]$. Requires Gaussian expectations of $\log \int \Rightarrow$ (usually) Monte-Carlo integration (later lecture).

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- ▶ Parametric variational: $\operatorname{argmin} \mathbf{KL}[\mathcal{N}(\hat{\mathbf{z}}_t, \hat{V}_t) \parallel \int d\mathbf{z}_{t-1} \dots]$. Requires Gaussian expectations of $\log \int \Rightarrow$ (usually) Monte-Carlo integration (later lecture).
- ▶ The other KL: $\operatorname{argmin} \mathbf{KL}[\int d\mathbf{z}_{t-1} \parallel \mathcal{N}(\hat{\mathbf{z}}_t, \hat{V}_t)]$ needs only first and second moments of nonlinear message \Rightarrow EP.

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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:

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

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Consider q with the **same** factorisation, but potentially approximated sites:

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- ▶ **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:

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

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

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$$\begin{aligned} & \min_f \mathbf{KL}[f_i(\mathcal{Z}_i)q_{-i}(\mathcal{Z}) \| f(\mathcal{Z}_i)q_{-i}(\mathcal{Z})] \\ &= \max_f \int d\mathcal{Z} f_i(\mathcal{Z}_i)q_{-i}(\mathcal{Z}) \log f(\mathcal{Z}_i)q_{-i}(\mathcal{Z}) \\ &= \max_f \int d\mathcal{Z}_i d\mathcal{Z}_{-i} f_i(\mathcal{Z}_i)q_{-i}(\mathcal{Z}_i)q_{-i}(\mathcal{Z}_{-i}|\mathcal{Z}_i) (\log f(\mathcal{Z}_i)q_{-i}(\mathcal{Z}_i) + \log q_{-i}(\mathcal{Z}_{-i}|\mathcal{Z}_i)) \\ &= \max_f \int d\mathcal{Z}_i f_i(\mathcal{Z}_i)q_{-i}(\mathcal{Z}_i) (\log f(\mathcal{Z}_i)q_{-i}(\mathcal{Z}_i)) \int d\mathcal{Z}_{-i} q_{-i}(\mathcal{Z}_{-i}|\mathcal{Z}_i) \end{aligned}$$

Local updates

Each EP update involves a KL minimisation:

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

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

Expectation Propagation (EP)

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

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

repeat

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

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

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

Include: $q(\mathcal{Z}) \leftarrow \tilde{f}_i^{\text{new}}(\mathcal{Z}_i) q_{-i}(\mathcal{Z})$

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:

$$q_{\rightarrow i}(\mathcal{Z}_i) = \prod_{j \in \text{ne}(i)} M_{j \rightarrow i}(\mathcal{Z}_j \cap \mathcal{Z}_i)$$

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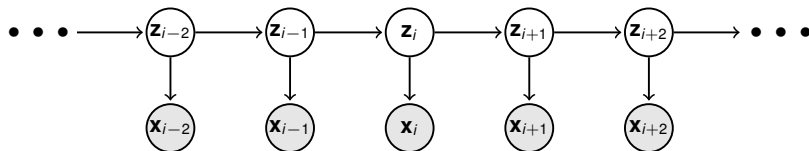
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- ▶ For some approximations (e.g. Gaussian) may be able to compute true loopy cavity using approximate sites, even if computing exact message would have been intractable.
- ▶ In either case, message updates can be scheduled in any order.
- ▶ No guarantee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

EP for a NLSSM



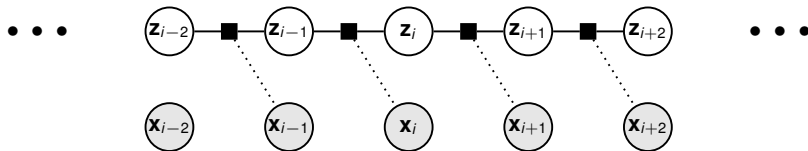
$$P(\mathbf{z}_i | \mathbf{z}_{i-1}) = \phi_i(\mathbf{z}_i, \mathbf{z}_{i-1})$$

$$\text{e.g. } \exp(-\|\mathbf{z}_i - h_s(\mathbf{z}_{i-1})\|^2 / 2\sigma^2)$$

$$P(\mathbf{x}_i | \mathbf{z}_i) = \psi_i(\mathbf{z}_i)$$

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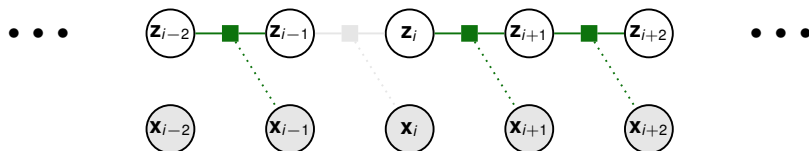
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Then $f_i(\mathbf{z}_i, \mathbf{z}_{i-1}) = \phi_i(\mathbf{z}_i, \mathbf{z}_{i-1})\psi_i(\mathbf{z}_i)$. As ϕ_i and ψ_i are non-linear, inference is not generally tractable.

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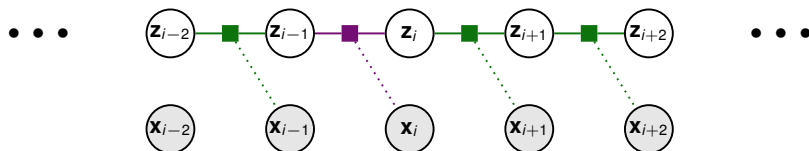
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Assume $\tilde{f}_i(\mathbf{z}_i, \mathbf{z}_{i-1})$ is Gaussian. Then,

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

with both α and β Gaussian.

EP for a NLSSM



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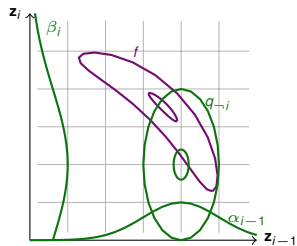
$$\tilde{f}_i(\mathbf{z}_i, \mathbf{z}_{i-1}) = \operatorname{argmin}_{f \in \mathcal{N}} \text{KL} [\phi_i(\mathbf{z}_i, \mathbf{z}_{i-1}) \psi_i(\mathbf{z}_i) \alpha_{i-1}(\mathbf{z}_{i-1}) \beta_i(\mathbf{z}_i) \parallel f(\mathbf{z}_i, \mathbf{z}_{i-1}) \alpha_{i-1}(\mathbf{z}_{i-1}) \beta_i(\mathbf{z}_i)]$$

NLSSM EP message updates

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

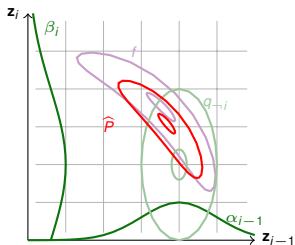
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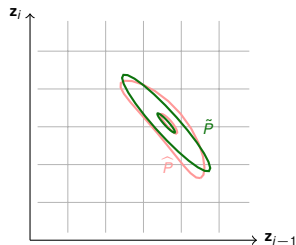
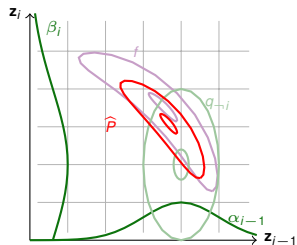
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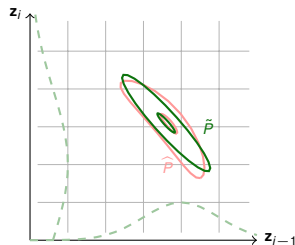
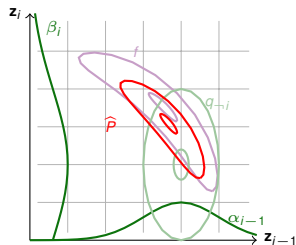
$$\tilde{P}(\mathbf{z}_{i-1}, \mathbf{z}_i) = \operatorname{argmin}_{P \in \mathcal{N}} [\hat{P}(\mathbf{z}_{i-1}, \mathbf{z}_i) \parallel P(\mathbf{z}_{i-1}, \mathbf{z}_i)]$$



NLSSM EP message updates

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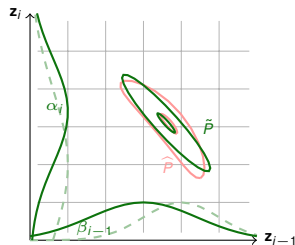
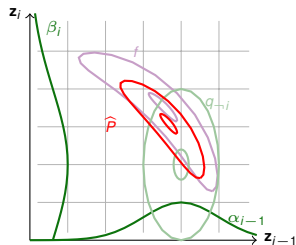
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$$\alpha_i(\mathbf{z}_i) = \int \prod_{\mathbf{z}_1 \dots \mathbf{z}_{i-1} \mid i' < i+1} \tilde{f}_{i'}(\mathbf{z}_{i'}, \mathbf{z}_{i'-1}) = \int_{\mathbf{z}_{i-1}} \alpha_{i-1}(\mathbf{z}_{i-1}) \tilde{f}_i(\mathbf{z}_i, \mathbf{z}_{i-1}) = \frac{1}{\beta_i(\mathbf{z}_i)}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

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



Moment Matching

Each EP update involves a KL minimisation:

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

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

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

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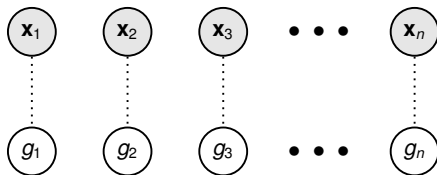
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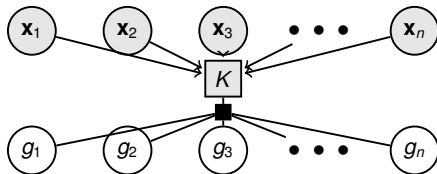


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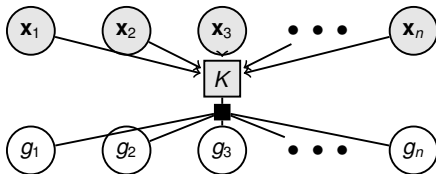


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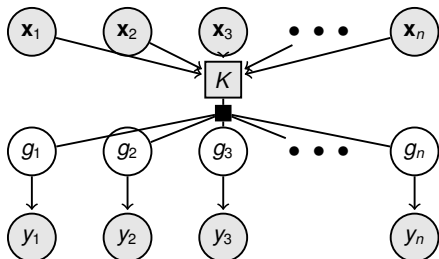


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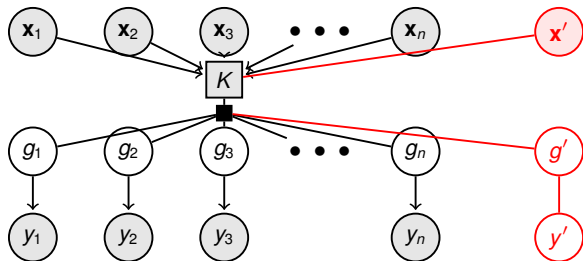


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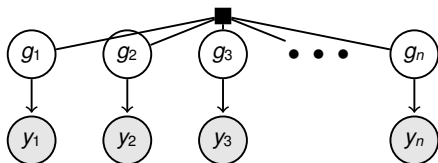


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- ▶ In a GP regression model, noisy observations y_i are conditionally independent given g_i .
- ▶ No parameters to learn (though often hyperparameters); instead, we make predictions on test data directly: [assuming $\boldsymbol{\mu} = 0$, and matrix $\boldsymbol{\Sigma}$ incorporates diagonal noise]

$$P(y' | \mathbf{x}', D) = \mathcal{N}(\boldsymbol{\Sigma}_{\mathbf{x}', X} \boldsymbol{\Sigma}_{X, X}^{-1} \mathbf{z}, \boldsymbol{\Sigma}_{\mathbf{x}', \mathbf{x}'} - \boldsymbol{\Sigma}_{\mathbf{x}', X} \boldsymbol{\Sigma}_{X, X}^{-1} \boldsymbol{\Sigma}_{X, \mathbf{x}'})$$

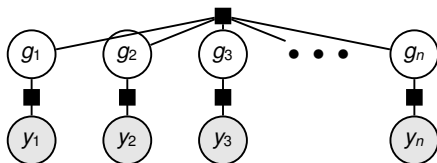
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- ▶ We can write the GP joint on g_i and y_i as a factor graph:

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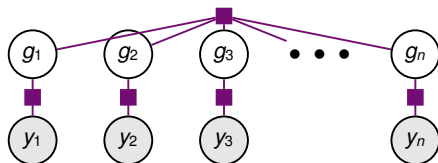
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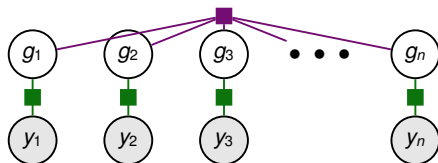


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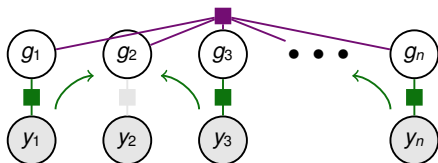


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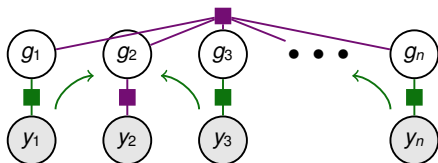
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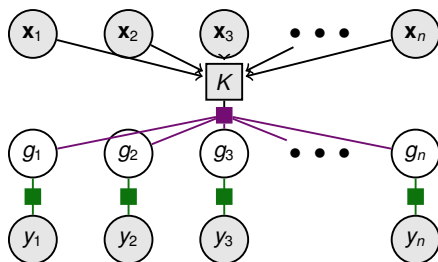
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- ▶ The EP updates thus require calculating Gaussian expectations of $f_i(g)g^{\{1,2\}}$:

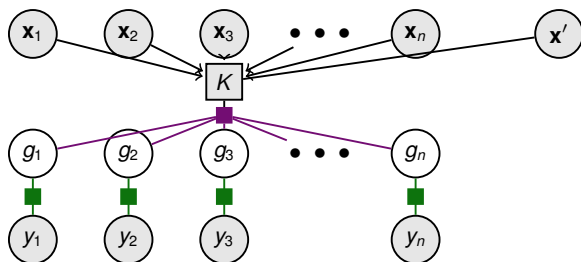
$$\tilde{f}_i^{\text{new}}(g_i) = \mathcal{N}\left(\int dg q_{-i}(g) f_i(g) g, \int dg q_{-i}(g) f_i(g) g^2 - (\tilde{\mu}_i^{\text{new}})^2\right) / q_{-i}(g_i)$$

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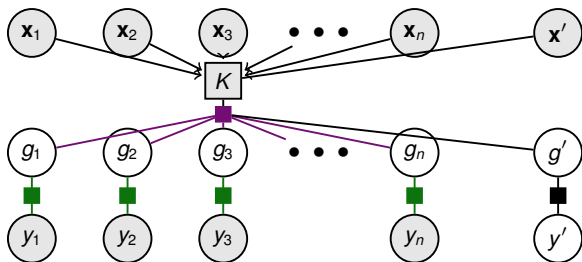
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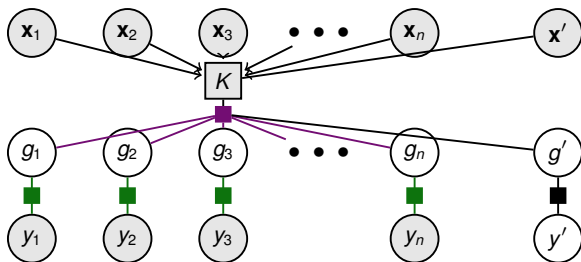
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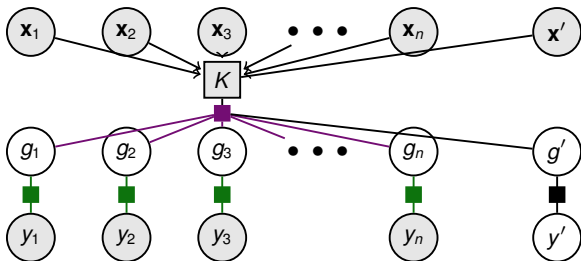
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- ▶ Predictions are obtained by marginalising the approximation: [let $\tilde{\Psi} = \text{diag}[\tilde{\psi}_1^2 \dots \tilde{\psi}_n^2]$]

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

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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 $\tilde{f}_i = \tilde{C}_i e^{\mathbf{T}(\mathcal{Z}) \cdot \theta_i}$.

Write $\theta = \sum \theta_j$ for the natural parameters of $q(\mathcal{Z})$ and $\theta_{-i} = \sum_{j \neq i} \theta_j$ for the natural parameters of $q_{-i}(\mathcal{Z})$.

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

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

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

$$\int \tilde{C}_i e^{\mathbf{T}(\mathcal{Z}) \cdot \theta_i} \prod_{-i} \tilde{C}_j e^{\mathbf{T}(\mathcal{Z}) \cdot \theta_j} = \int f_i(\mathcal{Z}_i) \prod_{-i} \tilde{C}_j e^{\mathbf{T}(\mathcal{Z}) \cdot \theta_j} \Rightarrow \tilde{C}_i = e^{\Phi_i(\theta_{-i}) - \Phi(\theta)}$$

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

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 - ▶ However, proves to be simpler than it sounds.

EP log-likelihood optimisation for learning

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by EP moment matching at convergence!

EP log-likelihood optimisation for learning

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

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