Probabilistic & Unsupervised Learning

Expectation Propagation

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Term 1, Autumn 2014

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 methods
- Learning – intractable partition function
  - Constrastive divergence
  - Sampling parameters
  - Score-matching
- Model selection
  - Laplace approximation / BIC
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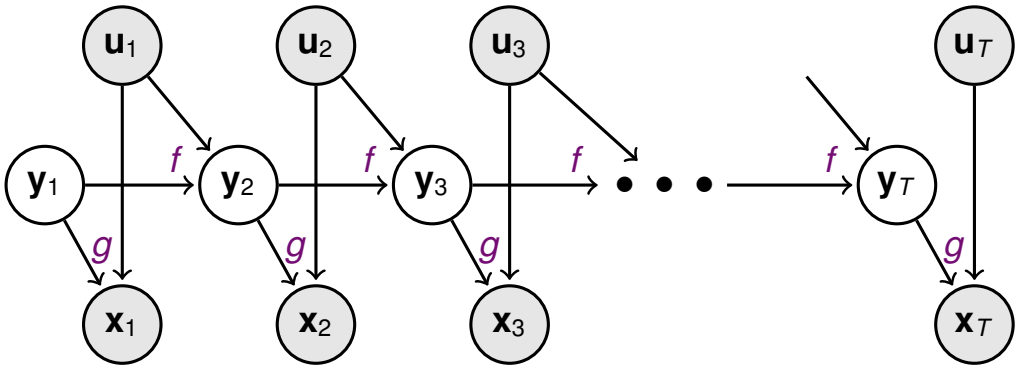
Nonlinear state-space model (NLSSM)



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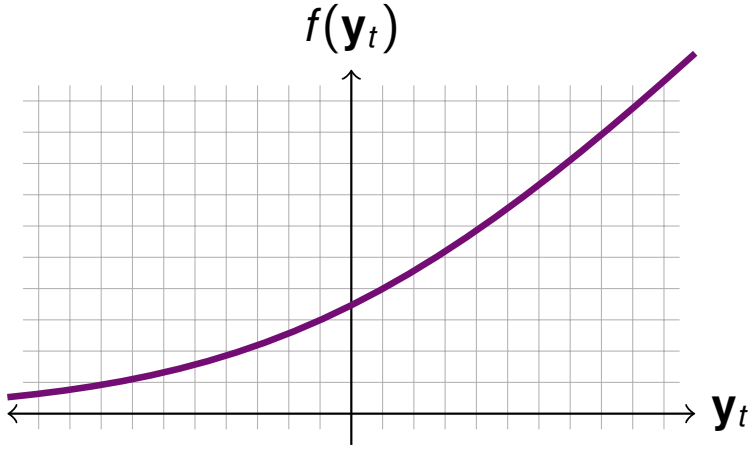
$\mathbf{w}_t, \mathbf{v}_t$ usually still Gaussian.



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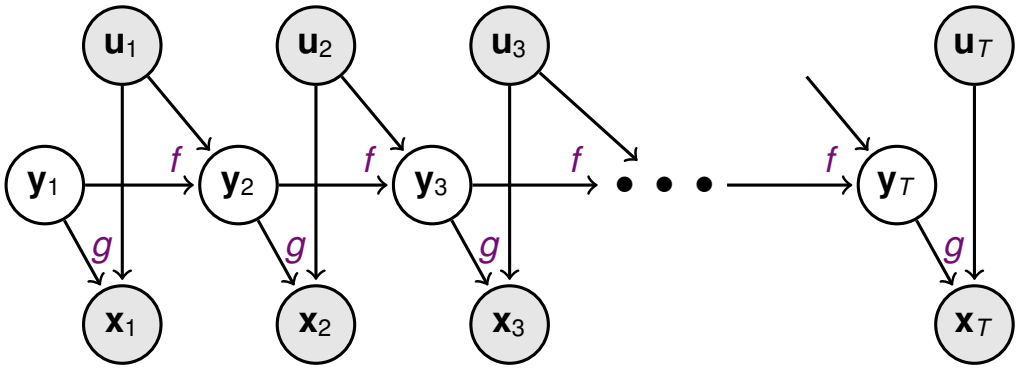

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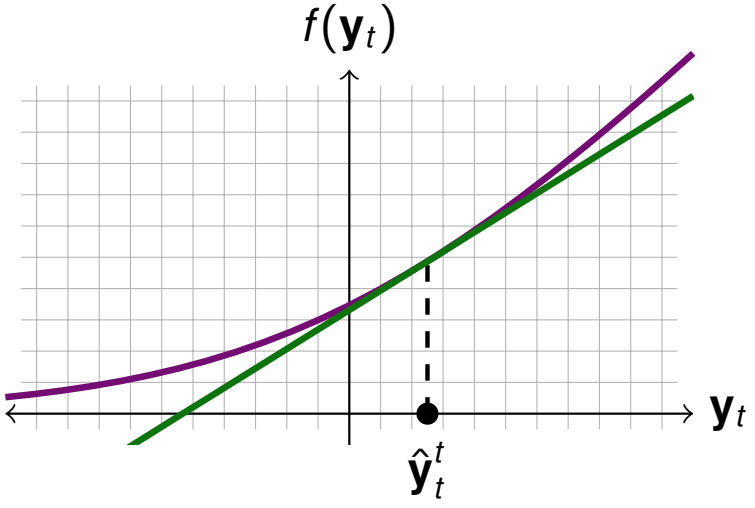

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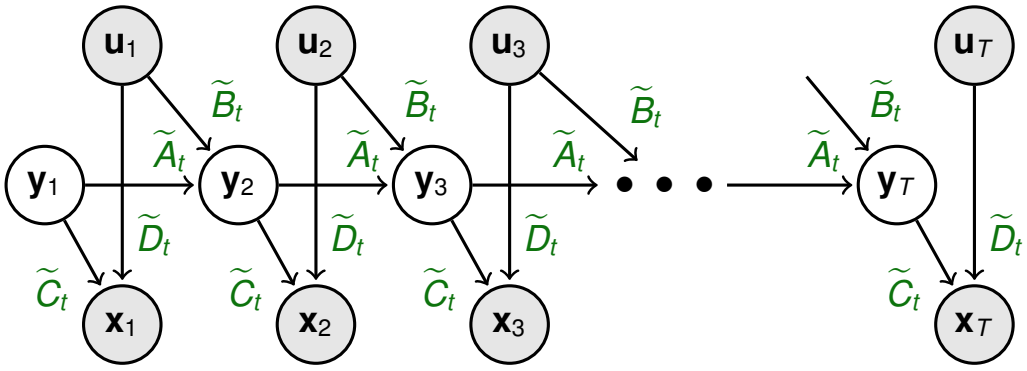

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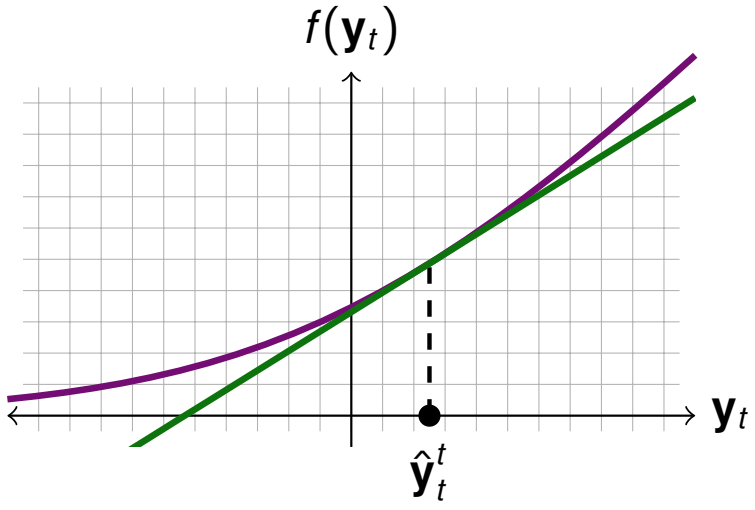

Run the Kalman filter (smoother) on non-stationary linearised system ($\widetilde{A}_t, \widetilde{B}_t, \widetilde{C}_t, \widetilde{D}_t$):

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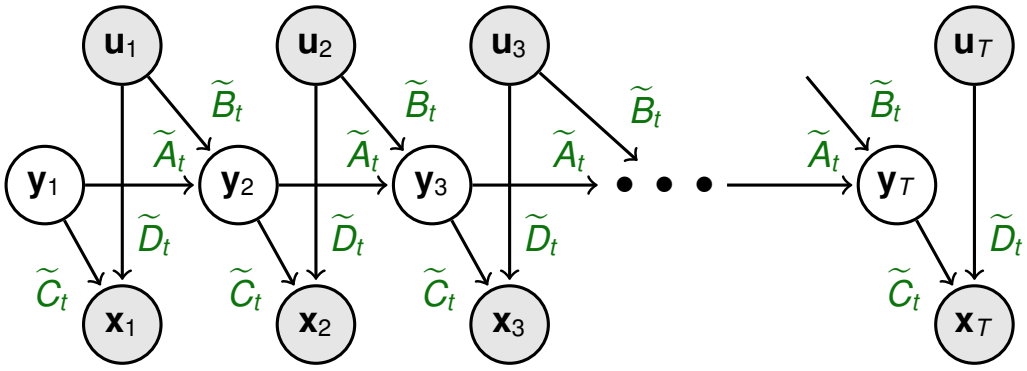

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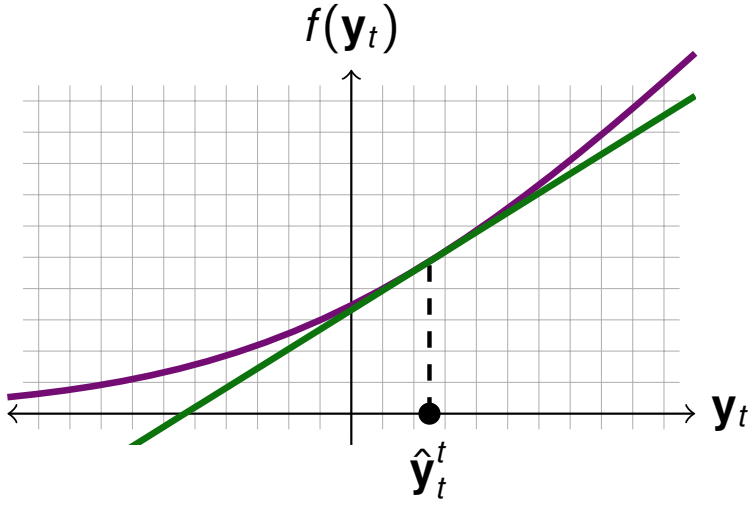

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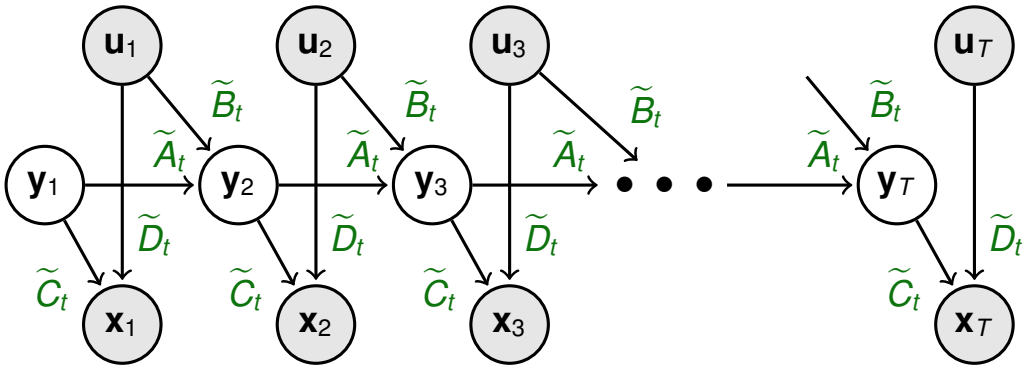

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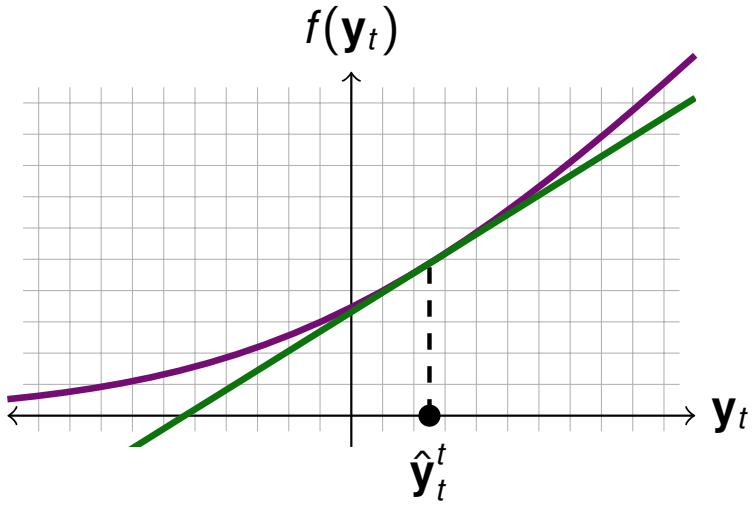

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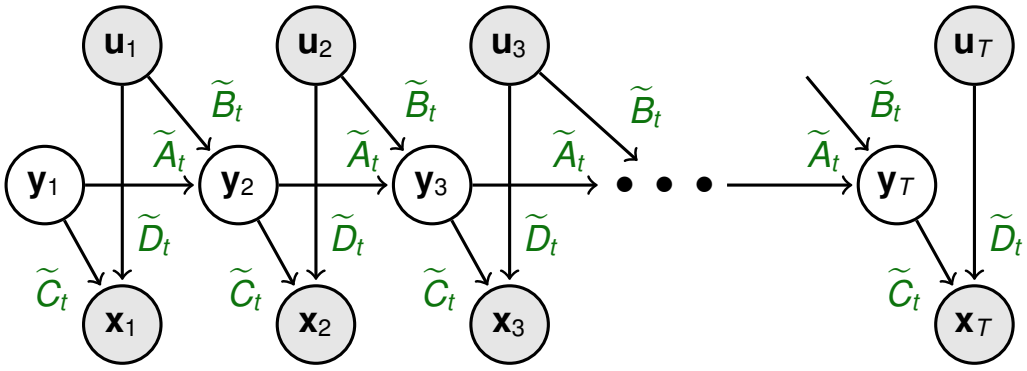

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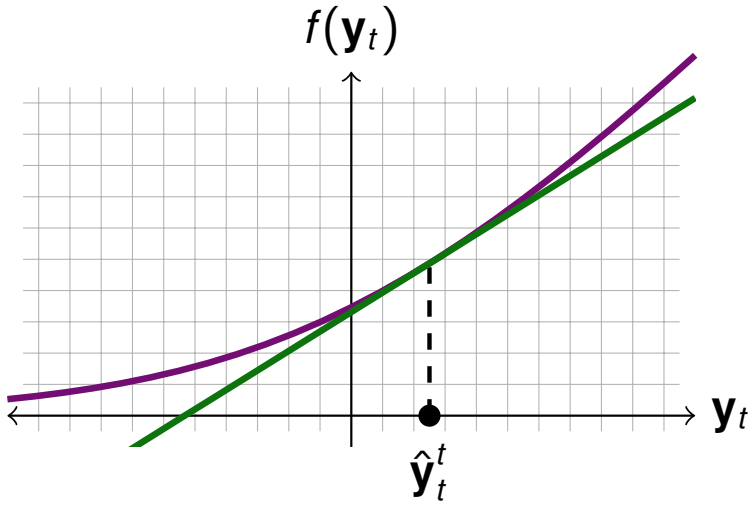

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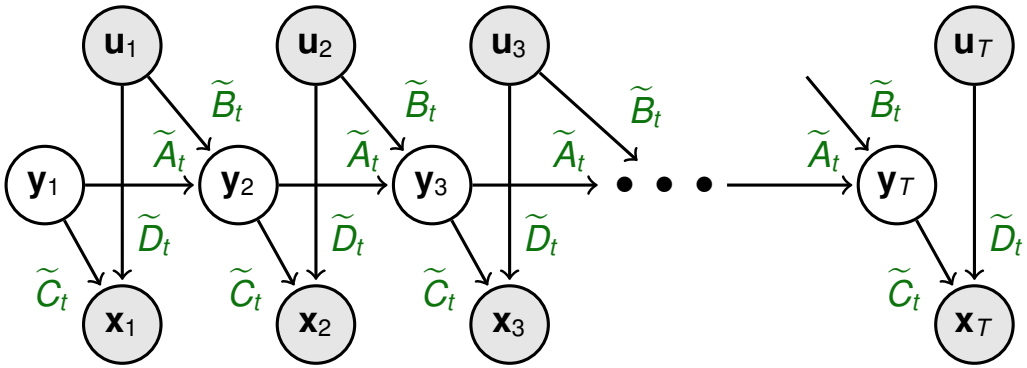

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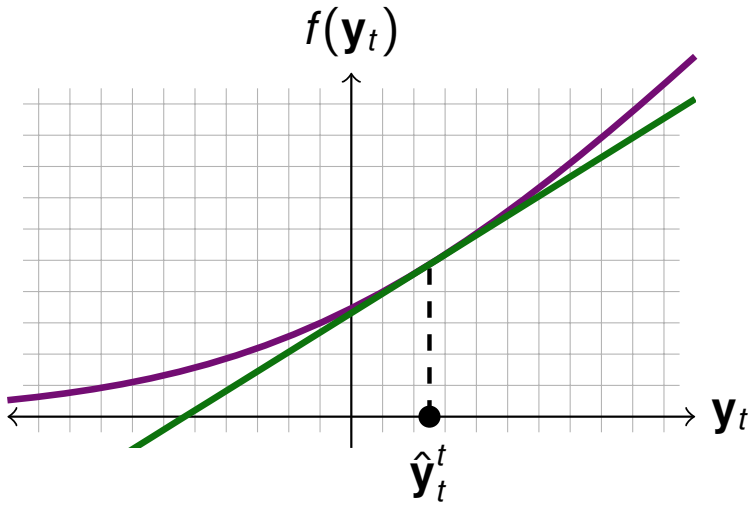

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Can base EM-like algorithm on EKF/EKS (or alternatives).

Other message approximations

Consider the forward messages on a latent chain:

$$P(y_t|x_{1:t}) = \frac{1}{Z} P(x_t|y_t) \int dy_{t-1}\; P(y_t|y_{t-1}) P(y_{t-1}|x_{1:t-1})$$

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

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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: argmin $\mathbf{KL}\left[\mathcal{N}\left(\hat{\mathbf{y}}_t, \hat{V}_t\right) \middle\| \int dy_{t-1} \ldots\right]$. Requires Gaussian expectations of log $\int \Rightarrow$ may be challenging.

Other message approximations

Consider the forward messages on a latent chain:

$$P(y_t|x_{1:t}) = \frac{1}{Z} P(x_t|y_t) \int dy_{t-1}\; P(y_t|y_{t-1}) P(y_{t-1}|x_{1:t-1})$$

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

$$\tilde{P}(y_t|x_{1:t}) \approx \frac{1}{Z} P(x_t|y_t) \int dy_{t-1} \quad \underbrace{P(y_t|y_{t-1})}_{\mathcal{N}\left(f(\mathbf{y}_{t-1}), Q\right)} \quad \underbrace{\tilde{P}(y_{t-1}|x_{1:t-1})}_{\mathcal{N}\left(\hat{\mathbf{y}}_{t-1}, V_{t-1}\right)}$$

- Linearisation at the peak (EKF) is only one approach.
- Laplace filter: use mode and curvature of integrand.
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- The other KL: argmin $\mathbf{KL}\left[\int dy_{t-1} \left\|\mathcal{N}\left(\hat{\mathbf{y}}_t, \hat{V}_t\right)\right.\right]$ needs only first and second moments of nonlinear message $\Rightarrow$ EP.

Variational learning

Free energy:

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

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  - Usually no guarantees, but if learning converges if is frequently more accurate than the factored approximation

Approximating the posterior

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- Can we use other divergences?

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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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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:

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

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Consider q with the same factorisation, but potentially approximated sites: $q(\mathcal{Y}) \stackrel{\mathrm{def}}{=} \prod_{i=1}^{N} \tilde{f}_i(\mathcal{Y}_i)$.

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- Approximation of factors.
  - Usually by “projection” to exponential families.
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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:

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

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

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

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

Expectation Propagation (EP)

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

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

repeat

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

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

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

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

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:

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

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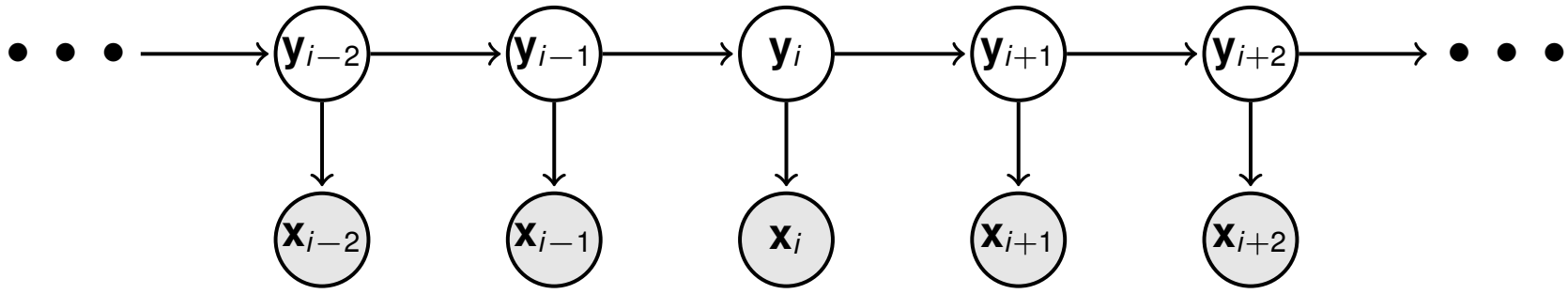
- For some approximations (e.g. Gaussian) may be able to compute true loopy cavity using approximate sites, even if computing exact message would have been intractable.
- In either case, message updates can be scheduled in any order.
- No guarantee of convergence (but see “power-EP” methods).

EP for a NLSSM



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

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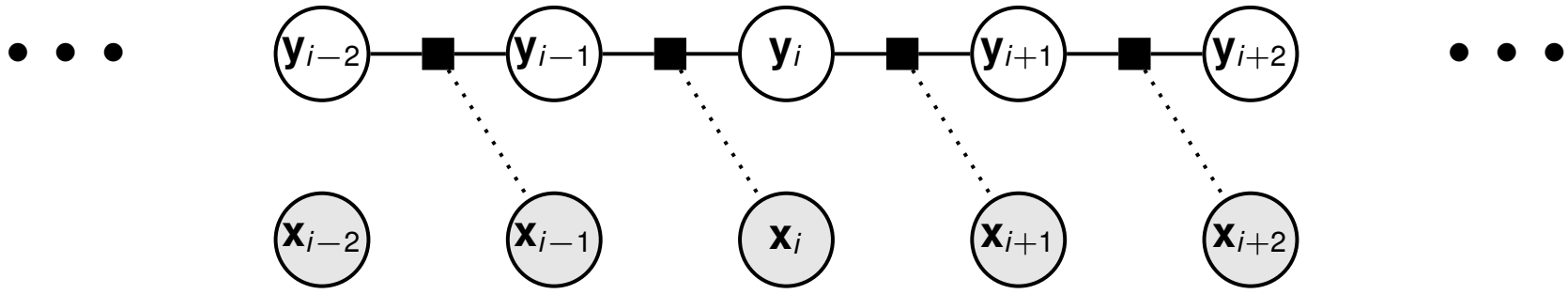

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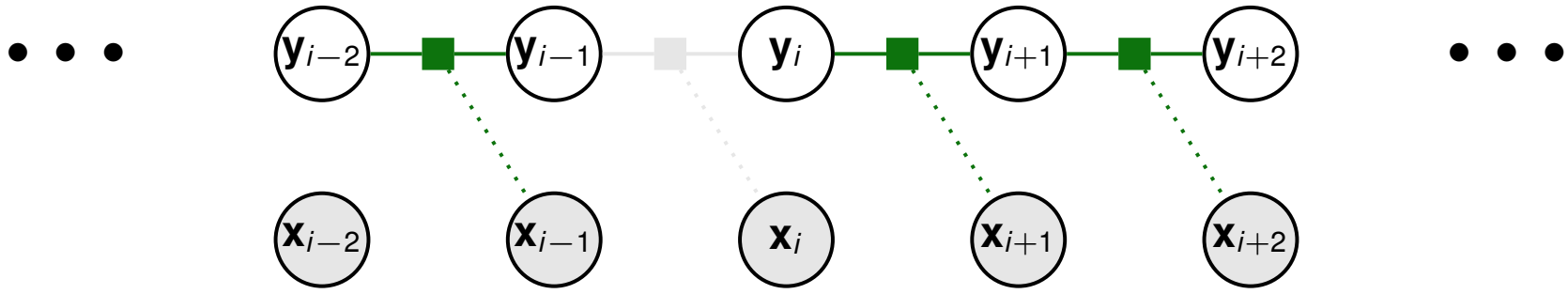

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with both α and β Gaussian.

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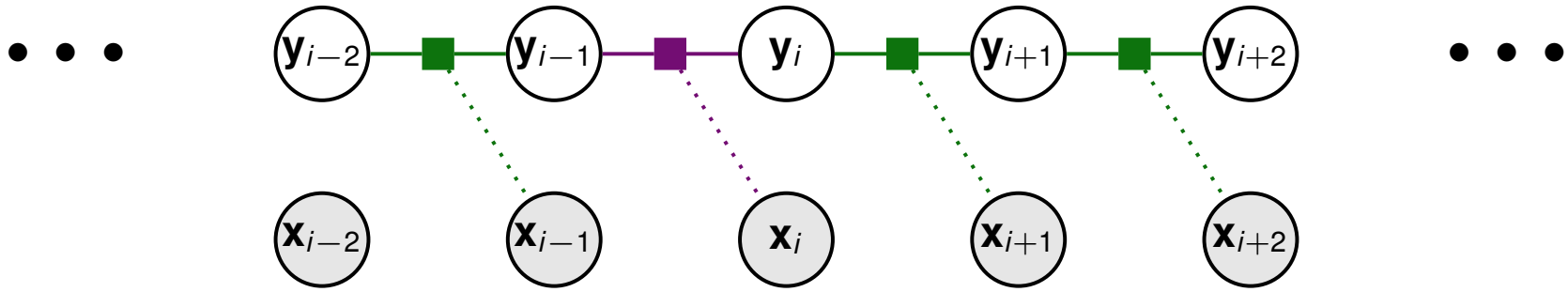

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NLSSM EP message updates

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

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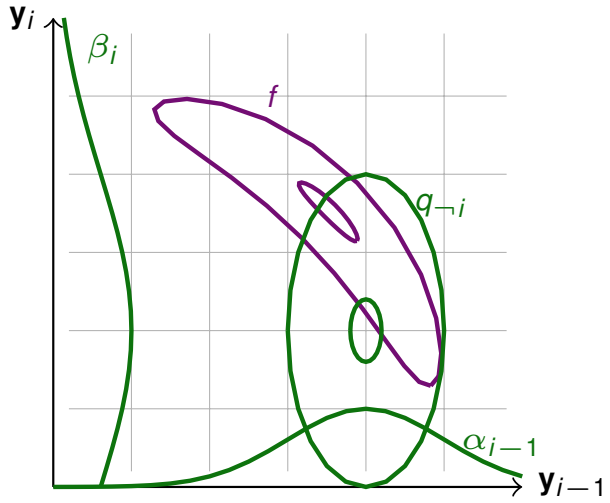

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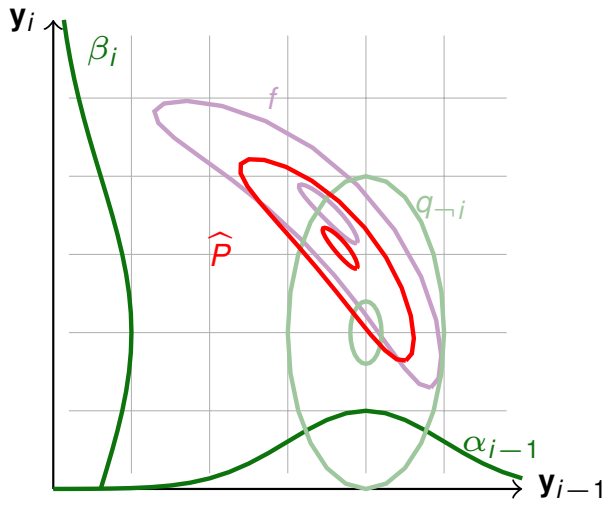

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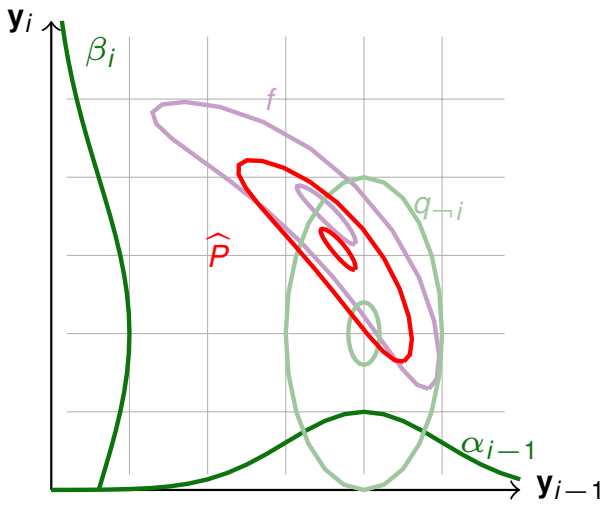

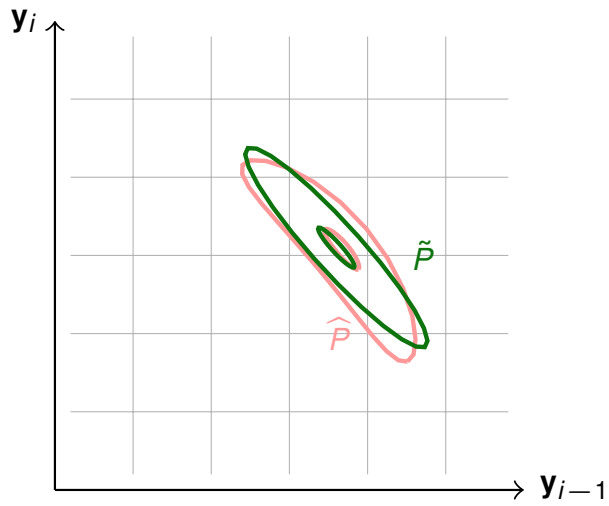

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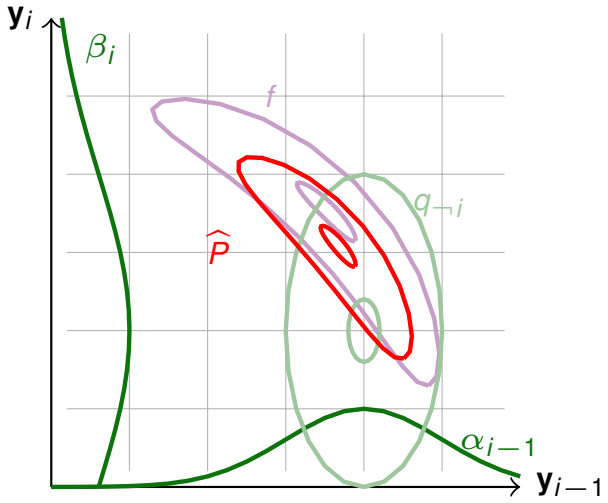

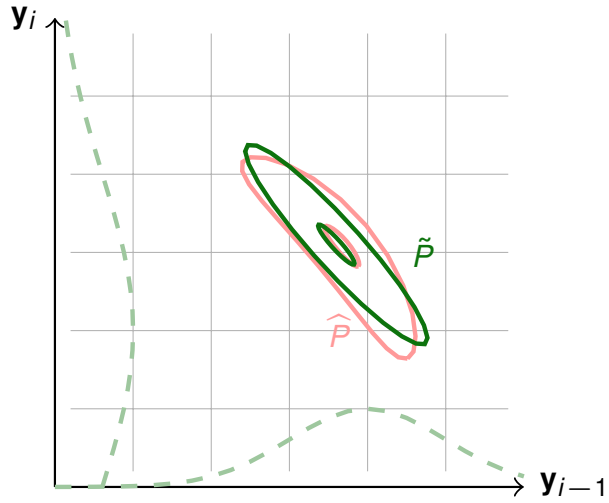

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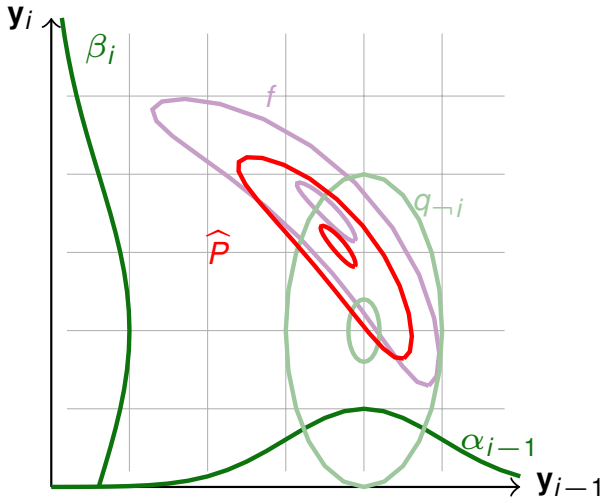

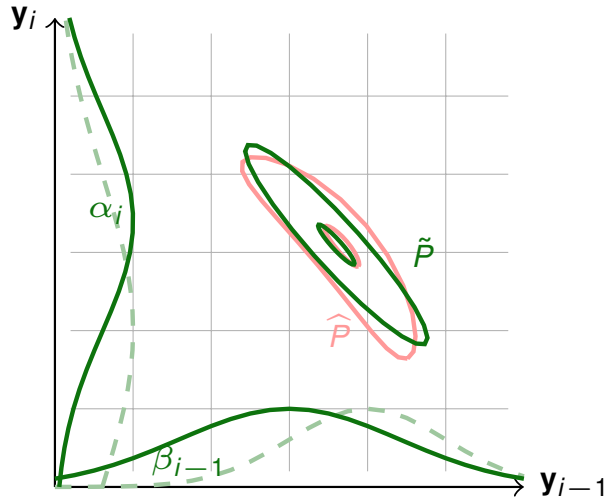

Moment Matching

Each EP update involves a KL minimisation:

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

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

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

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

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- Laplace approximation.
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  - As long as messages remain positive definite will converge to global Laplace approximation.

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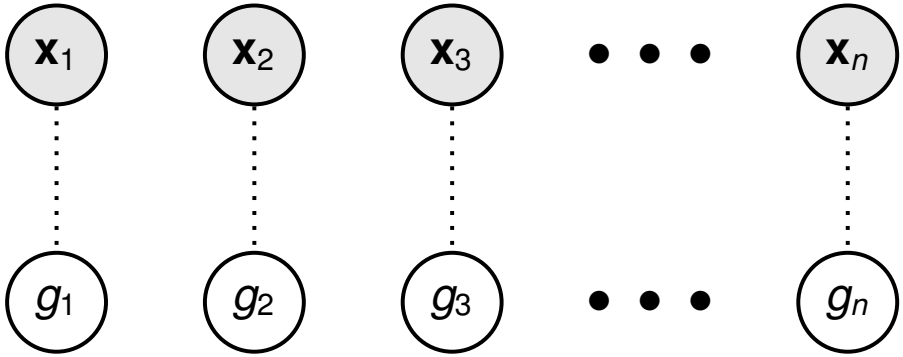

Recall:

- 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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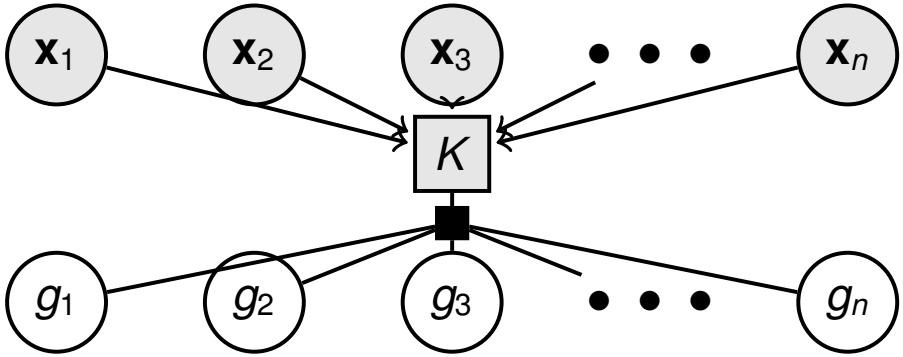

Recall:

- 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" $\mathbf{x}_i$.
- The Gaussian parameters depend on the inputs: $(\boldsymbol{\mu} = [\mu(\mathbf{x}_i)],\ \Sigma = [K(\mathbf{x}_i, \mathbf{x}_j)])$.

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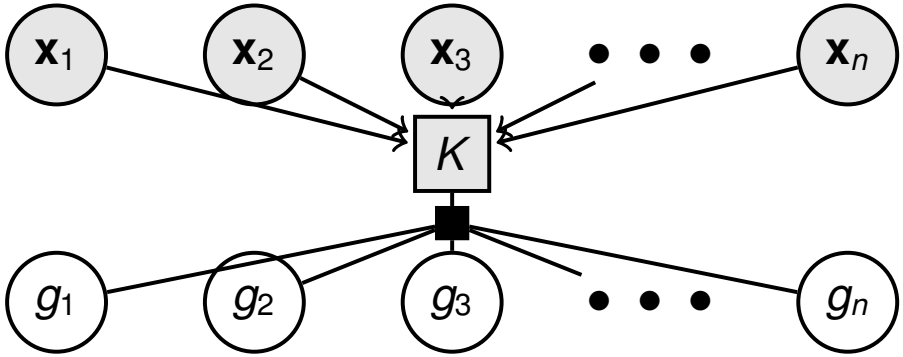

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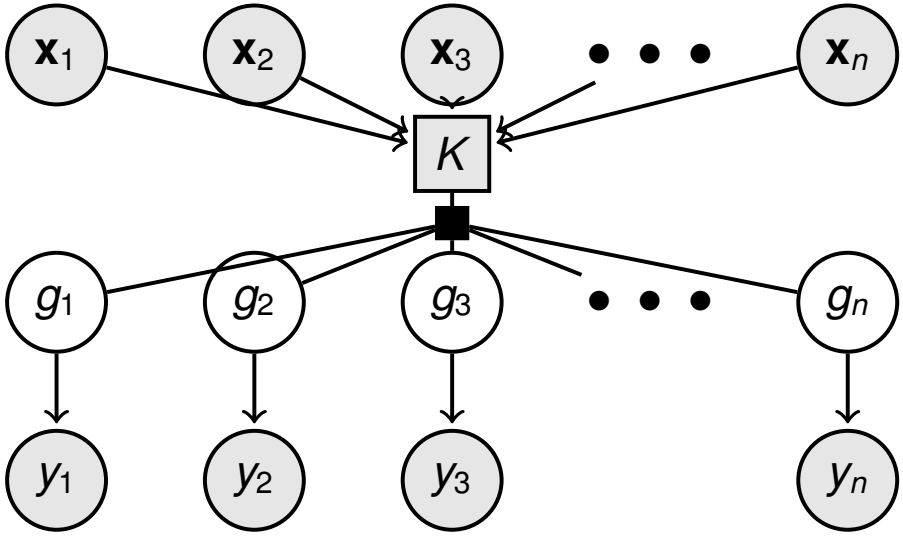

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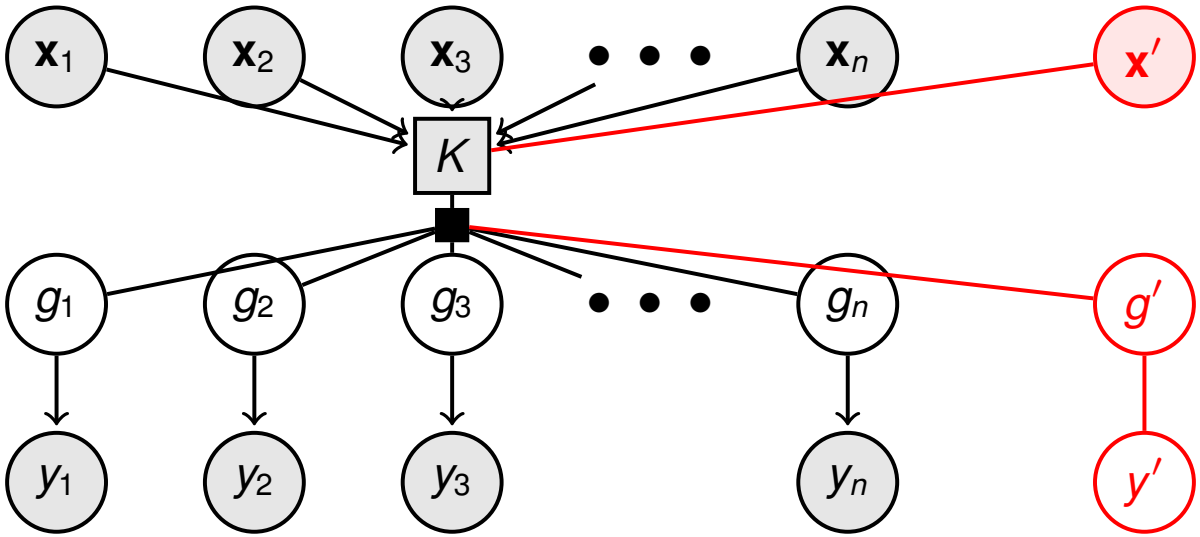

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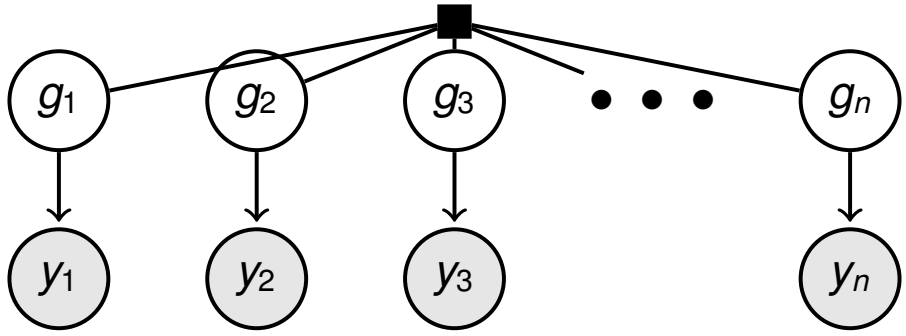
- In a GP regression model, noisy observations y_i are conditionally independent given g_i.
- No parameters to learn (though often hyperparameters); instead, we make predictions on test data directly: [assuming $\mu = 0$, and matrix Σ incorporates diagonal noise]

$$P(y'|\mathbf{x}', \mathcal{D}) = \mathcal{N}\left(\Sigma_{x',X}\Sigma_{X,X}^{-1}\mathbf{y},\ \Sigma_{x',x'} - \Sigma_{x',X}\Sigma_{X,X}^{-1}\Sigma_{X,x'}\right)$$

GP EP updates



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

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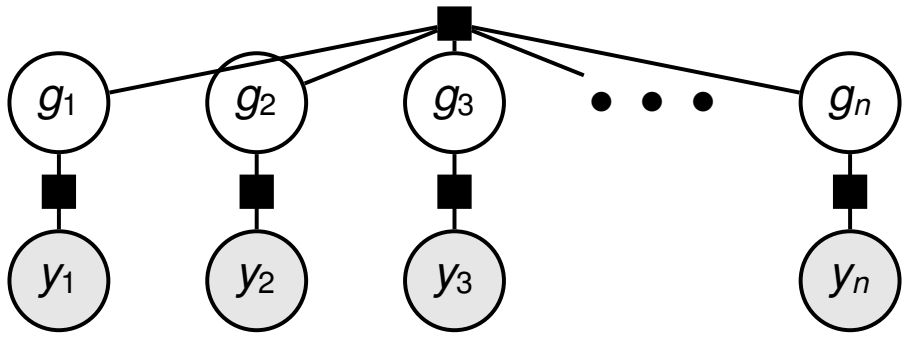

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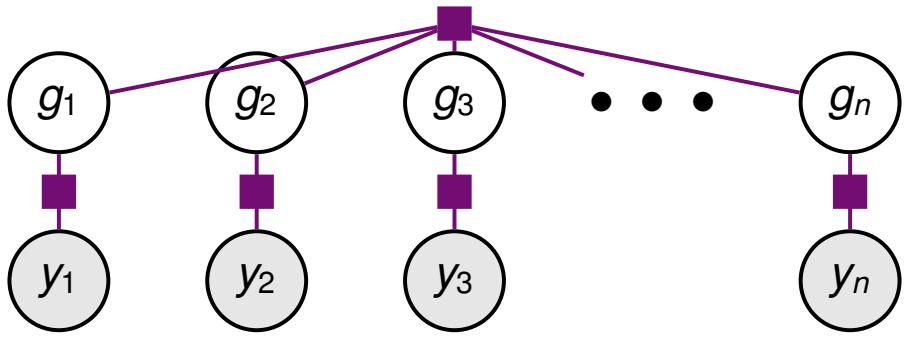

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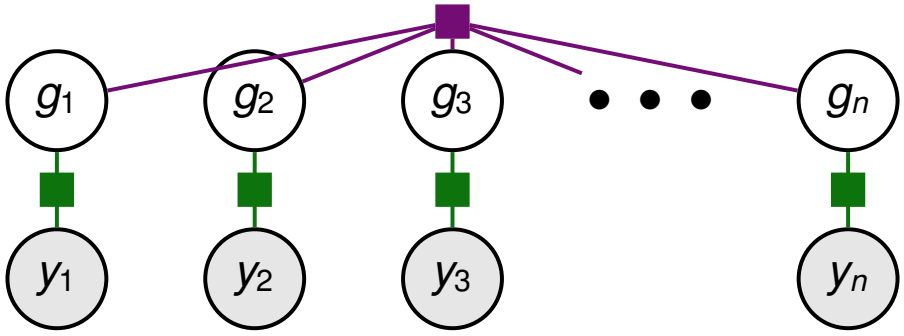

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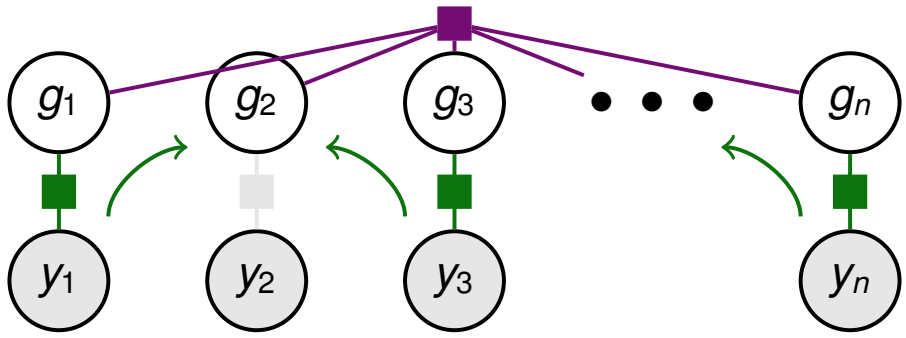

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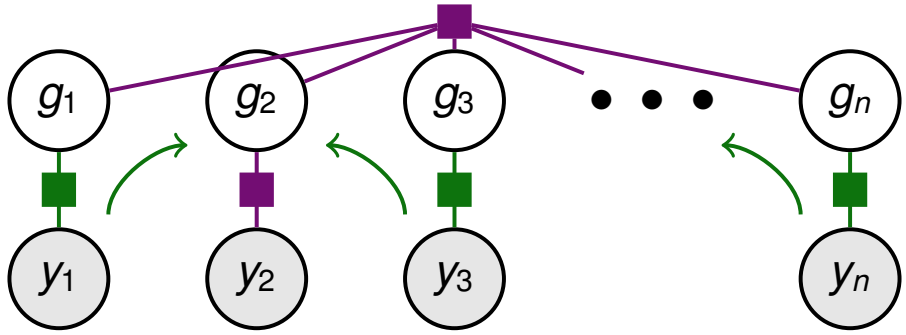

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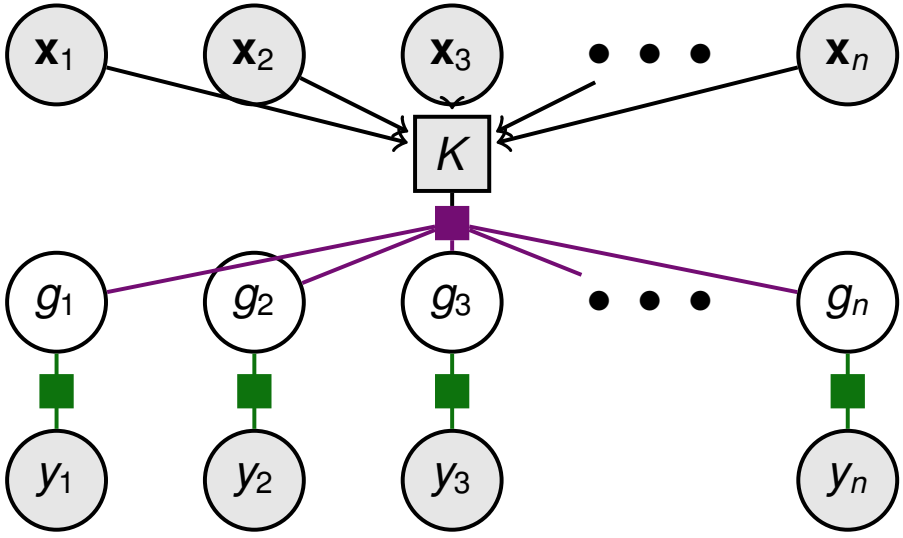
- The EP updates thus require calculating Gaussian expectations of $f_i(g)g^{\{1,2\}}$:

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

EP GP prediction



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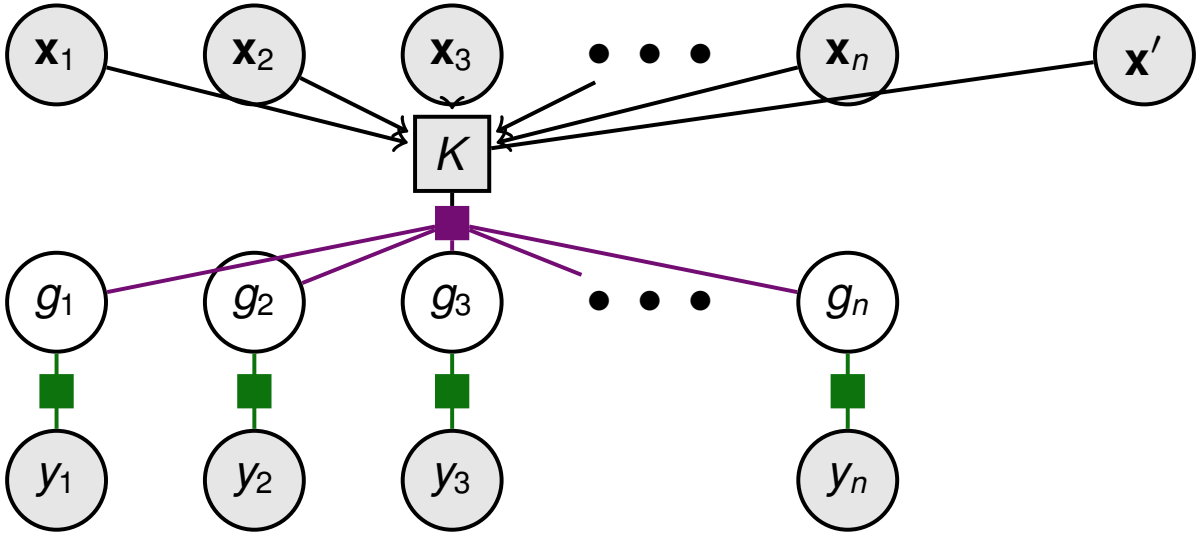

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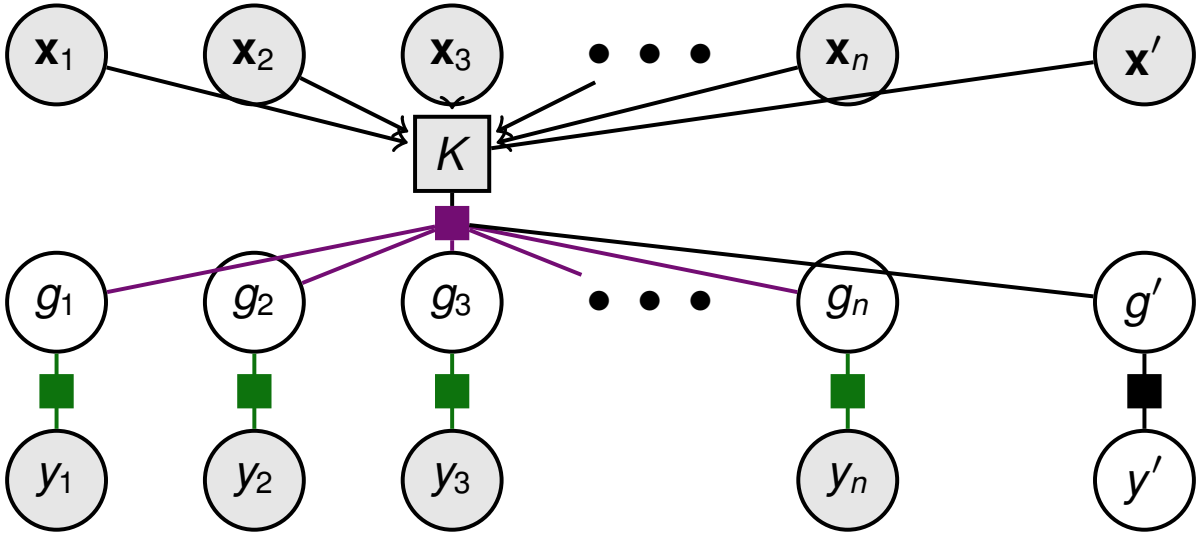

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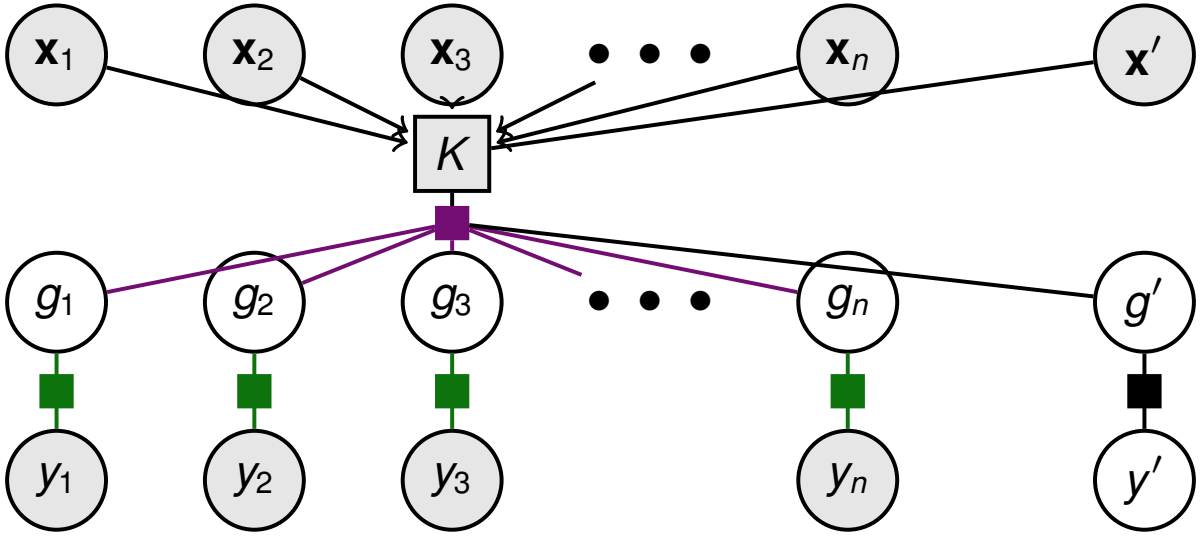

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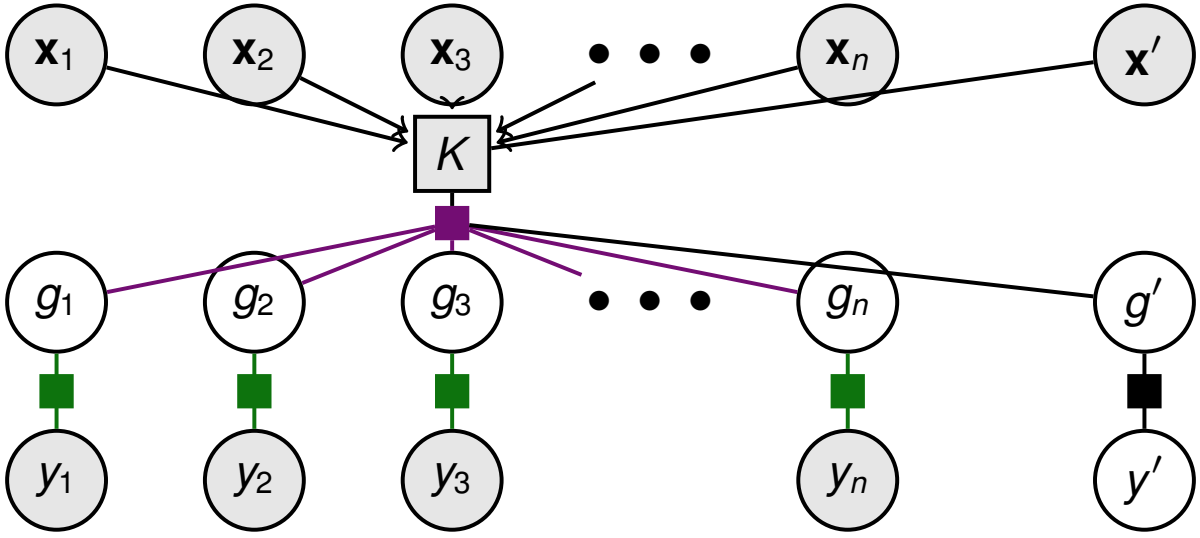

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- Thus no change is needed to the approximating potentials $\tilde{f}_i$.
- Predictions are obtained by marginalising the approximation: [let $\tilde{\Psi} = \text{diag}[\tilde{\psi}_1^2 \ldots \tilde{\psi}_n^2]$]

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

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  as well as the overall normaliser of $\prod_i \tilde{f}_i(\mathcal{Y}_i)$.

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

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