Fast and scalable spike and slab variable selection in high-dimensional Gaussian processes

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- High-dimensional inputs - which are relevant to $f(\cdot)$?
- Variable selection:
  1. improve predictive accuracy
  2. reduce downstream data collection costs
  3. understand 'meaningful' relationships

Gaussian process regression (GPR)

$$
\begin{aligned}
y &= f(x) + \epsilon : \epsilon \sim \mathcal{N}(0, \sigma^2) \\
f(x) &\sim \mathcal{GP}(m(x), k(x, x'))
\end{aligned}
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- A Gaussian process $f(x)$ is a random function where any $f(x_1), ..., f(x_n)$ are MVN
- Properties determined by mean $m(x)$, covariance (kernel) $k_\alpha(x, x')$

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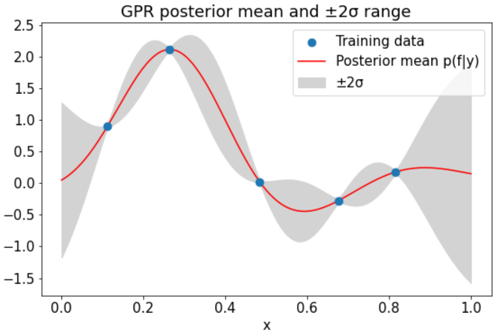
2. $\underbrace{p(f(\cdot)|y)}_{\text{posterior}} = \frac{p(y|f(\cdot))p(f(\cdot)|\alpha)}{p(y)}$



GPR variable selection with automatic relevance determination (ARD)[3]

1. Use 'automatic relevance determination' (ARD) kernel[2]

$$k_{ARD}(x, x) = k(\theta \odot x, \theta \odot x') : \theta \in \mathbb{R}_+^d$$

[2] e.g. stationary isotropic monotone $k(\cdot, \cdot) : \frac{\partial}{\partial \theta_j} \mathbb{E}[(f(x + he_j) - f(x))^2] > 0 \implies \theta$ as relevance measure

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ML-II complexity penalty $\implies$ irrelevant $\theta_j \to 0$

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ARD limitations[4] - toy example

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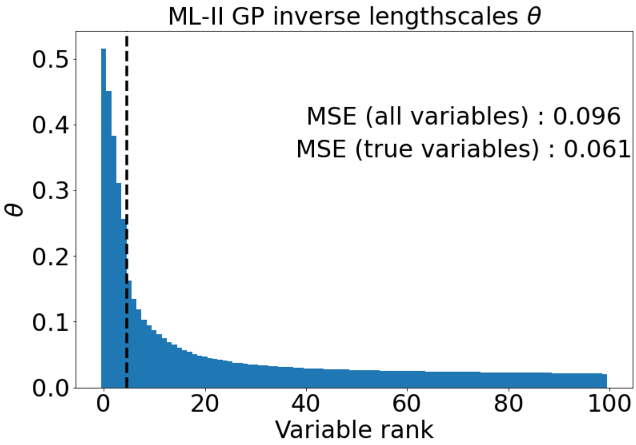
$x \sim \mathcal{N}_{100}(0, I)$, $y \sim \mathcal{N}(\sum_{j=1}^{5} sin(a_j x_j)), \sigma^2), \sigma^2 = \frac{\sigma_y^2}{20}$



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1. Place spike and slab prior on inverse lengthscales θ:

$$p(\theta_j|\gamma_j) = \gamma_j \underbrace{\tilde{p}(\theta_j)}_{\text{slab}} + (1-\gamma_j)\underbrace{\delta_0(\theta_j)}_{\text{spike}} \quad , \quad p(\gamma_j) = \mathcal{B}ern(\gamma_j|\pi)$$

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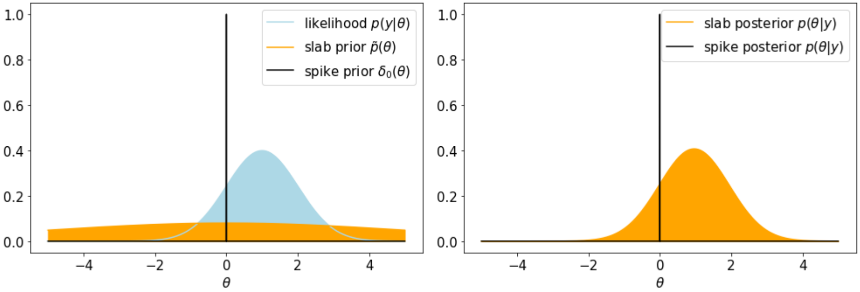

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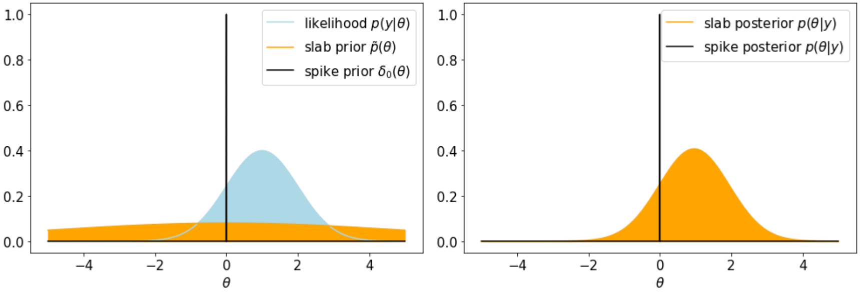

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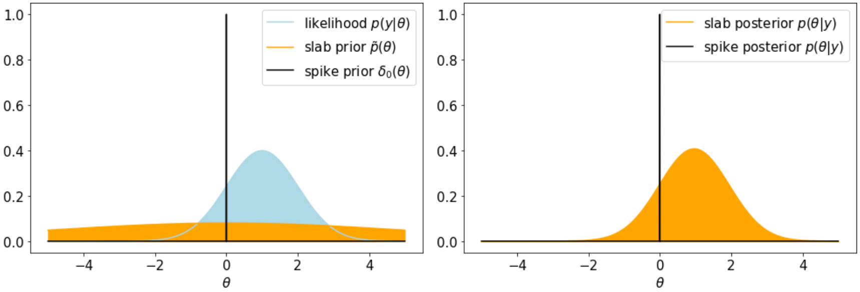

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3. Variable select based on $q(\gamma_j = 1|y)$ or $\text{argmax}_\gamma\{q(\gamma)\}$.

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Existing implementations

- **Supervised GPR**[5]: MCMC based $\implies$ costly in high-dimensions (2^d search $+$ no HMC)

[5] Savitsky et al. (2011); Linkletter et al. (2006); Qamar and Tokdar (2014)
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Variational inference for spike and slab GPR

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- Want $q^*(\theta, \gamma) = \text{argmin}_{q \in \mathcal{Q}}\{KL[q(\theta, \gamma)|p(\theta, \gamma|y)]\}$
- Equivalent to maximising free energy / evidence lower bound:

$$\mathcal{F} = \langle \log p(y|\theta) \rangle_{q(\theta,\gamma)} - KL[q(\theta, \gamma)||p(\theta, \gamma)]\}$$

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$$\langle \log \delta_0(\theta_j) \rangle_{q(\theta_j)} = -\infty \quad \forall q(\cdot) \neq \delta_0(\cdot)$$

Our variational inference strategy

1. Gaussian approximation to the Dirac spike:

$$p(\theta_j|\gamma_j) = \gamma_j \underbrace{\mathcal{N}(0, \sigma_1^2)}_{\text{slab}} + (1 - \gamma_j) \underbrace{\mathcal{N}(0, \sigma_0^2)}_{\text{spike}} \quad : \quad \sigma_0^2 \ll 1 \ll \sigma_1^2$$

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$\implies$ fast approximate co-ordinate ascent strategy available

aCAVI: approximate coordinate ascent variational inference (CAVI)

(Exact) CAVI update to $q(\gamma)$:

$$q(\gamma) \propto exp\{\langle logp(\theta|\gamma)\rangle_{q(\theta)}\}p(\gamma) = \prod_j \mathcal{B}ern(\gamma_j|\lambda_j)$$

$\mathcal{O}(d)$ cost

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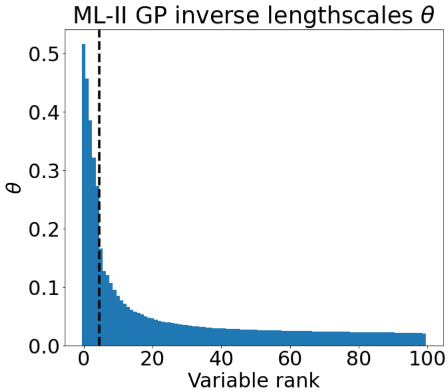
(Approximate) CAVI update to $q_\psi(\theta)$ using rep-grad SVI:

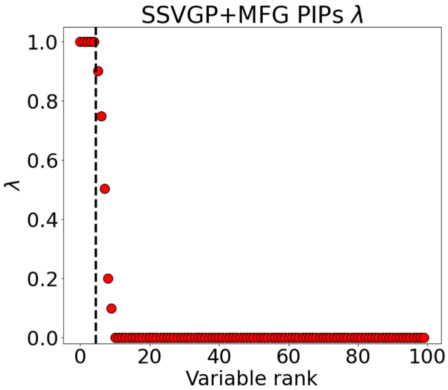
For $t = 1, \ldots T$:

$$\psi \leftarrow \psi + \eta \odot \hat{\nabla}_\psi \mathcal{F}$$

$\mathcal{O}(sn^2 d) + \mathcal{O}(sn^3)$ cost

Toy example results





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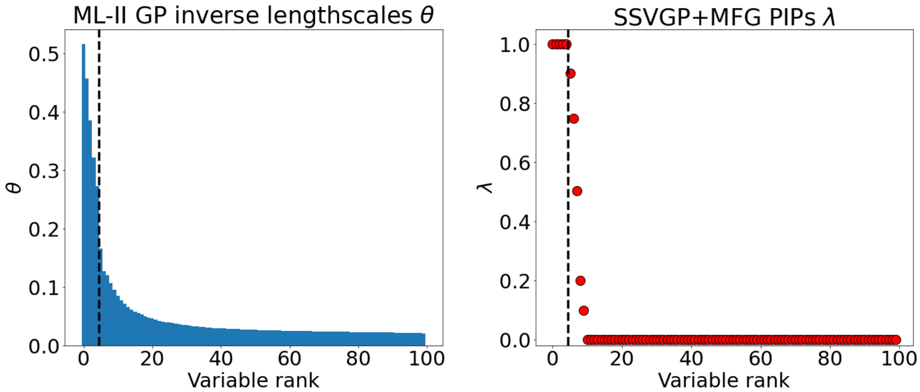

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ML-II GP	0.096 ± 0.014	$\mathbf{5.0} \pm 0.7$
SSVGP+MFG	$\mathbf{0.068} \pm 0.011$	27.8 ± 0.5

Addressing hyperparameter sensitivity

$$v = \frac{1}{\sigma_0^2}, c = \frac{\sigma_0^2}{\sigma_1^2}$$

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v	10^2	10^3	10^4	10^5	10^6
$\bar{\lambda}$ (toy example)	0	0.05	0.07	0.34	1

Bayesian model averaging

$$\mathcal{M}_k = \{v_k, c, \pi\}$$

$$\begin{tikzcd}
q(\theta, \gamma|\mathcal{M}_1) \arrow[dr] & q(\theta, \gamma|\mathcal{M}_2) \arrow[d] & \cdots & q(\theta, \gamma|\mathcal{M}_K) \arrow[dll] \\
& \boxed{\sum_k^K p(\mathcal{M}_k|y)(\cdot)} \arrow[d] & & \\
& q(\theta, \gamma) & &
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... but expensive and $p(\mathcal{M}_k | y)$ intractable

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   - Reduces complexity from $\mathcal{O}(d)$ to $\mathcal{O}(q)$: $q = \{\#\lambda > \epsilon\}$
   - Under certain conditions $\mu_j \to N_\delta(0)$ if $\lambda_j \leq \epsilon$ during a-CAVI

Using the leave-one-out predictive density to approximate posterior weights

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- Under ZT approximation:

$$\text{LOO-PD} = \prod_i \underbrace{p(y_i | y_{\neg i}, \theta = \mu_k)}_{\text{standard GPR posterior}}$$

$$\implies \mathcal{O}(n^3) \text{ using Bürkner et al. (2021)}$$

Nearest neighbour truncations for large-n scalability[7]

Marginal likelihood:

$$\log p(y|\theta) \approx \frac{n}{m} \log p(y_i, y_{NN(i)}|\theta)$$

Predictive distribution:

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For m-nearest neighbours we get $\mathcal{O}(n^3) \to \mathcal{O}(n \log n + m^3)$

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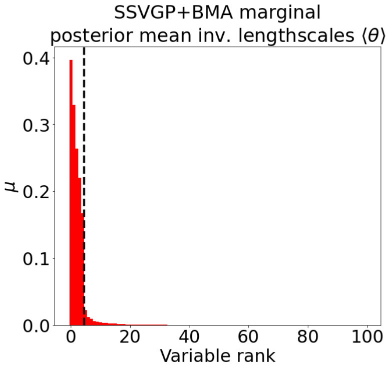
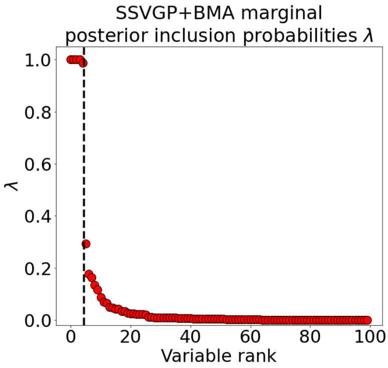
Returning to the toy example





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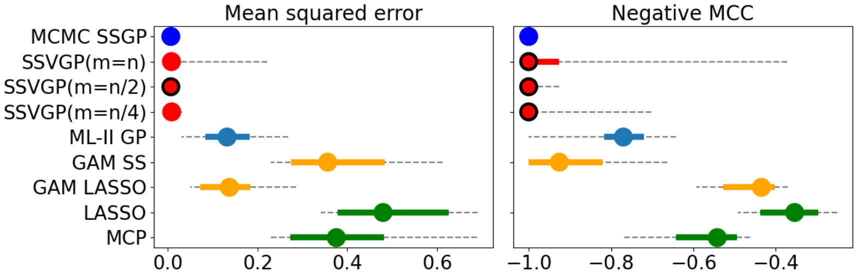
SSVGP original	0.068 ± 0.011	27.8 ± 0.5
SSVGP+BMA	$\mathbf{0.064} \pm 0.01$	14.6 ± 0.4

[8] nearest neighbour truncation with m=n/4 neighbours used for BMA

"Ground truth" simulation comparison

Savitsky et al. (2011) experiment:

- Draw $n = 100$ samples of $x \sim Unif[0,1]^{1000}$
- Set $y = x_1 + x_2 + x_3 + x_4 + sin(3x_5) + sin(5x_6) + \epsilon$ for $\epsilon \sim \mathcal{N}(0, 0.05^2)$.



Method:	Savitsky et al. (2011)	SSVGP(n)	SSVGP(n/2)	SSVGP(n/4)	ML-II
Runtime:	10224s	20.3s	11.0s	8.4s	3.9s

Large-scale dataset results

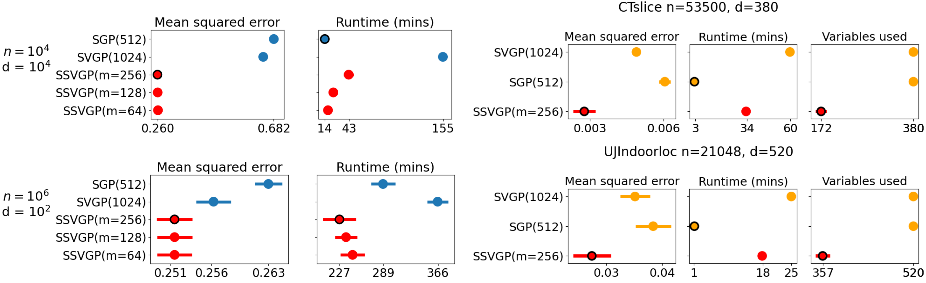


Figure: LHS: synthetic datasets, RHS: real datasets from UCI repository

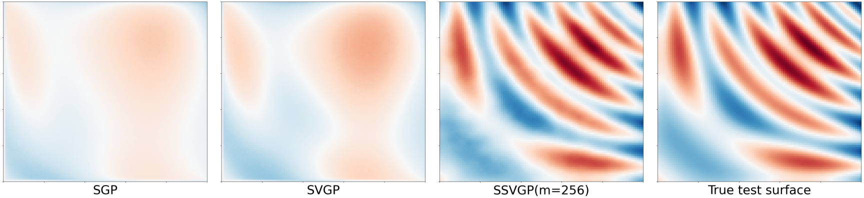


Figure: Synthetic experiment: average prediction surfaces for $n = d = 10^4$.

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https://github.com/HWDance/SSVGP

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