

Probabilistic & Unsupervised Learning

Expectation Propagation

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MSc ML/CSML, Dept Computer Science
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Term 1, Autumn 2015

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
 - ▶ Contrastive divergence
 - ▶ Sampling parameters
 - ▶ Score-matching
- ▶ Model selection
 - ▶ Laplace approximation / BIC
 - ▶ Variational Bayes
 - ▶ (Annealed) importance sampling
 - ▶ Reversible jump MCMC

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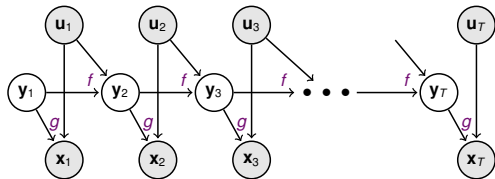
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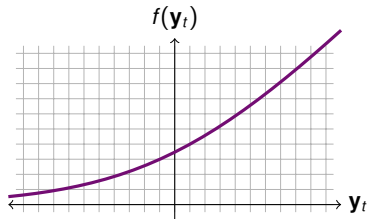
Nonlinear state-space model (NLSSM)



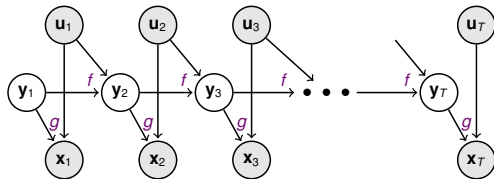
$$\mathbf{y}_{t+1} = f(\mathbf{y}_t, \mathbf{u}_t) + \mathbf{w}_t$$

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

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



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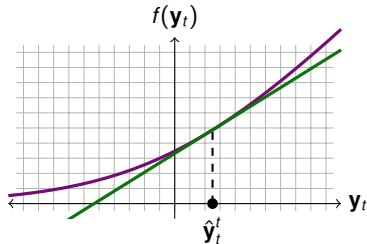
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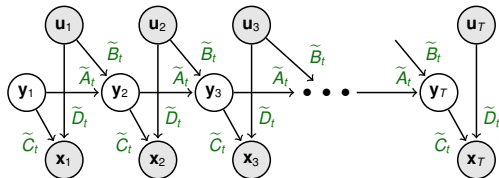
Extended Kalman Filter (EKF): linearise nonlinear functions about current estimate, $\hat{\mathbf{y}}_t^t$:

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

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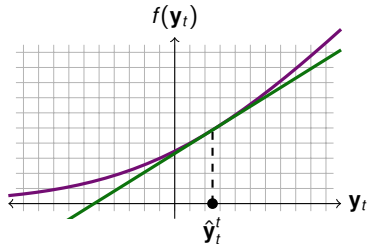
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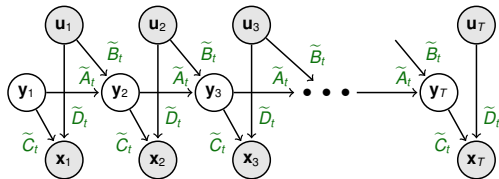
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Run the Kalman filter (smoother) on non-stationary linearised system ($\tilde{\mathbf{A}}_t, \tilde{\mathbf{B}}_t, \tilde{\mathbf{C}}_t, \tilde{\mathbf{D}}_t$):

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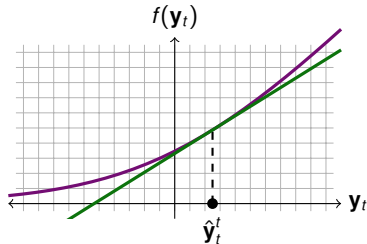
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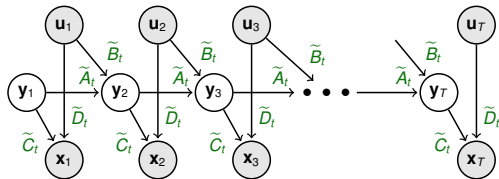
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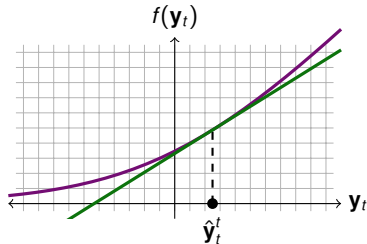
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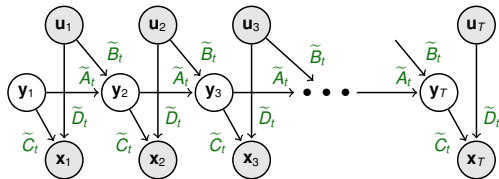
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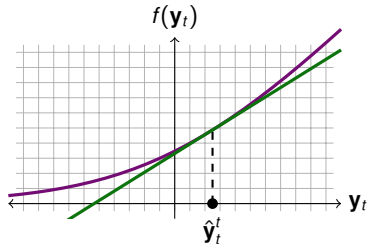
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Can base EM-like algorithm on EKF/EKS (or alternatives).

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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- ▶ The other KL: $\text{argmin}_{\mathbf{KL}} [\int dy_{t-1} \parallel \mathcal{N}(\hat{\mathbf{y}}_t, \hat{V}_t)]$ 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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- ▶ Exact EM: $q(\mathcal{Y}) = \operatorname{argmax}_q \mathcal{F} = P(\mathcal{Y} | \mathcal{X}, \theta)$

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Free energy:

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- ▶ Other approximations: $q(\mathcal{Y}) \approx P(\mathcal{Y} | \mathcal{X}, \theta)$
 - ▶ Usually no guarantees, but if learning converges it is frequently more accurate than the factored approximation

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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:

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

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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:

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

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

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

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

Expectation Propagation (EP)

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

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

repeat

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

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

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

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

end for

until convergence

Message Passing

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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.

Message Passing

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

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

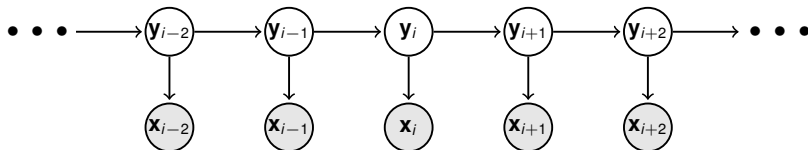
- ▶ Once the i th site has been approximated, the messages can be passed on to neighbouring cliques by marginalising to the shared variables (SSM example follows).
 \Rightarrow belief propagation.
- ▶ In loopy graphs, we can use loopy belief propagation. In that case

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

becomes an approximation to the **true** cavity distribution (or we can recast the approximation directly in terms of messages \Rightarrow later lecture).

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

EP for a NLSSM



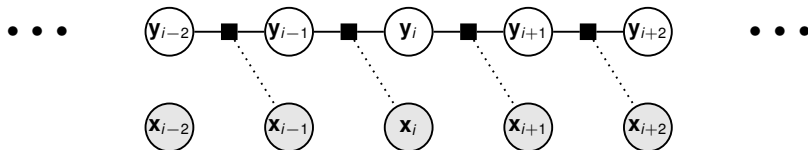
$$P(\mathbf{y}_i | \mathbf{y}_{i-1}) = \phi_i(\mathbf{y}_i, \mathbf{y}_{i-1})$$

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

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

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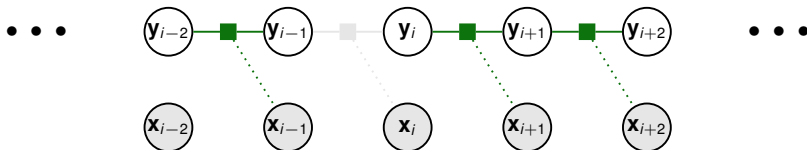
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Then $f_i(\mathbf{y}_i, \mathbf{y}_{i-1}) = \phi_i(\mathbf{y}_i, \mathbf{y}_{i-1})\psi_i(\mathbf{y}_i)$. As ϕ_i and ψ_i are non-linear, inference is not generally tractable.

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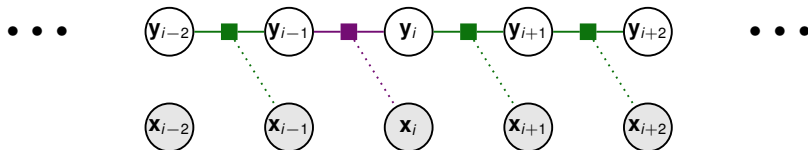
Then $f_i(\mathbf{y}_i, \mathbf{y}_{i-1}) = \phi_i(\mathbf{y}_i, \mathbf{y}_{i-1})\psi_i(\mathbf{y}_i)$. As ϕ_i and ψ_i are non-linear, inference is not generally tractable.

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

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

with both α and β Gaussian.

EP for a NLSSM



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

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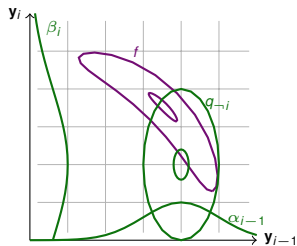
$$\tilde{f}_i(\mathbf{y}_i, \mathbf{y}_{i-1}) = \operatorname{argmin}_{f \in \mathcal{N}} \mathbf{KL}[\phi_i(\mathbf{y}_i, \mathbf{y}_{i-1})\psi_i(\mathbf{y}_i)\alpha_{i-1}(\mathbf{y}_{i-1})\beta_i(\mathbf{y}_i) \| f(\mathbf{y}_i, \mathbf{y}_{i-1})\alpha_{i-1}(\mathbf{y}_{i-1})\beta_i(\mathbf{y}_i)]$$

NLSSM EP message updates

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

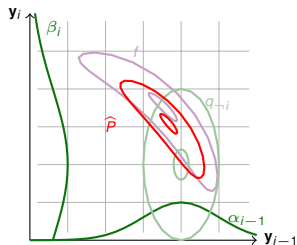
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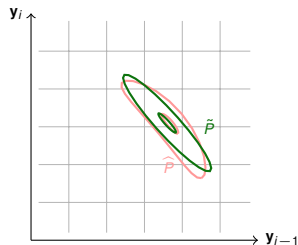
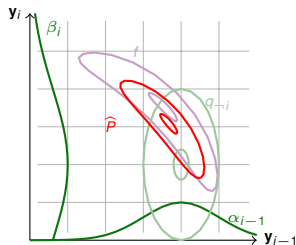
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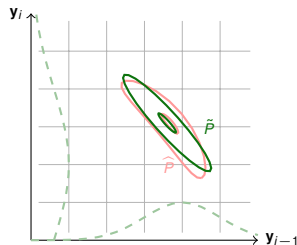
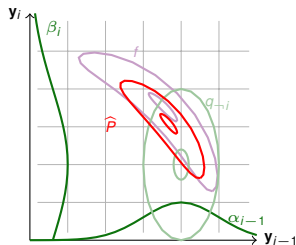
$$\tilde{P}(\mathbf{y}_{i-1}, \mathbf{y}_i) = \operatorname{argmin}_{P \in \mathcal{N}} [\hat{P}(\mathbf{y}_{i-1}, \mathbf{y}_i) \parallel P(\mathbf{y}_{i-1}, \mathbf{y}_i)]$$



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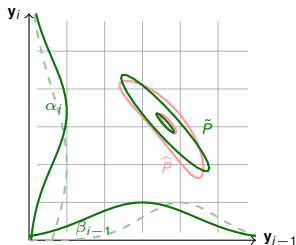
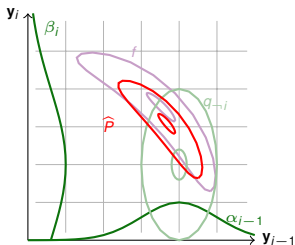
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Moment Matching

Each EP update involves a KL minimisation:

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

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

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

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

Numerical issues

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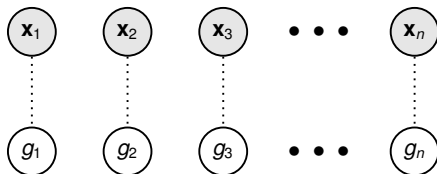
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- ▶ Laplace approximation.
 - ▶ Equivalent to Laplace propagation.
 - ▶ As long as messages remain positive definite will converge to global Laplace approximation.

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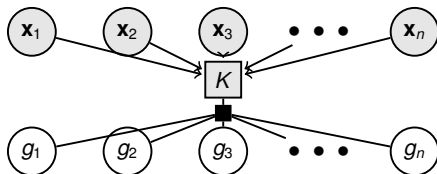


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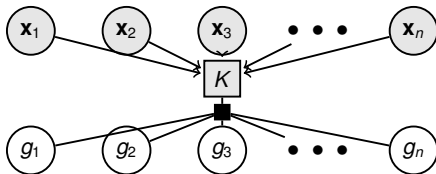


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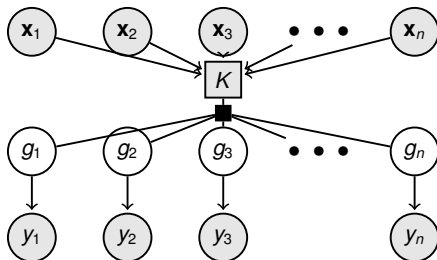


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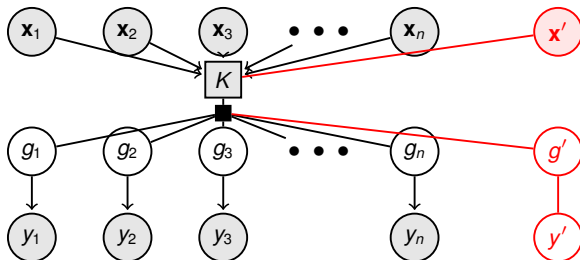


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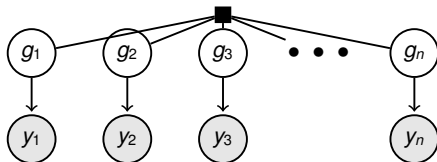


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- ▶ If we think of the g_s as function values, a GP provides a prior over functions.
- ▶ In a GP regression model, noisy observations y_i are conditionally independent given g_i .
- ▶ No parameters to learn (though often hyperparameters); instead,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

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

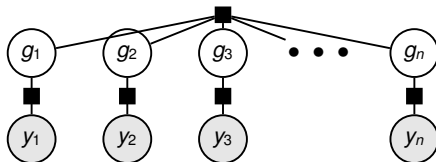
GP EP updates



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

$$P(g_1 \dots g_n, y_1, \dots y_n) = \mathcal{N}(g_1 \dots g_n | \mathbf{0}, K) \prod_i \mathcal{N}(y_i | g_i, \sigma_i^2)$$

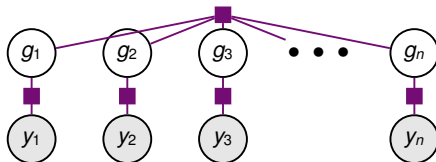
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GP EP updates

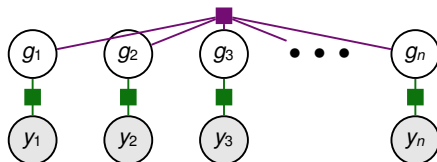


- ▶ We can write the GP joint on g_i and y_i as a factor graph:

$$P(g_1 \dots g_n, y_1, \dots y_n) = \underbrace{\mathcal{N}(g_1 \dots g_n | \mathbf{0}, K)}_{f_0(\mathcal{G})} \prod_i \underbrace{\mathcal{N}(y_i | g_i, \sigma_i^2)}_{f_i(g_i)}$$

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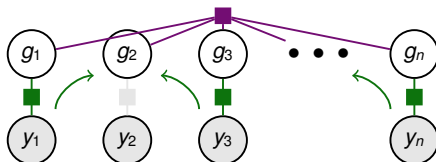


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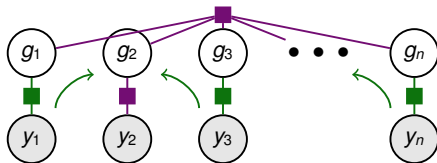
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- ▶ $q_{\neg i}(g_i)$ can be constructed by the usual GP marginalisation. If $\Sigma = K + \text{diag}[\tilde{\psi}_1^2 \dots \tilde{\psi}_n^2]$

$$q_{\neg i}(g_i) = \mathcal{N}(\Sigma_{i, \neg i} \Sigma_{\neg i, \neg i}^{-1} \tilde{\mu}_{\neg i}, K_{i,i} - \Sigma_{i, \neg i} \Sigma_{\neg i, \neg i}^{-1} \Sigma_{\neg i, i})$$

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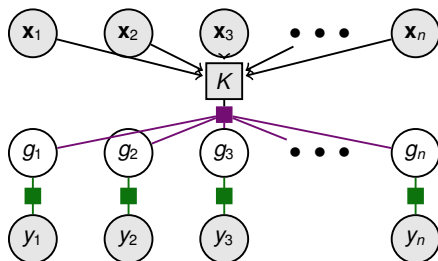
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- ▶ The EP updates thus require calculating Gaussian expectations of $f_i(g)g^{\{1,2\}}$:

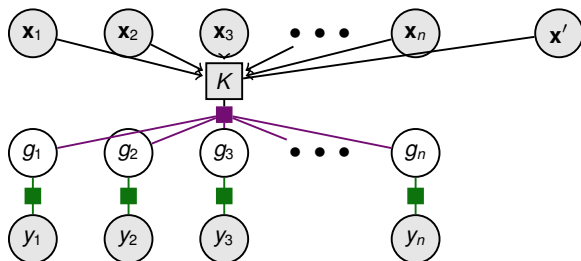
$$\tilde{f}_i^{\text{new}}(g_i) = \mathcal{N}\left(\int dg q_{-i}(g) f_i(g) g, \int dg q_{-i}(g) f_i(g) g^2 - (\tilde{\mu}_i^{\text{new}})^2\right) / q_{-i}(g_i)$$

EP GP prediction



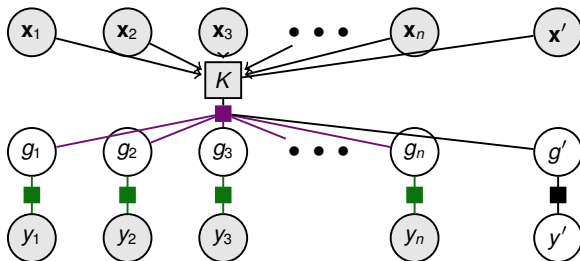
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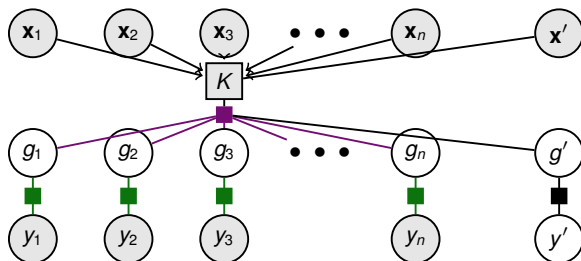
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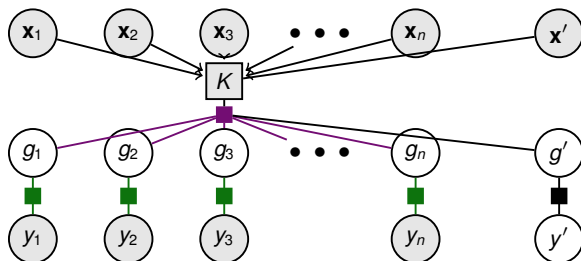
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- ▶ Thus no change is needed to the approximating potentials \tilde{f}_i .
- ▶ Predictions are obtained by marginalising the approximation: [let $\tilde{\Psi} = \text{diag}[\tilde{\psi}_1^2 \dots \tilde{\psi}_n^2]$]

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

$$K_{x',x'} - K_{x',x} (K_{x,x} + \tilde{\Psi})^{-1} K_{x,x'})$$

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

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.