Probabilistic & Unsupervised Learning

Expectation Propagation

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Term 1, Autumn 2018

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
  - Parametric variational approx (for special cases).
  - Message approximations (linearised, sigma-point, Laplace)
  - Assumed-density methods and Expectation-Propagation
  - Recognition models
- Learning – intractable partition function
  - Sampling parameters
  - Constrastive divergence
  - Score-matching
- Posterior estimation and model selection
  - Laplace approximation / BIC
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  - (Annealed) importance sampling
  - Reversible jump MCMC
  - Variational Bayes

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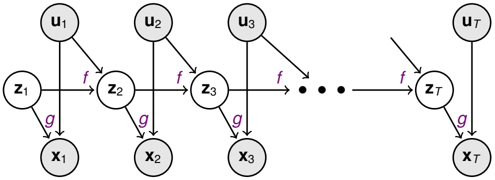
Nonlinear state-space model (NLSSM)



$$\mathbf{z}_{t+1} = f(\mathbf{z}_t, \mathbf{u}_t) + \mathbf{w}_t$$
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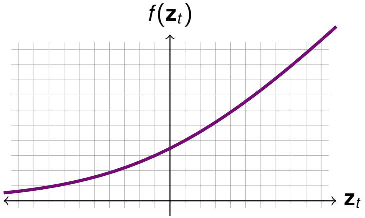
$\mathbf{w}_t, \mathbf{v}_t$ usually still Gaussian.



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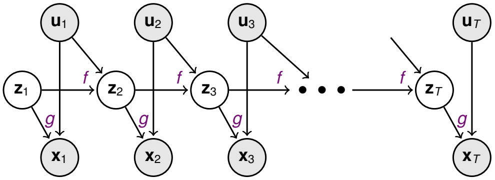

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Extended Kalman Filter (EKF): linearise nonlinear functions about current estimate, $\hat{\mathbf{z}}_t^t$:

$$\mathbf{z}_{t+1} \approx f(\hat{\mathbf{z}}_t^t, \mathbf{u}_t) + \left.\frac{\partial f}{\partial \mathbf{z}_t}\right|_{\hat{\mathbf{z}}_t^t} (\mathbf{z}_t - \hat{\mathbf{z}}_t^t) + \mathbf{w}_t$$

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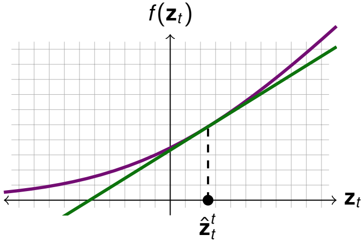

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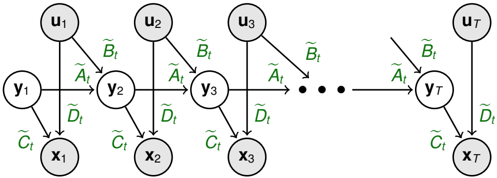

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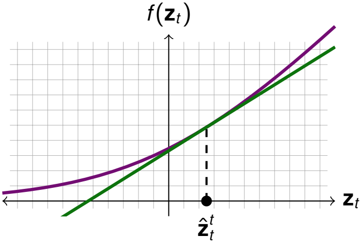

Run the Kalman filter (smoother) on non-stationary linearised system $(\widetilde{A}_t, \widetilde{B}_t, \widetilde{C}_t, \widetilde{D}_t)$:

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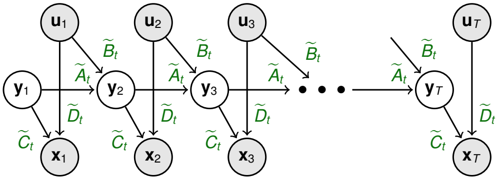

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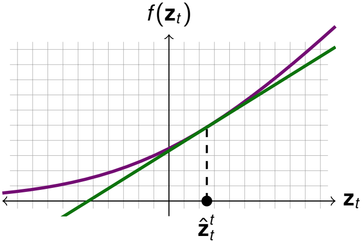

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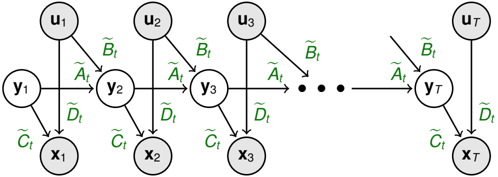

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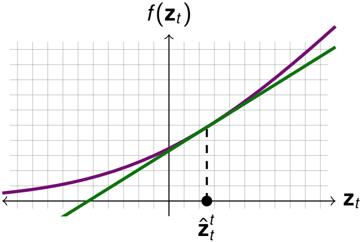

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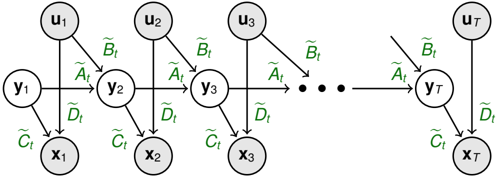

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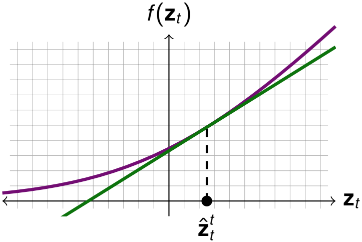

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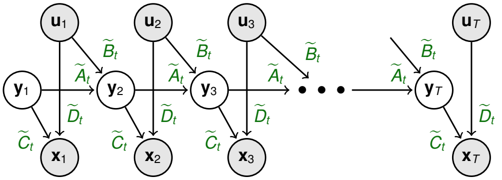

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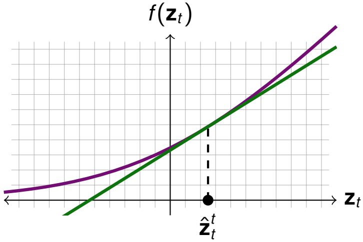

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Can base EM-like algorithm on EKF/EKS (or alternatives).

Other message approximations

Consider the forward messages on a latent chain:

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  - Equivalent to numerical evaluation of mean and covariance by Gaussian quadrature.
  - One form of "Assumed Density Filtering" and EP.

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- Linearisation at the peak (EKF) is only one approach.
- Laplace filter: use mode and curvature of integrand.
- Sigma-point ("unscented") filter:
  - Evaluate $f(\hat{\mathbf{z}}_{t-1})$, $f(\hat{\mathbf{z}}_{t-1} \pm \sqrt{\lambda}\mathbf{v})$ for eigenvalues, eigenvectors $\hat{V}_{t-1}\mathbf{v} = \lambda\mathbf{v}$.
  - "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: argmin $\mathbf{KL}\left[\mathcal{N}\left(\hat{\mathbf{z}}_t, \hat{V}_t\right) \middle\| \int d\mathbf{z}_{t-1} \;\ldots\right]$. Requires Gaussian expectations of $\log \int \Rightarrow$ may be challenging.

Other message approximations

Consider the forward messages on a latent chain:

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

Variational learning

Free energy:

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

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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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- 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:

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

Write $q_{\neg i}(\mathcal{Z}) = q_{\neg i}(\mathcal{Z}_i)q_{\neg i}(\mathcal{Z}_{\neg i}|\mathcal{Z}_i)$. Then: $\quad [\mathcal{Z}_{\neg i} \stackrel{\text{def}}{=} \mathcal{Z} \backslash \mathcal{Z}_i]$

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

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

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

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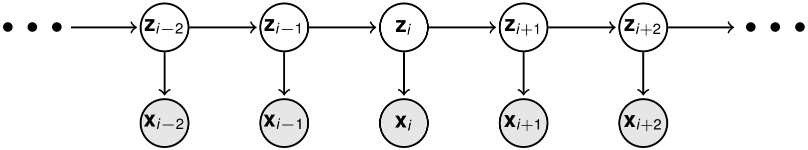
- For some approximations (e.g. Gaussian) may be able to compute true loopy cavity using approximate sites, even if computing exact message would have been intractable.
- In either case, message updates can be scheduled in any order.
- No guarantee of convergence (but see “power-EP” methods).

EP for a NLSSM



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

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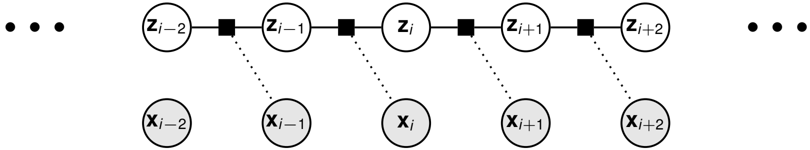
EP for a NLSSM



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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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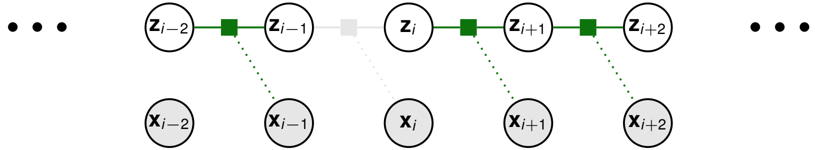

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Assume $\tilde{f}_i(\mathbf{z}_i, \mathbf{z}_{i-1})$ is Gaussian. Then,

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

with both α and β Gaussian.

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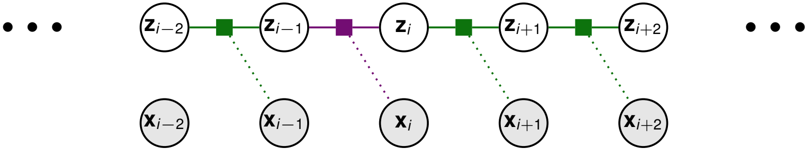

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with both α and β Gaussian.

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

NLSSM EP message updates

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

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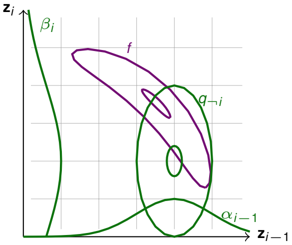

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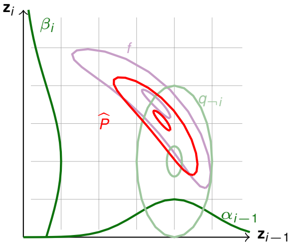

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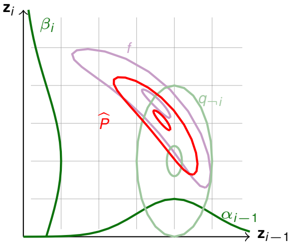

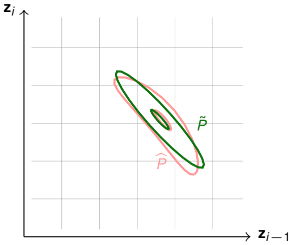

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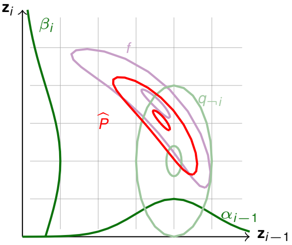

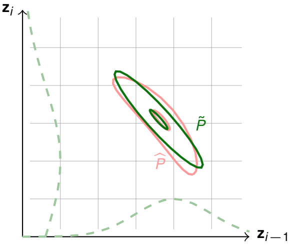

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$$\alpha_i(\mathbf{z}_i) = \int_{\mathbf{z}_1 \ldots \mathbf{z}_{i-1}} \prod_{i' < i+1} \tilde{f}_{i'}(\mathbf{z}_{i'}, \mathbf{z}_{i'-1}) = \int_{\mathbf{z}_{i-1}} \alpha_{i-1}(\mathbf{z}_{i-1}) \tilde{f}_i(\mathbf{z}_i, \mathbf{z}_{i-1}) = \frac{1}{\beta_i(\mathbf{z}_i)}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

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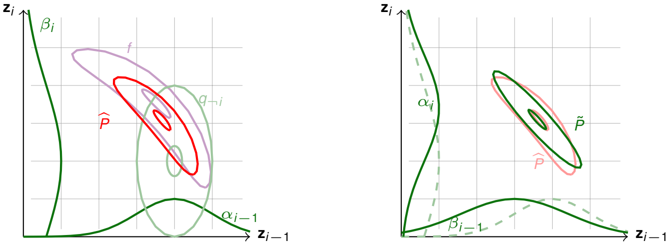

Moment Matching

Each EP update involves a KL minimisation:

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

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

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

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

Numerical issues

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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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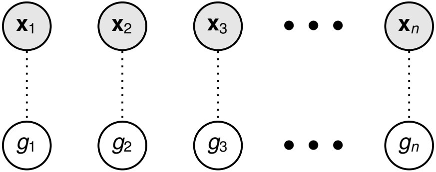

Recall:

- 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" $\mathbf{x}_i$.

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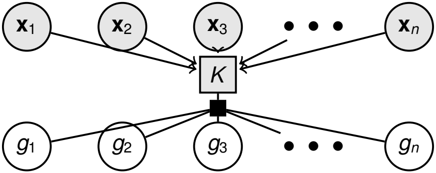

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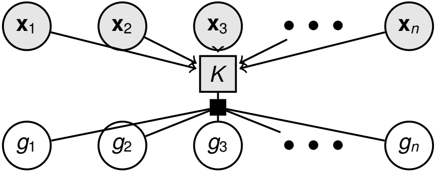
EP for Gaussian process classification

EP provides a succesful framework for Gaussian-process modelling of non-Gaussian observations (*e.g.* for classification).



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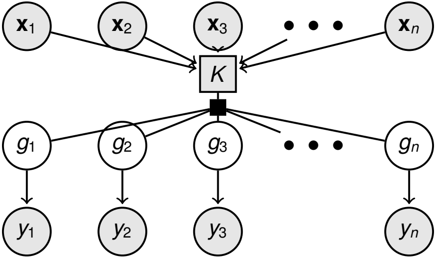

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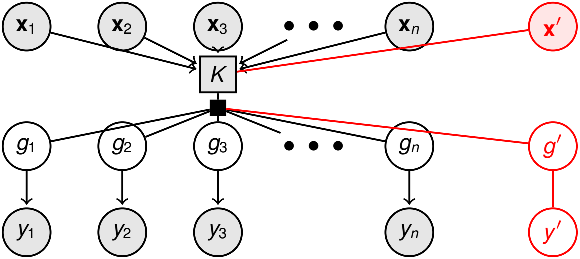

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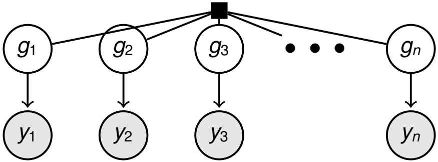

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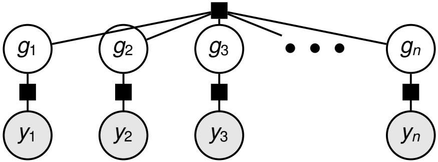

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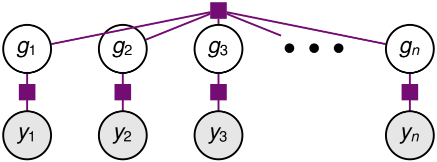

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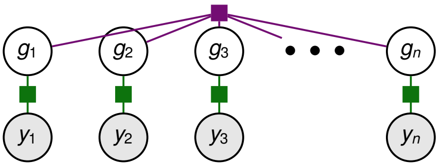

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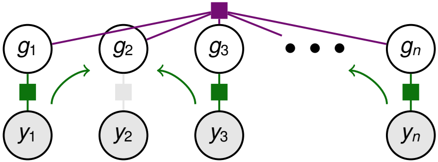

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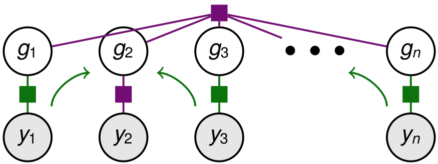

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- The EP updates thus require calculating Gaussian expectations of $f_i(g)g^{\{1,2\}}$:

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

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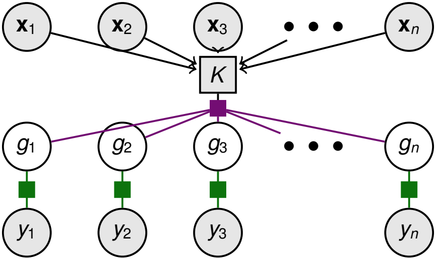

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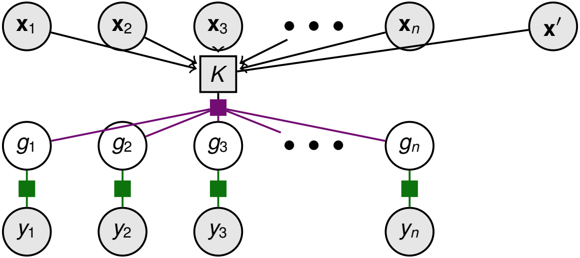

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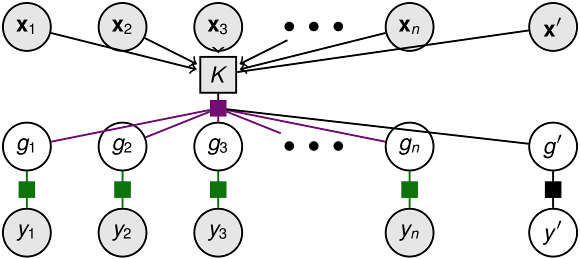

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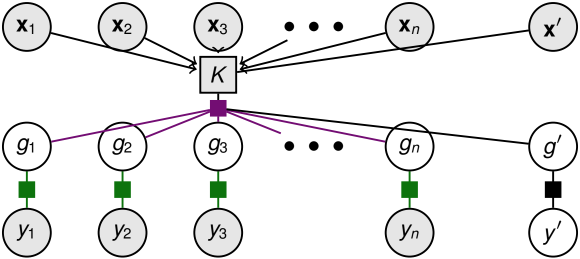

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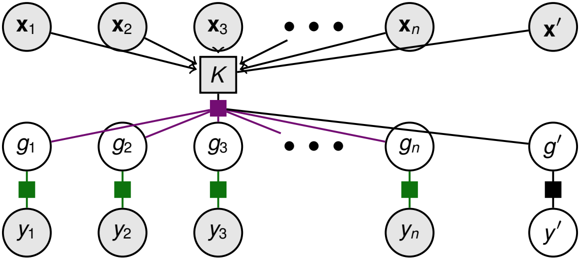

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- Predictions are obtained by marginalising the approximation: [let $\tilde{\Psi} = \text{diag}[\tilde{\psi}_1^2 \dots \tilde{\psi}_n^2]$]

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

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