Probabilistic & Unsupervised Learning

Expectation Propagation

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University College London

Term 1, Autumn 2016

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
- Learning – intractable partition function
  - Constrastive divergence
  - Sampling parameters
  - Score-matching
- Posterior estimation and model selection
  - Laplace approximation / BIC
  - Variational Bayes
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  - (Annealed) importance sampling
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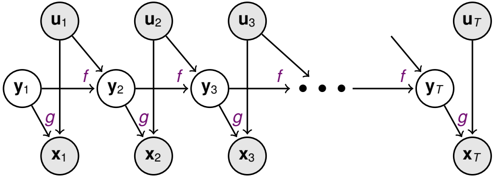
Nonlinear state-space model (NLSSM)



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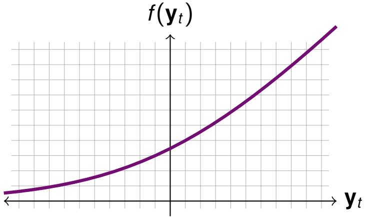
$\mathbf{w}_t, \mathbf{v}_t$ usually still Gaussian.



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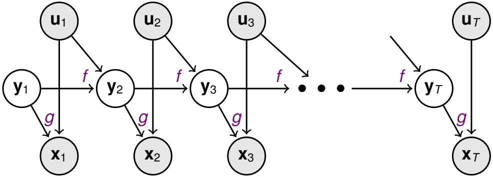

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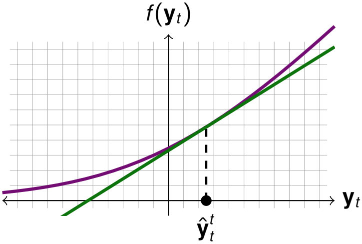

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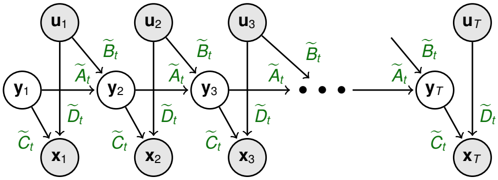

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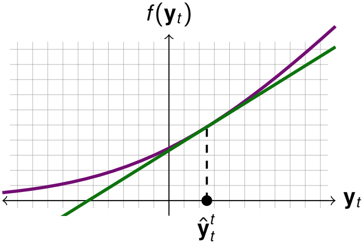

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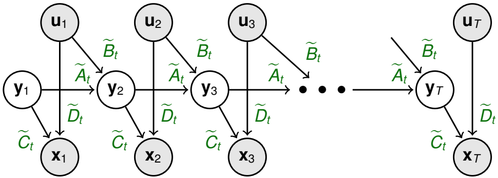

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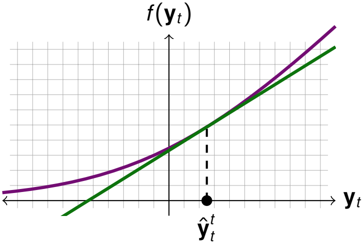

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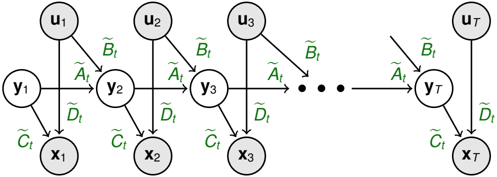

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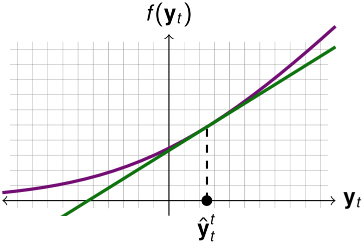

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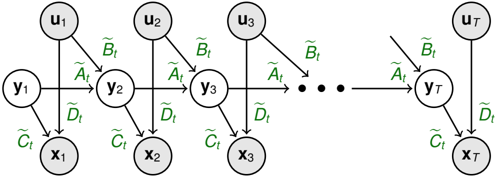

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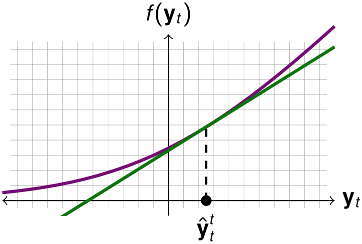

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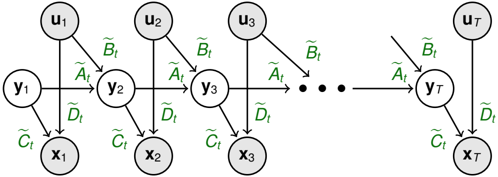

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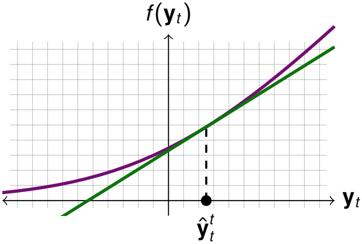

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Can base EM-like algorithm on EKF/EKS (or alternatives).

Other message approximations

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

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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.
- Sigma-point ("unscented") filter:
  - Evaluate $f(\hat{\mathbf{y}}_{t-1})$, $f(\hat{\mathbf{y}}_{t-1} \pm \sqrt{\lambda}\mathbf{v})$ 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 $\mathbf{KL}\left[\mathcal{N}\left(\hat{\mathbf{y}}_t, \hat{V}_t\right) \middle\| \int dy_{t-1} \;\ldots\right]$. Requires Gaussian expectations of log $\int \Rightarrow$ may be challenging.
- The other KL: argmin $\mathbf{KL}\left[\int dy_{t-1} \middle\| \mathcal{N}\left(\hat{\mathbf{y}}_t, \hat{V}_t\right)\right]$ needs only first and second moments of nonlinear message $\Rightarrow$ EP.

Variational learning

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 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:

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

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

We would like to minimise (at least in some sense) $\mathbf{KL}[P\|q]$.

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- Approximation of factors.
  - Usually by “projection” to exponential families.
  - This involves finding expected sufficient statistics, hence expectation.
- 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:

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

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

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

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

Expectation Propagation (EP)

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

Initialize $\tilde{f}_1(\mathcal{Y}_1) = \underset{f \in \{\tilde{f}\}}{\operatorname{argmin}} \, \mathbf{KL}[f_1(\mathcal{Y}_1) \| f_1(\mathcal{Y}_1)]$, $\tilde{f}_i(\mathcal{Y}_i) = 1$ 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: $\tilde{f}_i^{\mathrm{new}}(\mathcal{Y}) \leftarrow \underset{f \in \{\tilde{f}\}}{\operatorname{argmin}} \, \mathbf{KL}[f_i(\mathcal{Y}_i) q_{\neg i}(\mathcal{Y}_i) \| f(\mathcal{Y}_i) q_{\neg i}(\mathcal{Y}_i)]$

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

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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- Once the ith 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.

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- Once the ith 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

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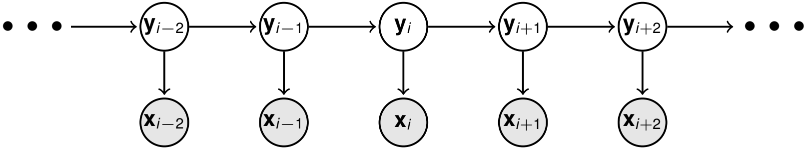
- For some approximations (e.g. Gaussian) may be able to compute true loopy cavity using approximate sites, even if computing exact message would have been intractable.
- In either case, message updates can be scheduled in any order.
- No guarantee of convergence (but see “power-EP” methods).

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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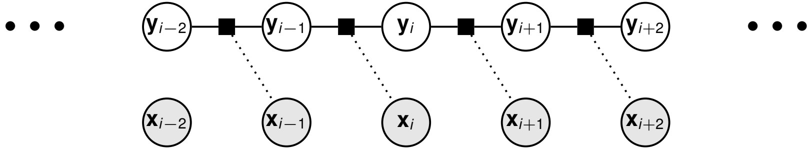

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Then $f_i(\mathbf{y}_i, \mathbf{y}_{i-1}) = \phi_i(\mathbf{y}_i, \mathbf{y}_{i-1})\psi_i(\mathbf{y}_i)$. As ϕ_i and ψ_i are non-linear, inference is not generally tractable.

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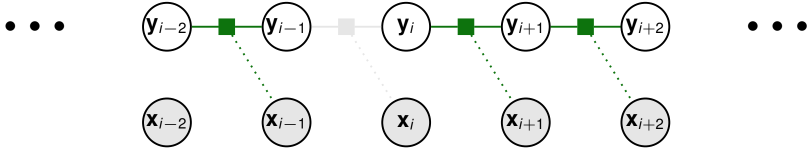

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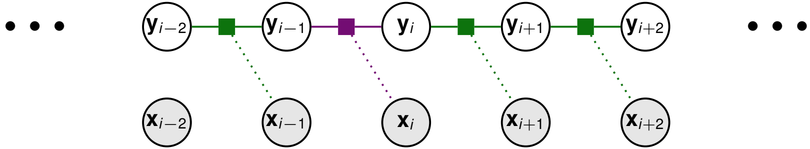
Assume $\tilde{f}_i(\mathbf{y}_i, \mathbf{y}_{i-1})$ is Gaussian. Then,

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

with both α and β Gaussian.

EP for a NLSSM



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with both α and β Gaussian.

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

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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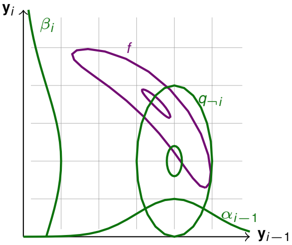

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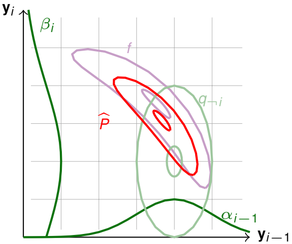

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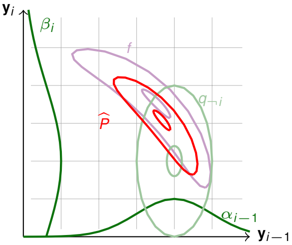

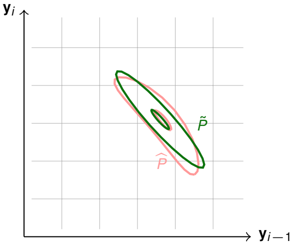

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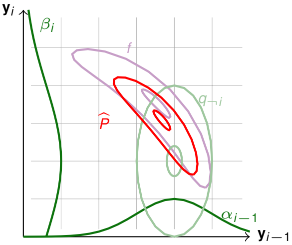

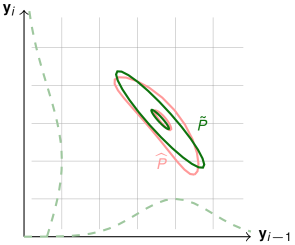

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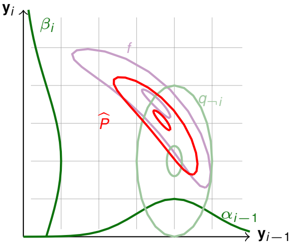

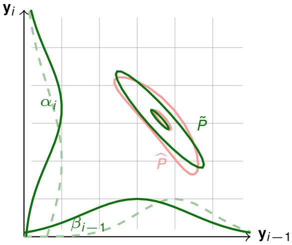

Moment Matching

Each EP update involves a KL minimisation:

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

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

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

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

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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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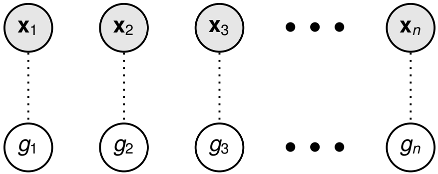

Recall:

- A GP defines a multivariate Gaussian distribution on any finite subset of random vars $\{g_1 \dots g_n\}$ drawn from a (usually uncountable) potential set indexed by "inputs" $\mathbf{x}_i$.

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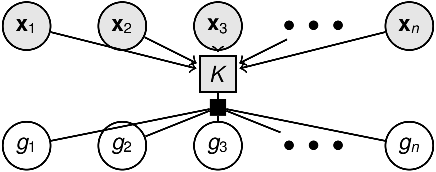

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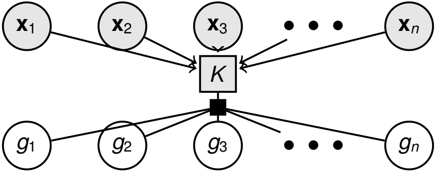

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- If we think of the gs as function values, a GP provides a prior over functions.

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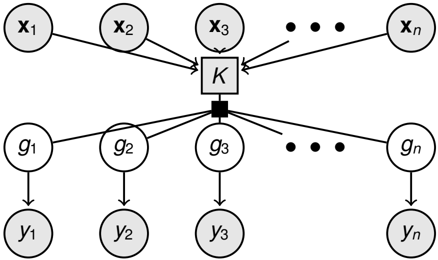

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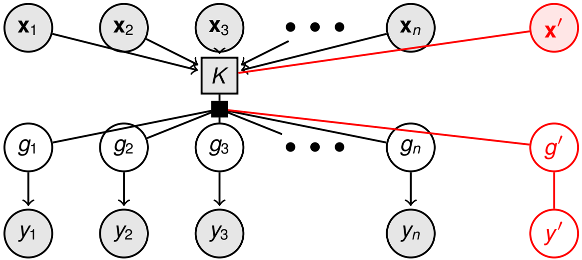
- A GP defines a multivariate Gaussian distribution on any finite subset of random vars $\{g_1 \ldots g_n\}$ drawn from a (usually uncountable) potential set indexed by "inputs" $\mathbf{x}_i$.
- The Gaussian parameters depend on the inputs: $(\boldsymbol{\mu} = [\mu(\mathbf{x}_i)],\ \Sigma = [K(\mathbf{x}_i, \mathbf{x}_j)])$.
- If we think of the gs 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.

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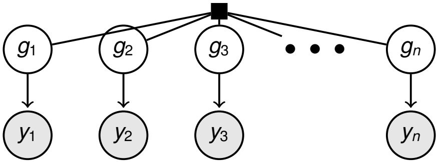
- No parameters to learn (though often hyperparameters); instead, we make predictions on test data directly: [assuming $\mu = 0$, and matrix Σ incorporates diagonal noise]

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

GP EP updates



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

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

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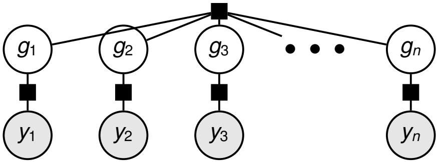

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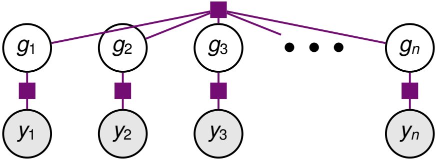

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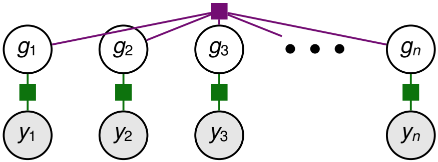

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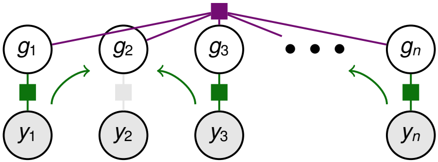

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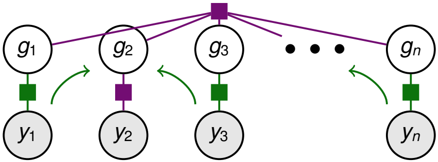

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- The EP updates thus require calculating Gaussian expectations of $f_i(g)g^{\{1,2\}}$:

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

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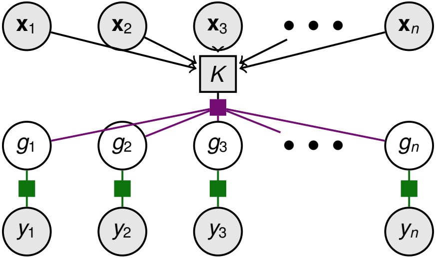

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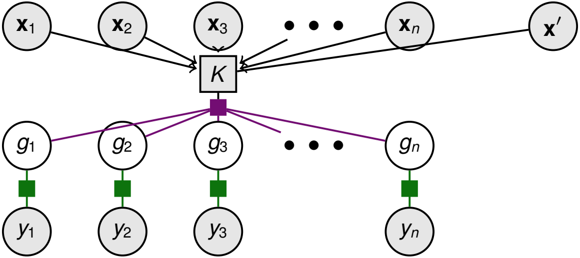

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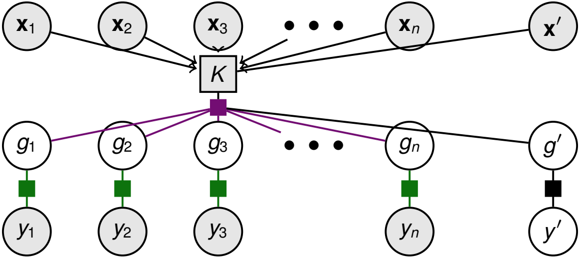

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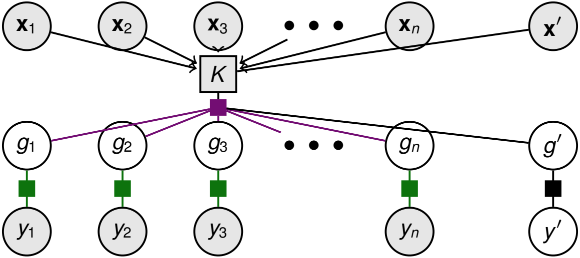

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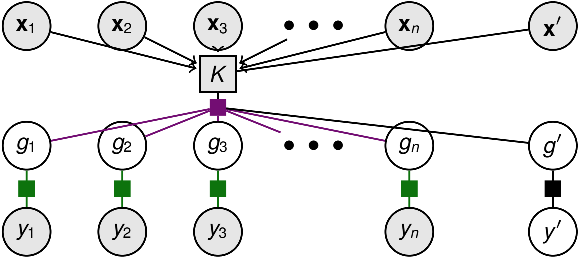

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- Predictions are obtained by marginalising the approximation: [let $\tilde{\Psi} = \text{diag}[\tilde{\psi}_1^2 \dots \tilde{\psi}_n^2]$]

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

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Alpha divergences and Power EP

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

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

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