

Modern Gaussian Processes: Scalable Inference and Novel Applications

(Part II-b) Approximate Inference

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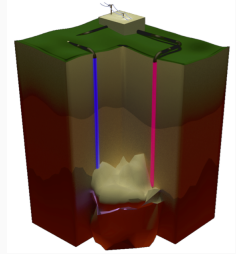
July 14th, 2019



Challenges in Bayesian Reasoning with Gaussian Process Priors

$p(\mathbf{f})$: prior over geology and rock properties

$p(\mathbf{y} | \mathbf{f})$: observation model's likelihood



\$20 Million geothermal well



Geol. surveys and explorations

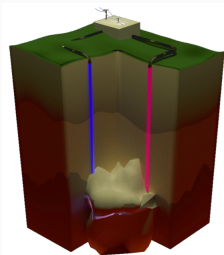
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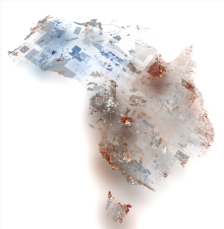
$p(\mathbf{y} | \mathbf{f})$: observation model's likelihood

$p(\mathbf{f} | \mathbf{y})$: posterior geological model:

$$p(\mathbf{f} | \mathbf{y}, \boldsymbol{\theta}) = \frac{p(\mathbf{f} | \boldsymbol{\theta})p(\mathbf{y} | \mathbf{f})}{\underbrace{\int p(\mathbf{f} | \boldsymbol{\theta})p(\mathbf{y} | \mathbf{f})d\mathbf{f}}_{\text{hard bit}}}$$



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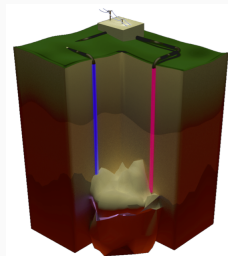
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Challenges:

- ▶ Non-linear likelihood models
- ▶ Large datasets



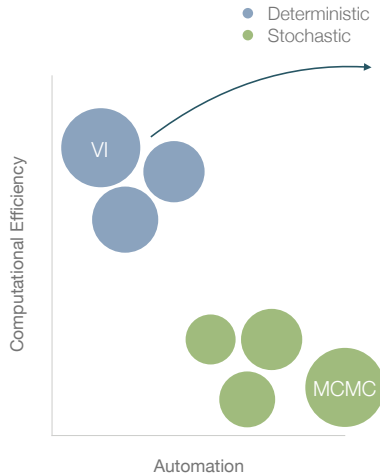
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Geol. surveys and explorations

Automated Probabilistic Reasoning

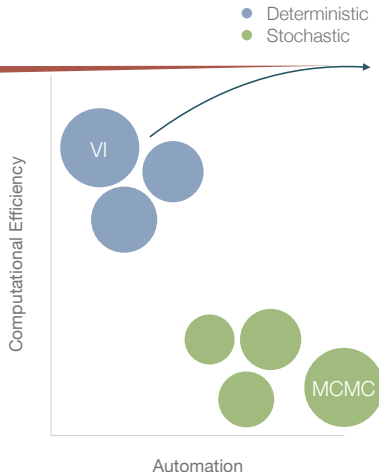
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Automated Probabilistic Reasoning

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Goal: Build generic yet practical inference tools for practitioners and researchers

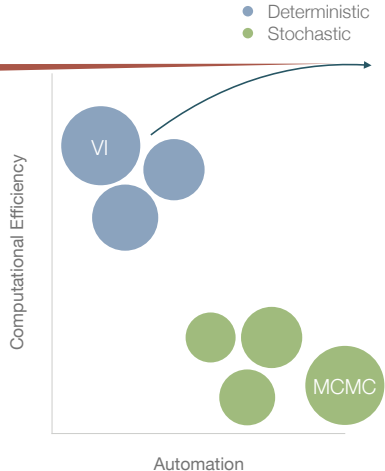


Automated Probabilistic Reasoning

- Approximate inference

Goal: Build generic yet practical inference tools for practitioners and researchers

- Other dimensions:
 - ▶ Accuracy
 - ▶ Convergence



- ① Latent Gaussian Process Models (LGPMs)
- ② Variational Inference
- ③ Scalability through Inducing Variables and Stochastic Variational Inference (SVI)

Latent Gaussian Process Models (LGPMs)

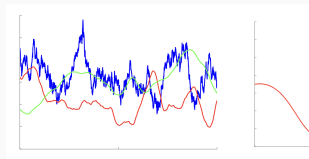
Latent Gaussian Process Models (LGPMs)

Supervised learning $\mathcal{D} = \{\mathbf{x}_n, \mathbf{y}_n\}_{n=1}^N$

- Factorised GP priors over Q latent functions:

$$f_j(\mathbf{x}) \sim \mathcal{GP}(0, \kappa_j(\mathbf{x}, \mathbf{x}'; \boldsymbol{\theta}))$$

$$p(\mathbf{F} | \mathbf{X}, \boldsymbol{\theta}) = \prod_{j=1}^Q \mathcal{N}(\mathbf{F}_{.j}; \mathbf{0}, \mathbf{K}_j)$$



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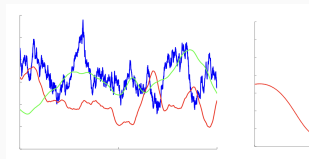
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- Factorised likelihood over observations

$$p(\mathbf{Y} | \mathbf{X}, \mathbf{F}, \phi) = \prod_{n=1}^N p(\mathbf{Y}_n | \mathbf{F}_{n\cdot}, \phi)$$



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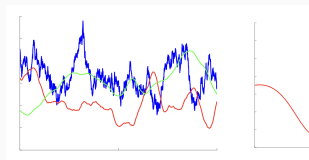
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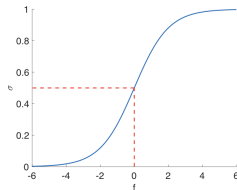
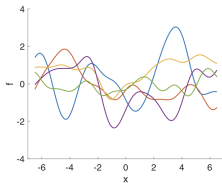
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What can we model within this framework?



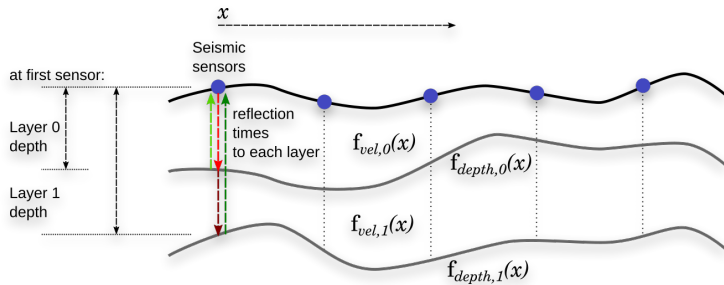
Examples of LGPMs (1)

- Multi-output regression
- Multi-class classification
 - ▶ $P = Q$ classes
 - ▶ softmax likelihood



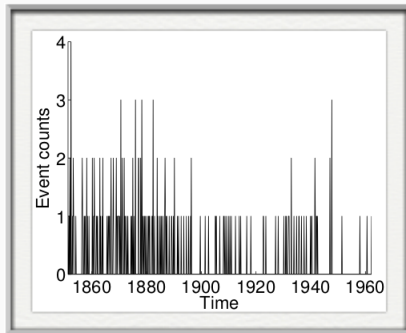
Examples of LGPMs (2)

- Inversion problems



Examples of LGPMs (3)

- Log Gaussian Cox processes (LGCPs)



We only require access to 'black-box' likelihoods. *How can we carry out inference in these general models?*

Variational Inference

Variational Inference (VI): Optimise Rather than Integrate

Recall our posterior estimation problem:

$$\underbrace{p(\mathbf{F} | \mathbf{Y})}_{\text{posterior}} = \frac{1}{\underbrace{p(\mathbf{Y})}_{\text{marginal likelihood}}} \underbrace{p(\mathbf{F})}_{\text{prior}} \underbrace{p(\mathbf{Y} | \mathbf{F})}_{\text{conditional likelihood}}$$

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- Instead, approximate $q(\mathbf{F} | \lambda) \approx p(\mathbf{F} | \mathbf{Y})$ to minimize:

$$\text{KL} [q(\mathbf{F} | \lambda) \parallel p(\mathbf{F} | \mathbf{Y})] \stackrel{\text{def}}{=} \mathbb{E}_{q(\mathbf{F} | \lambda)} \log \frac{q(\mathbf{F} | \lambda)}{p(\mathbf{F} | \mathbf{Y})}$$

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Properties:

$$\text{KL} [q \parallel p] \geq 0,$$

$$\text{KL} [q \parallel p] = 0 \text{ iff } q = p.$$

Decomposition of the Marginal Likelihood

$$\log p(\mathbf{Y}) = \text{KL} [q(\mathbf{F} | \lambda) \parallel p(\mathbf{F} | \mathbf{Y})] + \mathcal{L}_{\text{ELBO}}(\lambda)$$

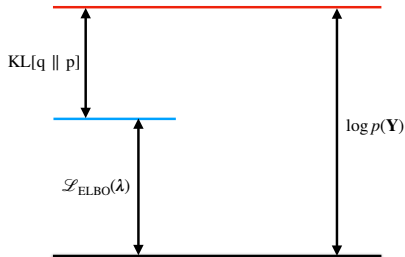


Fig reproduced from Bishop (2006)

- $\mathcal{L}_{\text{ELBO}}(\lambda)$ is a lower bound on the log marginal likelihood
- The optimum is achieved when $q = p$
- Maximizing $\mathcal{L}_{\text{ELBO}}(\lambda) \equiv \text{minimizing } \text{KL} [q(\mathbf{F} | \lambda) \parallel p(\mathbf{F} | \mathbf{Y})]$

Variational Inference Strategy

- The evidence lower bound $\mathcal{L}_{\text{ELBO}}(\lambda)$ can be written as:

$$\mathcal{L}_{\text{ELBO}}(\lambda) \stackrel{\text{def}}{=} \underbrace{\mathbb{E}_{q(\mathbf{F} | \lambda)} \log p(\mathbf{Y} | \mathbf{F})}_{\text{expected log likelihood (ELL)}} - \underbrace{\text{KL}[q(\mathbf{F} | \lambda) \parallel p(\mathbf{F})]}_{\text{KL(approx. posterior} \parallel \text{prior)}}$$

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- ELL is a model-fit term and KL is a penalty term
- What family of distributions?
 - ▶ As flexible as possible
 - ▶ Tractability is the main constraint
 - ▶ No risk of over-fitting

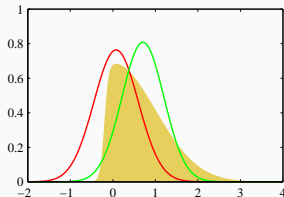


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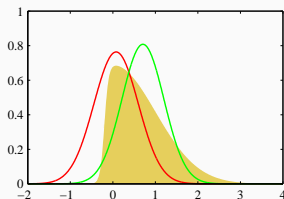


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We want to maximise $\mathcal{L}_{\text{ELBO}}(\lambda)$ wrt variational parameters λ

Goal: Approximate intractable posterior $p(\mathbf{F} | \mathbf{Y})$ with variational distribution

$$q(\mathbf{F} | \boldsymbol{\lambda}) = \sum_{k=1}^K \pi_k q_k(\mathbf{F} | \boldsymbol{\lambda}) = \sum_{k=1}^K \pi_k \prod_{j=1}^Q \mathcal{N}(\mathbf{F}_k; \mathbf{m}_{kj}, \mathbf{S}_{kj})$$

with variational parameters $\boldsymbol{\lambda} = \{\mathbf{m}_{kj}, \mathbf{S}_{kj}\}$,

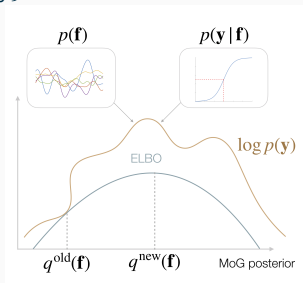
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Recall $\mathcal{L}_{\text{ELBO}}(\lambda) = -\text{KL} + \text{ELL}$:

- KL term can be bounded using Jensen's inequality
 - ▶ Exact gradients of parameters



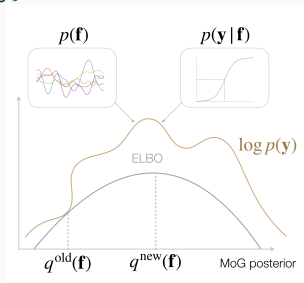
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ELL and its gradients can be estimated *efficiently*

Expected Log Likelihood Term

Th.1: Efficient estimation

The ELL and its gradients can be estimated using expectations over univariate Gaussian distributions.

$$q_{k(n)} \stackrel{\text{def}}{=} q_{k(n)}(\mathbf{F}_{\cdot n} | \boldsymbol{\lambda}_{k(n)})$$

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Practical consequences

- Can use unbiased Monte Carlo estimates
- Gradients of the likelihood are not required (only likelihood evaluations)
- Holds $\forall Q \geq 1$

Scalability through Inducing Variables and Stochastic Variational Inference (SVI)

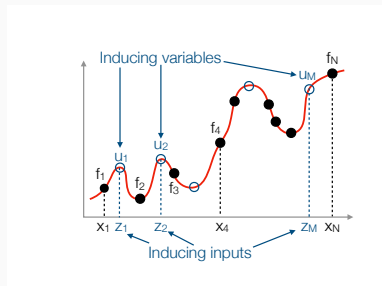
Inducing Variables in GP Models

Inducing variables \mathbf{u}

- Latent values of the GP, as \mathbf{f} and \mathbf{f}_*
- Usually marginalized (integrated out)

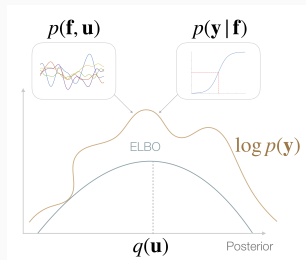
Inducing inputs \mathbf{Z}

- Corresponding input location, as \mathbf{x}
- Imprint on final solution

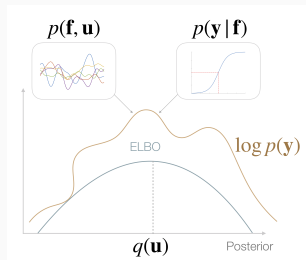


Generalization of “support points”, “active set”, “pseudo-inputs”

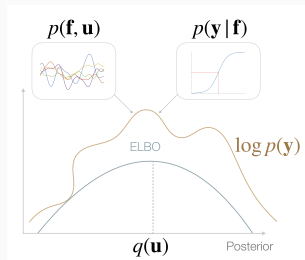
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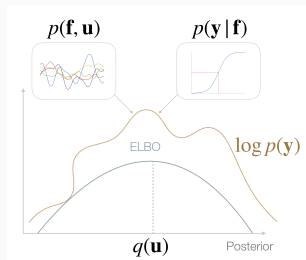
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- Hyper-parameters and inducing inputs optimized *jointly*

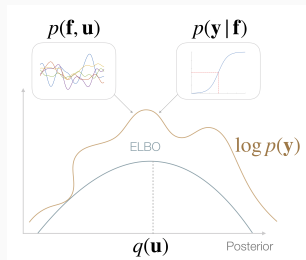


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Computation dominated by:

$$\mathbf{K}_{\mathbf{x}\mathbf{z}}\mathbf{K}_{\mathbf{z}\mathbf{z}}^{-1}\mathbf{K}_{\mathbf{z}\mathbf{x}}$$

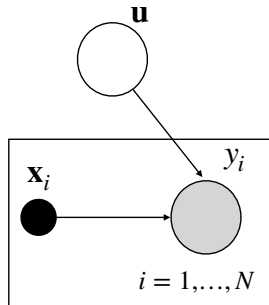
Time cost $\mathcal{O}(NM^2)$, can we do better?



Stochastic Variational Inference for GP Models

Maintain an explicit representation of $q(\mathbf{u}) = \mathcal{N}(\mathbf{m}, \mathbf{S})$

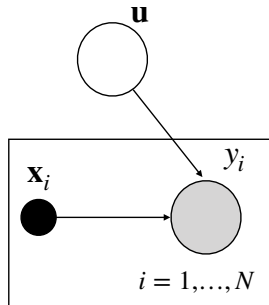
- Inducing variables act as global variables
- ELBO decomposes across observations
- Use stochastic optimization
- $\mathbf{K}_{\mathbf{x}_i \mathbf{z}} \mathbf{K}_{\mathbf{z} \mathbf{z}}^{-1} \mathbf{K}_{\mathbf{z} \mathbf{x}_i}$: Time cost $\mathcal{O}(M^3) \rightarrow$ big data!



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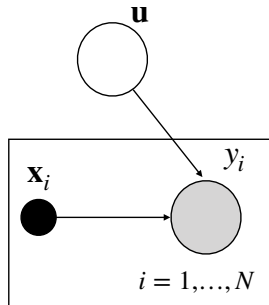


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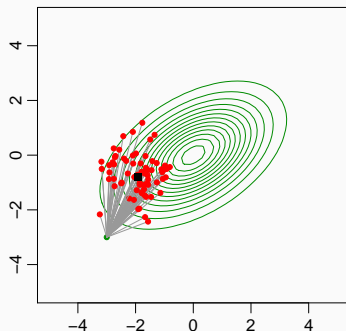
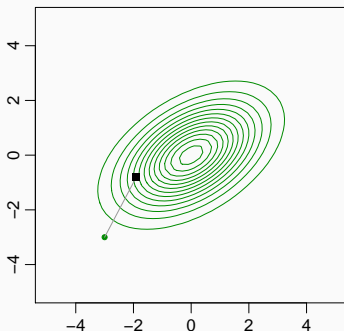
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- Converge to optimal solution for Gaussian likelihoods (Hensman et al, UAI, 2013)
- Generalization to LGPMs (Dezfouli & Bonilla, NeurIPS, 2015)

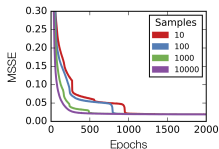
Stochastic Gradient Optimization

$$\mathbb{E} \left\{ \widetilde{\nabla_{\text{vpar}} \text{LowerBound}} \right\} = \nabla_{\text{vpar}} \text{LowerBound}$$



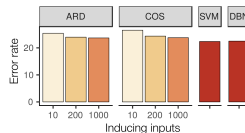
Robbins and Monro, *AoMS*, 1951

$$\text{vpar}' = \text{vpar} + \frac{\alpha_t}{2} \widetilde{\nabla_{\text{vpar}}}(\text{LowerBound}) \quad \alpha_t \rightarrow 0$$



Scalability & efficient computation
Low-variance gradient estimates

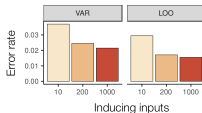
- ★ Breaks error-barrier on MNIST for GP models
- ★ Unprecedented scale



Well-targeted objective functions
Leave-one-out hyper-parameter learning

The holy trinity of machine learning

Representational power
Flexible kernels



- LGPMs: General framework for GP priors and non-linear likelihoods
- Applications in multi-class classification, multi-output regression, modelling count data and more
- Generic inference via optimisation of the variational objective (ELBO)
- Scalability via inducing-variable approach
- AutoGP