

# Learning from the dual parameterization

## Approximate inference and learning in Gaussian process models

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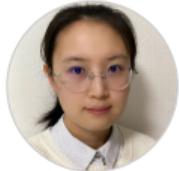
Bern, 28 June 2023



Aalto University



Joint work...



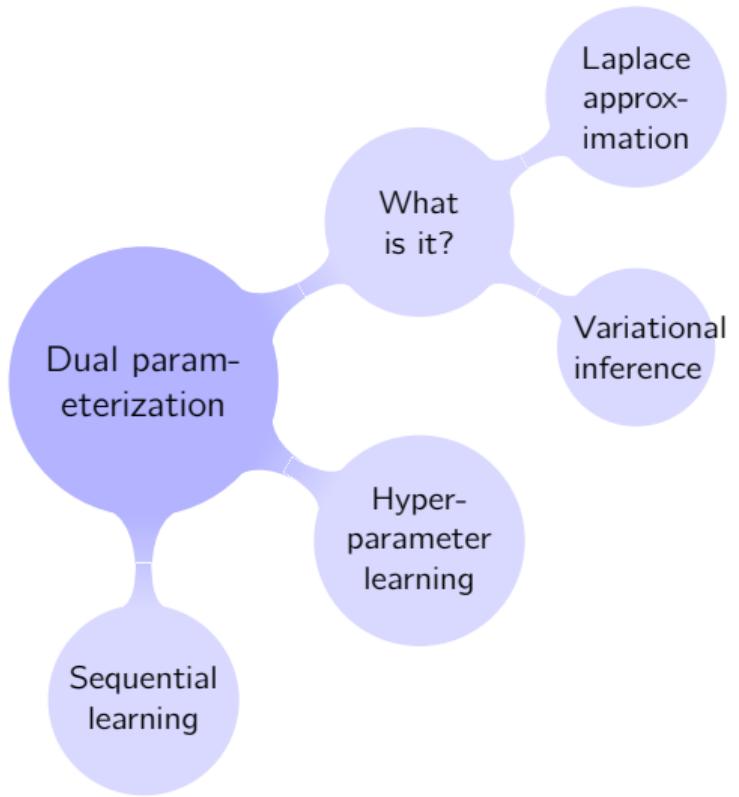
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# Outline

Gaussian process model

Laplace approximation

Variational inference

Hyperparameter learning

Sparse approximation

Sequential learning

## Gaussian process model

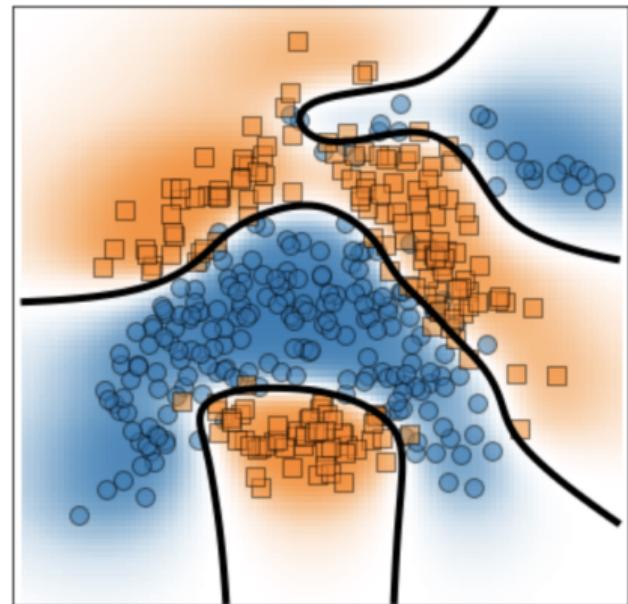
prior:  $p(f(\cdot)) = \mathcal{GP}(\mu(\cdot), \kappa(\cdot, \cdot))$

likelihood:  $p(\mathbf{y} | \mathbf{f}) = \prod_{i=1}^n p(y_i | f_i)$ , e.g. Bernoulli for classification

posterior:  $p(f(\cdot) | \mathbf{y}) \propto p(\mathbf{y} | \mathbf{f}) p(f(\cdot))$  intractable  
 $\approx q(f(\cdot))$  approximate inference

# Approximate inference for non-conjugate likelihood models

- ▶ **MCMC (sampling) methods**  
(accurate but generally heavy)
- ▶ **Laplace approximation (LA)**  
(fast and simple)
- ▶ **Expectation propagation (EP)**  
(efficient but tricky)
- ▶ **Variational methods (VB/VI)**  
(popular but not problem-free)



GP classification with a Bernoulli likelihood

## Gaussian approximate posterior

$$p(\mathbf{f} \mid \mathbf{y}) \approx q(\mathbf{f})$$

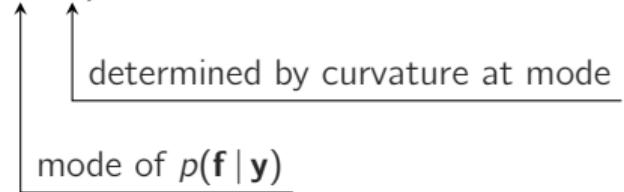
$$q(\mathbf{f}) = N(\mathbf{f}; \mathbf{m}, S)$$

How to find  $\mathbf{m}$  and  $S$ ?

# Laplace approximation

$$p(\mathbf{f} | \mathbf{y}) \approx q(\mathbf{f})$$

$$q(\mathbf{f}) = N(\mathbf{f}; \mathbf{m}, S)$$



How to find  $\mathbf{m}$  and  $S$ ?

“Point estimate++”

## Laplace approximation, mean parameter $\mathbf{m}$

posterior:

$$p(\mathbf{f} | \mathbf{y}) \propto p(\mathbf{y} | \mathbf{f}) p(\mathbf{f})$$

Laplace objective:

$$\mathcal{L}_{\text{Lap}} = \log p(\mathbf{y} | \mathbf{f}) + \log p(\mathbf{f})$$

mode of posterior:

$$\mathbf{m} = \mathbf{f}^* = \arg \max_{\mathbf{f}} \mathcal{L}_{\text{Lap}}(\mathbf{f})$$

(log-concave likelihoods: convex optimization, unique global maximum)

We can find a different (**dual**) parameterization!

Stationary point of  $\mathcal{L}_{\text{Lap}} = \log p(\mathbf{y} | \mathbf{f}) + \log p(\mathbf{f})$

At the optimum:

$$\log p(\mathbf{f}) = -\frac{1}{2}\mathbf{f}^T \mathbf{K}^{-1} \mathbf{f} + \text{const.}$$

$$\begin{aligned} 0 &= \nabla_{\mathbf{f}} \mathcal{L}_{\text{Lap}} \Big|_{\mathbf{f}=\mathbf{f}^*} \\ &= \underbrace{\nabla_{\mathbf{f}} \log p(\mathbf{y} | \mathbf{f}) \Big|_{\mathbf{f}=\mathbf{f}^*}}_{\text{likelihood term}} + \underbrace{\nabla_{\mathbf{f}} \log p(\mathbf{f}) \Big|_{\mathbf{f}=\mathbf{f}^*}}_{\text{prior term}} \\ &= \underbrace{\nabla_{\mathbf{f}} \log p(\mathbf{y} | \mathbf{f}) \Big|_{\mathbf{f}=\mathbf{f}^*}}_{=: \boldsymbol{\alpha}(\mathbf{f}^*)} - \mathbf{K}^{-1} \mathbf{f} \Big|_{\mathbf{f}=\mathbf{f}^*} \end{aligned}$$

$$0 = \boldsymbol{\alpha}^* - \mathbf{K}^{-1} \mathbf{f}^* \quad \Leftrightarrow \quad \mathbf{f}^* = \mathbf{K} \boldsymbol{\alpha}^*$$

- ⇒ mode can equivalently be parameterized through the **derivatives of the likelihood**
- ⇒ **dual** parameterization

## What about the covariance S?

Laplace approximation: 2<sup>nd</sup>-order Taylor approximation to log posterior.

$$\text{precision} \quad S^{-1} = -\nabla_{\mathbf{f}}^2 \mathcal{L}_{\text{Lap}} \Big|_{\mathbf{f}=\mathbf{f}^*}$$

Hessian of negative log posterior,  $-\mathcal{L}_{\text{Lap}} = -\log p(\mathbf{y} | \mathbf{f}) - \log p(\mathbf{f})$ :

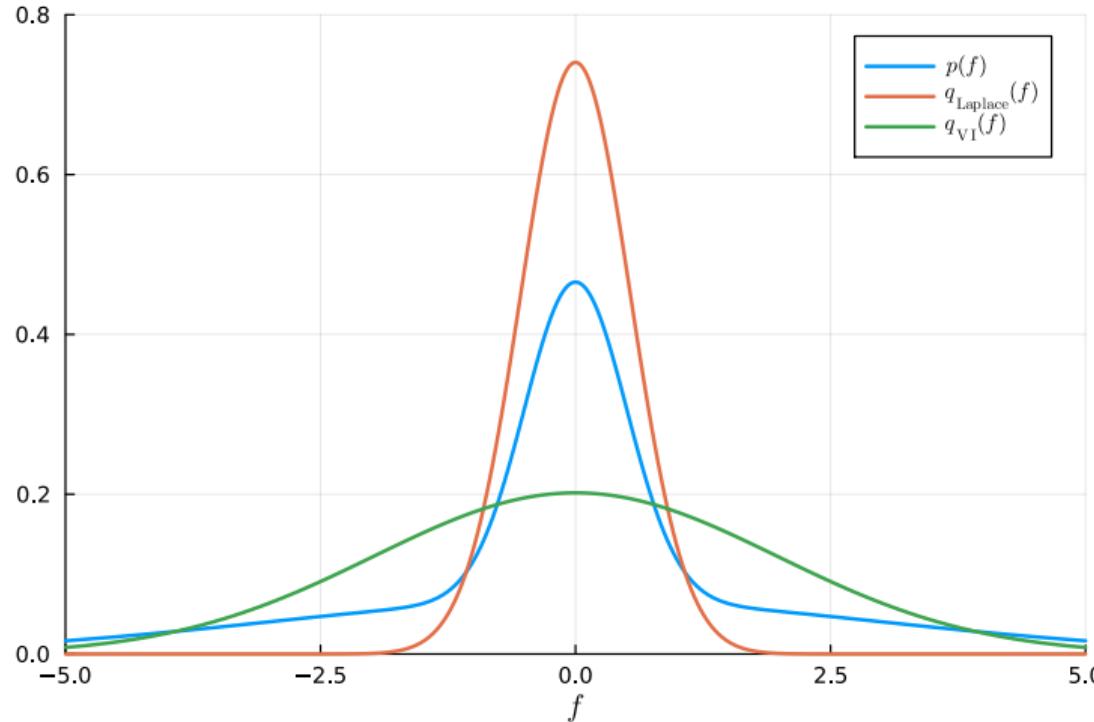
$$-\nabla_{\mathbf{f}}^2 \mathcal{L}_{\text{Lap}} \Big|_{\mathbf{f}=\mathbf{f}^*} = \underbrace{-\nabla_{\mathbf{f}}^2 \log p(\mathbf{y} | \mathbf{f}) \Big|_{\mathbf{f}=\mathbf{f}^*}}_{=:W} + K^{-1}$$

For factorizing likelihood,  $p(\mathbf{y} | \mathbf{f}) = \prod_{i=1}^n p(y_i | f_i)$ :

$$W = -\nabla_{\mathbf{f}}^2 \log p(\mathbf{y} | \mathbf{f}) \Big|_{\mathbf{f}=\mathbf{f}^*} = \text{diag}(\boldsymbol{\beta}), \quad \beta_i = -\frac{\partial^2}{\partial f_i^2} \log p(y_i | f_i)$$

$$\Rightarrow S_{\text{Lap}} = (W + K^{-1})^{-1}$$

## Laplace approximation is local



Instead of point estimate (and post-hoc uncertainty), we may prefer optimizing over a whole posterior distribution directly  $\Rightarrow$  **variational inference (VI)**

## Dual parameterization of VI

$$q(\mathbf{f}) = \mathcal{N}(\mathbf{f}; \mathbf{m}, \mathbf{S})$$

$$q^*(\mathbf{f}) \propto p(\mathbf{f}) \prod_{i=1}^n \underbrace{\exp(\langle \lambda_i^*, T(f_i) \rangle)}_{\text{1D sites}}$$

sufficient statistics  $(f_i, f_i^2)$

where  $\lambda_i^* = \underbrace{\nabla_{\mu_i} \mathbb{E}_{q^*(f_i)} [\log p(y_i | f_i)]}_{\text{nat.grad.}}$

$(\alpha_i, \beta_i)$

## From Laplace to VI

$$\mathcal{L}_{\text{Lap}}[\mathbf{f}] = \underbrace{\log p(\mathbf{y} | \mathbf{f})}_{\text{data fit}} + \underbrace{\log p(\mathbf{f})}_{\text{regularizer}}$$

$$\begin{aligned}\mathcal{L}_{\text{VI}}[q(\mathbf{f})] &= \mathbb{E}_{q(\mathbf{f})} \log p(\mathbf{y} | \mathbf{f}) + \mathbb{E}_{q(\mathbf{f})} \log p(\mathbf{f}) + \mathbb{H}[q(\mathbf{f})] \\ &= \mathbb{E}_{q(\mathbf{f})} \log p(\mathbf{y} | \mathbf{f}) - \underbrace{\mathbb{E}_{q(\mathbf{f})} \log \frac{q(\mathbf{f})}{p(\mathbf{f})}}_{\text{KL}\left[q(\mathbf{f}) \| p(\mathbf{f})\right]} \\ &\quad \uparrow \begin{array}{l} \text{entropy} \\ \Rightarrow \text{valid objective} \\ (\rightarrow \text{Generalized VI}) \end{array}\end{aligned}$$

$$\mathcal{L}_{\text{ELBO}}[q(\mathbf{f})] = \mathbb{E}_{q(\mathbf{f})} \log p(\mathbf{y} | \mathbf{f}) - \text{KL}\left[q(\mathbf{f}) \| p(\mathbf{f})\right]$$

## Stationary point

$$q^*(\mathbf{f}) = \arg \max_q \mathcal{L}_{\text{ELBO}}[q] \quad \text{for } q(\mathbf{f}) = \mathcal{N}(\mathbf{m}, \mathbf{S})$$

Now **two** stationary point equations:

$$0 = \nabla_{\mathbf{m}} \mathcal{L}_{\text{ELBO}}$$

$$0 = \nabla_{\mathbf{S}} \mathcal{L}_{\text{ELBO}}$$

## Equation for mean $\mathbf{m}$

$$\nabla_{\mathbf{m}} \mathcal{L}_{\text{ELBO}}[q(\mathbf{f})] = \nabla_{\mathbf{m}} \mathbb{E}_{q(\mathbf{f})}[\log p(\mathbf{y} | \mathbf{f})] - \nabla_{\mathbf{m}} \text{KL}[q(\mathbf{f}) \| p(\mathbf{f})]$$

$$\text{KL}[q(\mathbf{f}) \| p(\mathbf{f})] = \text{KL}[\mathcal{N}(\mathbf{m}, \mathbf{S}) \| \mathcal{N}(\mathbf{0}, \mathbf{K})] = \frac{1}{2} \left( \text{Tr}(\mathbf{K}^{-1} \mathbf{S}) - n + \mathbf{m}^T \mathbf{K}^{-1} \mathbf{m} + \log \frac{\det \mathbf{K}}{\det \mathbf{S}} \right)$$

$$\nabla_{\mathbf{m}} \text{KL}[q(\mathbf{f}) \| p(\mathbf{f})] = \mathbf{K}^{-1} \mathbf{m}$$

$$\nabla_{\mathbf{m}} \mathbb{E}_{q(\mathbf{f})}[\log p(\mathbf{y} | \mathbf{f})] = \mathbb{E}_{q(\mathbf{f})}[\nabla_{\mathbf{f}} \log p(\mathbf{y} | \mathbf{f})] =: \boldsymbol{\alpha}$$

↑  
Bonnet's theorem

At optimum:

$$0 = \boldsymbol{\alpha}^* - \mathbf{K}^{-1} \mathbf{m}^* \quad \Leftrightarrow \quad \mathbf{m}^* = \mathbf{K} \boldsymbol{\alpha}^*$$

## Equation for covariance S

more complicated...

## Reparameterizations

$$q(\mathbf{f}) = N(\mathbf{m}, S)$$

- ▶ mean–covariance:  $\xi = (\mathbf{m}, S)$  (and whitened reparameterization)
- ▶ natural parameters:  $\eta = (S^{-1}\mathbf{m}, -\frac{1}{2}S^{-1})$
- ▶ expectation parameters:  $\mu = (\mathbf{m}, \mathbf{m}\mathbf{m}^T + S)$

## Lagrangian dual

$$\mathcal{L}_{\text{ELBO}}[q(\mathbf{f})] = \mathbb{E}_{q(\mathbf{f})} \log p(\mathbf{y} | \mathbf{f}) - \text{KL}[q(\mathbf{f}) \| p(\mathbf{f})]$$

Introducing local  $\tilde{\mu}$  and moment-matching constraint:

$$\mathcal{L}_{\text{Lagrange}}(\tilde{\mu}, \mu, \lambda) = \sum_{i=1}^n \mathbb{E}_{\tilde{q}_i}(f_i; \tilde{\mu}_i) [\log p(y_i | f_i)] - \sum_{i=1}^n \langle \lambda_i, \tilde{\mu}_i - \mu_i \rangle - \text{KL}[q(\mathbf{f}; \boldsymbol{\mu}) \| p(\mathbf{f})]$$

Stationary point:

$q^*(\mathbf{f})$  has natural parameters  $\eta_q^* = \eta_p + \lambda^*$

$$0 = \nabla_{\lambda} \mathcal{L}_{\text{Lagrange}}$$

$$\Rightarrow \quad \mu^* = \tilde{\mu}^*$$

$$0 = \nabla_{\tilde{\mu}} \mathcal{L}_{\text{Lagrange}}$$

$$\Rightarrow \quad \lambda_i^* = \nabla_{\mu_i} \mathbb{E}_{q^*(f_i)} [\log p(y_i | f_i)]$$

$$0 = \nabla_{\mu} \mathcal{L}_{\text{Lagrange}}$$

$$\Rightarrow \quad \lambda^* = \underbrace{\nabla_{\mu} \text{KL}[q(\mathbf{f}; \mu^*) \| p(\mathbf{f})]}_{\eta_q - \eta_p}$$

## Optimal $q^*(\mathbf{f})$

Optimal  $q^*(\mathbf{f})$  has natural parameters  $\eta_q^* = \eta_p + \lambda^*$

Prior  $p(\mathbf{f})$  has natural parameters  $\eta_p = (0, -\frac{1}{2}\mathbf{K}^{-1})$

In mean–covariance parameterization:

$$\mathbf{m}^* = \mathbf{K}\boldsymbol{\alpha}^*$$

$$\boldsymbol{\alpha}^* = \mathbb{E}_{q^*(\mathbf{f})}[\nabla_{\mathbf{f}} \log p(\mathbf{y} | \mathbf{f})]$$

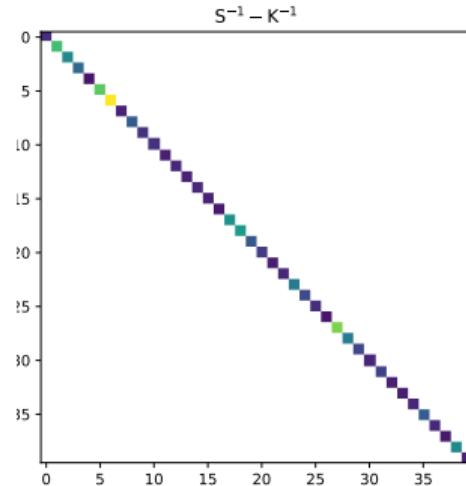
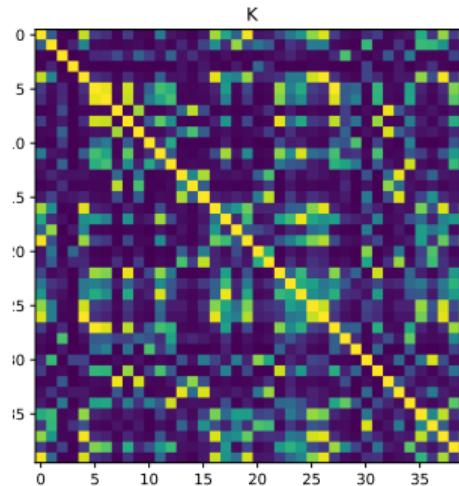
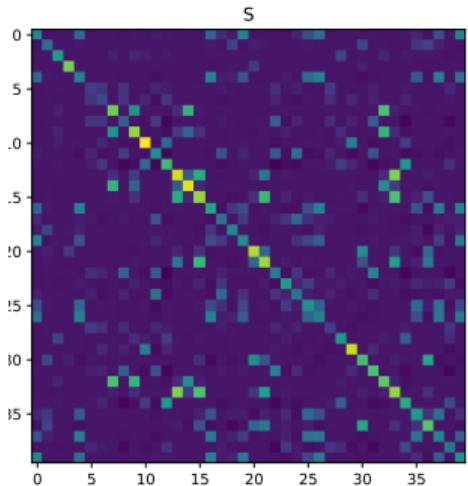
$$(\mathbf{S}^*)^{-1} = \mathbf{K}^{-1} + \boldsymbol{\beta}^*$$

$$\boldsymbol{\beta}^* = \mathbb{E}_{q^*(\mathbf{f})}[-\nabla_{\mathbf{f}}^2 \log p(\mathbf{y} | \mathbf{f})]$$

⇒ optimal Gaussian approximate posterior for factorizing likelihoods:

$$q^*(\mathbf{f}) = \frac{1}{Z} p(\mathbf{f}) \prod_{i=1}^n t_i(f_i)$$

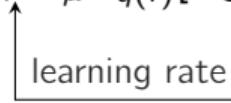
# Optimal posterior decomposition



# How to find $\alpha^*$ and $\beta_i^*$ ?

Natural gradient updates:

$$\lambda^{k+1} = (1 - \rho)\lambda^k + \rho \nabla_{\mu} \mathbb{E}_{q(\mathbf{f})} [\log p(\mathbf{y} | \mathbf{f})]$$

 learning rate

- ▶ cheap: same cost as standard gradient descent, no dense Hessian required!

## Learning hyperparameters $\theta$

$$p(\theta | \mathcal{D}) \propto \underbrace{p(\mathcal{D} | \theta)}_{\int p(\mathcal{D} | f) p(f | \theta) df} p(\theta)$$

- ▶  $p(\theta | \mathcal{D})$ : e.g. MCMC
- ▶ point estimate  $\theta^*$ 
  - ▶ maximum likelihood:  $\theta^* = \arg \max_{\theta} p(\mathcal{D} | \theta)$

## Marginal likelihood

$$\log p(\mathcal{D} \mid \theta) = \log \int p(\mathcal{D} \mid \mathbf{f}) p(\mathbf{f} \mid \theta) d\mathbf{f}$$

Laplace:

$$\begin{aligned}\log p(\mathbf{y} \mid \theta) &= \log \int \exp(\mathcal{L}_{\text{Lap}}(\mathbf{f})) d\mathbf{f} \\ &\approx \mathcal{L}_{\text{Lap}}(\mathbf{f}^*) - \frac{1}{2} \log \det S_{\text{Lap}} + \text{const.}\end{aligned}$$

VI:

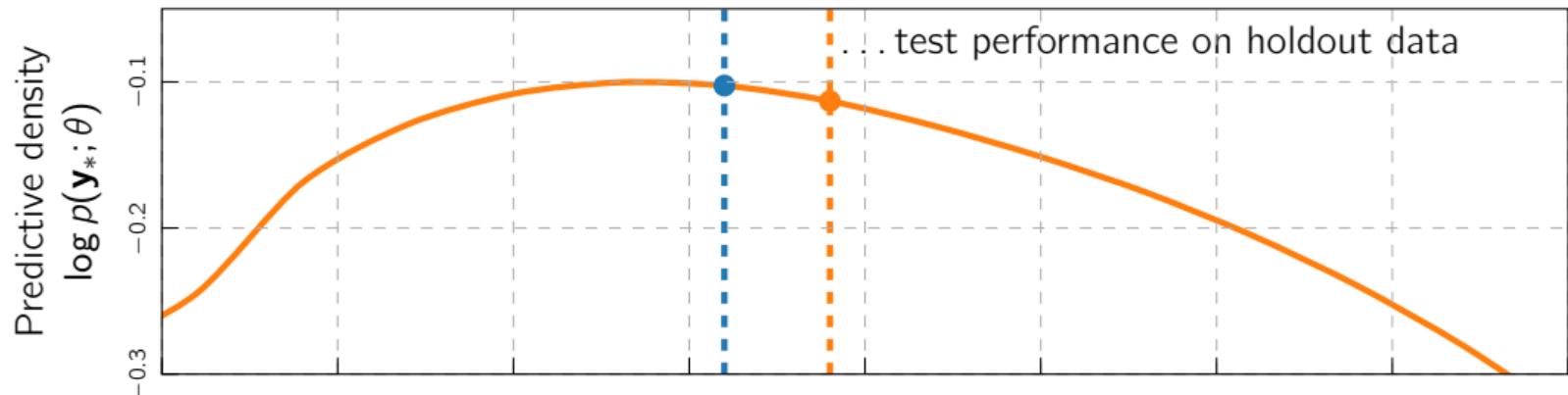
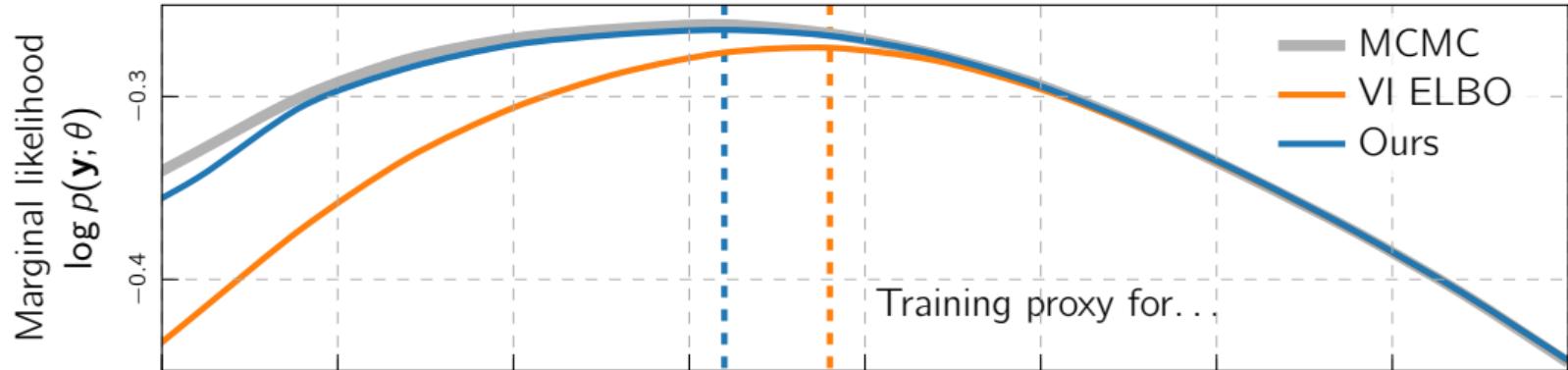
$$\log p(\mathbf{y} \mid \theta) \geq \mathcal{L}_{\text{ELBO}}[q^*]$$

EP:

$$\log p(\mathbf{y} \mid \theta) \approx \mathcal{L}_{\text{EP}}[q^*]$$

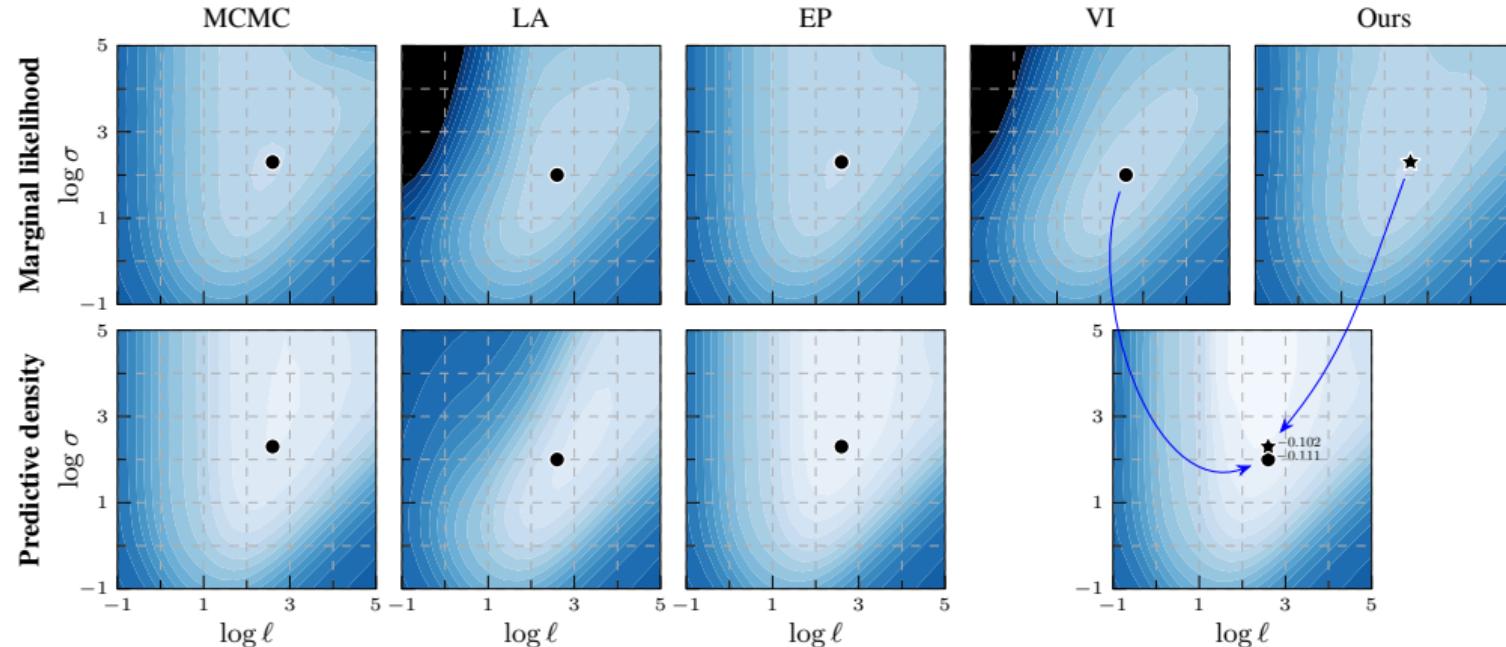
$$= \log \int p(\mathbf{f}) \prod_{i=1}^n t(f_i) d\mathbf{f}$$

Same form as dual parameterization!



Characteristic lengthscale,  $\log \theta$

# Marginal likelihood estimation



# Variational Expectation–Maximization

$$\text{E-step (inference): } \boldsymbol{\lambda}^{(k+1)} \leftarrow \arg \max_{\boldsymbol{\lambda}} \mathcal{L}_E(\boldsymbol{\lambda}, \boldsymbol{\theta}^{(k)})$$

$$\text{M-step (learning): } \boldsymbol{\theta}^{(k+1)} \leftarrow \arg \max_{\boldsymbol{\theta}} \mathcal{L}_M(\boldsymbol{\lambda}^{(k+1)}, \boldsymbol{\theta})$$

$$\mathcal{L}_E \equiv \mathcal{L}_{\text{ELBO}}$$

$$\mathcal{L}_M \equiv \mathcal{L}_{\text{EP}}$$

$(n, d)$	LA	EP	VI	Ours	MCMC
trains	(10, 30)	-0.702±0.025	-0.698±0.033	-0.702±0.037	-0.691±0.046
balloons	(16, 5)	-0.660±0.125	-0.650±0.128	-0.649±0.185	-0.607±0.227
fertility	(100, 10)	-0.388±0.122	-0.384±0.149	-0.393±0.136	-0.397±0.139
pittsburg-bridges-T-OR-D	(102, 8)	-0.299±0.081	-0.321±0.108	-0.290±0.110	-0.293±0.116
acute-nephritis	(120, 7)	-0.203±0.012	-0.046±0.007	-0.007±0.002	-0.005±0.002
acute-inflammation	(120, 7)	-0.184±0.018	-0.052±0.007	-0.007±0.002	-0.007±0.003
echocardiogram	(131, 11)	-0.424±0.093	-0.418±0.095	-0.425±0.110	-0.428±0.112
hepatitis	(155, 20)	-0.370±0.071	-0.372±0.072	-0.364±0.090	-0.367±0.094
parkinsons	(195, 23)	-0.260±0.031	-0.295±0.056	-0.160±0.050	-0.141±0.046
breast-cancer-wisc-prog	(198, 34)	-0.458±0.075	-0.473±0.091	-0.457±0.085	-0.460±0.088
spect	(265, 23)	-0.593±0.049	-0.590±0.055	-0.594±0.054	-0.595±0.054
statlog-heart	(270, 14)	-0.395±0.064	-0.389±0.061	-0.396±0.071	-0.397±0.071
haberman-survival	(306, 4)	-0.530±0.053	-0.532±0.059	-0.531±0.055	-0.531±0.055
ionosphere	(351, 34)	-0.224±0.042	-0.230±0.042	-0.170±0.048	-0.170±0.055
horse-colic	(368, 26)	-0.463±0.059	-0.452±0.057	-0.467±0.072	-0.473±0.082
congressional-voting	(435, 17)	-0.640±0.028	-0.639±0.030	-0.641±0.030	-0.642±0.029
cylinder-bands	(512, 36)	-0.488±0.038	-0.500±0.041	-0.465±0.049	-0.451±0.052
breast-cancer-wisc-diag	(569, 31)	-0.085±0.026	-0.140±0.020	-0.077±0.044	-0.075±0.045
ilpd-indian-liver	(583, 10)	-0.513±0.040	-0.520±0.041	-0.512±0.043	-0.512±0.043
monks-2	(601, 7)	-0.491±0.025	-0.512±0.028	-0.464±0.031	-0.442±0.033
statlog-australian-credit	(690, 15)	-0.630±0.026	-0.639±0.036	-0.630±0.026	-0.630±0.026
credit-approval	(690, 16)	-0.342±0.047	-0.342±0.050	-0.341±0.052	-0.342±0.052
breast-cancer-wisc	(699, 10)	-0.094±0.025	-0.093±0.023	-0.093±0.029	-0.093±0.029
blood	(748, 5)	-0.478±0.039	-0.479±0.040	-0.478±0.039	-0.478±0.039
pima	(768, 9)	-0.474±0.033	-0.476±0.038	-0.474±0.035	-0.474±0.035
mammographic	(961, 6)	-0.407±0.038	-0.407±0.040	-0.408±0.040	-0.408±0.040
statlog-german-credit	(1000, 25)	-0.491±0.030	-0.491±0.032	-0.492±0.032	-0.492±0.032

Bold Count

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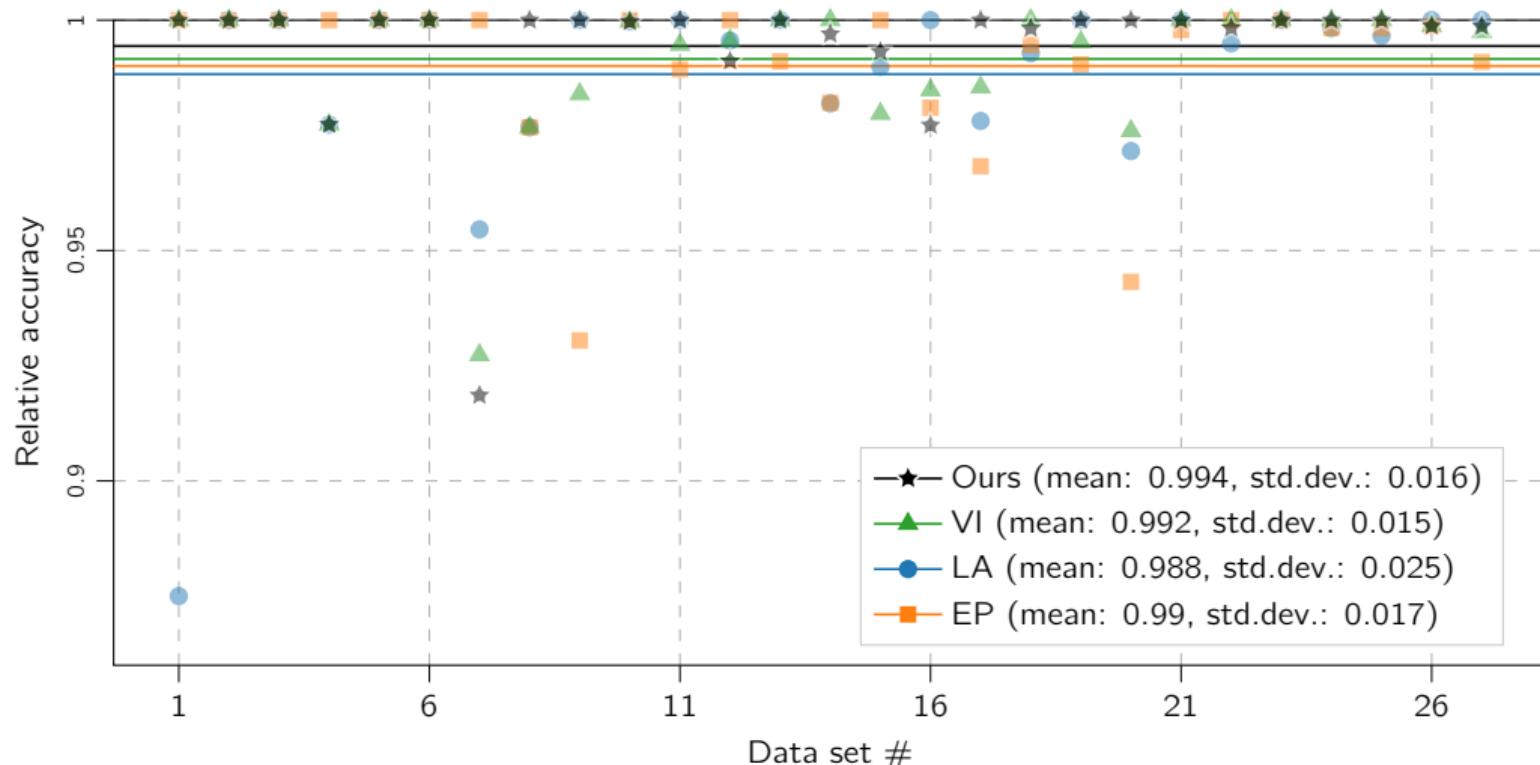
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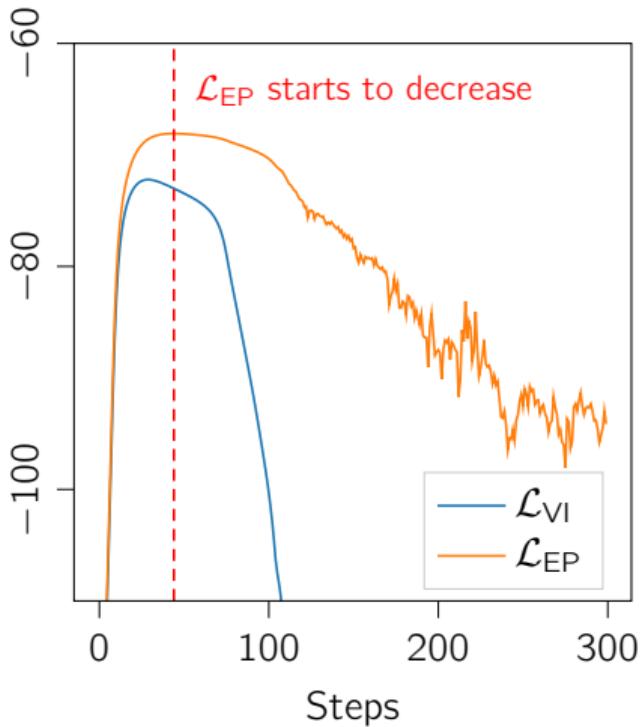
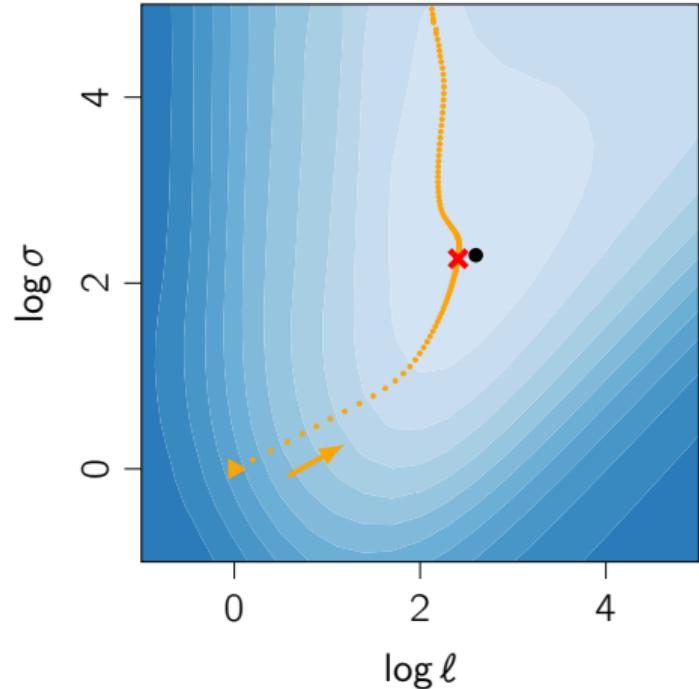
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## Relative accuracy (compared to best method on each data set)



## Optimization issues. . .



## What about big data?

Sparse approximation using  $\mathbf{u} = f(\mathbf{Z})$ :

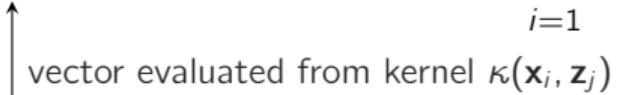
$$q_{\mathbf{u}}(f(\cdot); \boldsymbol{\xi}_{\mathbf{u}}, \boldsymbol{\theta}) = \int p(f(\cdot) | \mathbf{u}; \boldsymbol{\theta}) q(\mathbf{u}; \boldsymbol{\xi}_{\mathbf{u}}) d\mathbf{u},$$

Dual parameters:

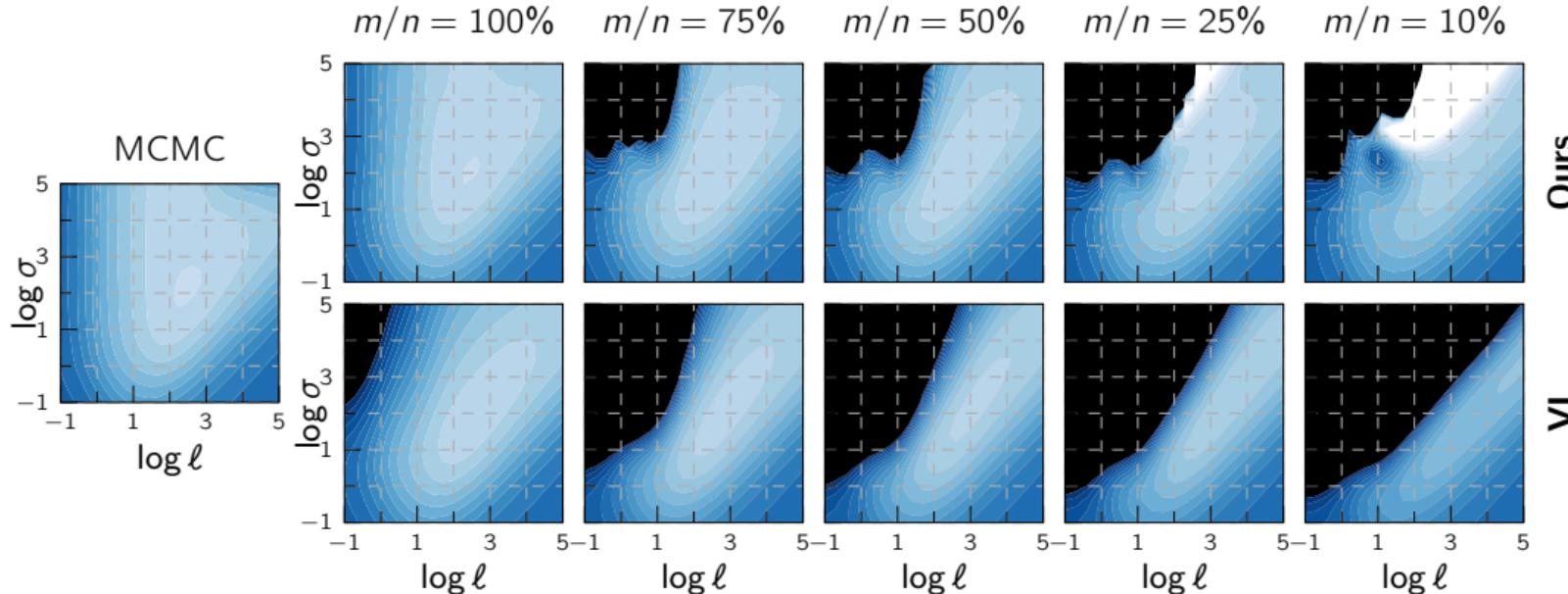
$$\hat{\alpha}_i = \mathbb{E}_{q_{\mathbf{u}}(f_i)}[\nabla_{f_i} \log p(y_i | f_i)] \quad \hat{\beta}_i = \mathbb{E}_{q_{\mathbf{u}}(f_i)}[-\nabla_{f_i}^2 \log p(y_i | f_i)]$$

Projection onto sparse inducing points:

$$\boldsymbol{\alpha}_{\mathbf{u}} = \sum_{i=1}^n \mathbf{k}_{z_i} \hat{\alpha}_i \quad \mathbf{B}_{\mathbf{u}} = \sum_{i=1}^n \mathbf{k}_{z_i} \hat{\beta}_i \mathbf{k}_{z_i}^{\top}$$

  
vector evaluated from kernel  $\kappa(\mathbf{x}_i, \mathbf{z}_j)$

# Sparse marginal likelihood approximations



## Additive structure of dual parameterization in sequential learning

$$\begin{aligned}\hat{\alpha}_i &= \mathbb{E}_{q_{\mathbf{u}}(f_i)}[\nabla_{f_i} \log p(y_i | f_i)] & \hat{\beta}_i &= \mathbb{E}_{q_{\mathbf{u}}(f_i)}[-\nabla_{f_i}^2 \log p(y_i | f_i)] \\ \boldsymbol{\alpha}_{\mathbf{u}} &= \sum_{i=1}^n \mathbf{k}_{z_i} \hat{\alpha}_i & \mathbf{B}_{\mathbf{u}} &= \sum_{i=1}^n \mathbf{k}_{z_i} \hat{\beta}_i \mathbf{k}_{z_i}^\top\end{aligned}$$

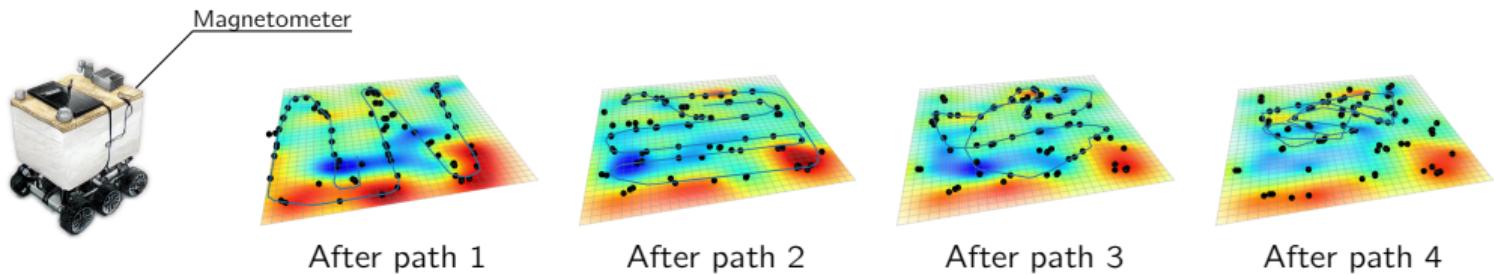
$$\mathcal{L}_{\text{batch}}(\mathbf{m}, S | \mathcal{D}) = \sum_{i \in \mathcal{D}} \mathbb{E}_{q_{\mathbf{u}}(f_i)}[\log p(y_i | f_i)] - \text{KL}[q_{\mathbf{u}}(\mathbf{u}) \| p_{\theta}(\mathbf{u})]$$

$$\mathcal{L}_{\text{batch}}(\mathbf{m}, S | \cancel{\mathcal{D}_{\text{old}}} \cup \mathcal{D}_{\text{new}}) = \sum_{i \in \cancel{\mathcal{D}_{\text{old}}} \cup \mathcal{D}_{\text{new}}} \mathbb{E}_{q_{\mathbf{u}}(f_i)}[\log p(y_i | f_i)] - \text{KL}[q_{\mathbf{u}}(\mathbf{u}) \| p_{\theta}(\mathbf{u})]$$

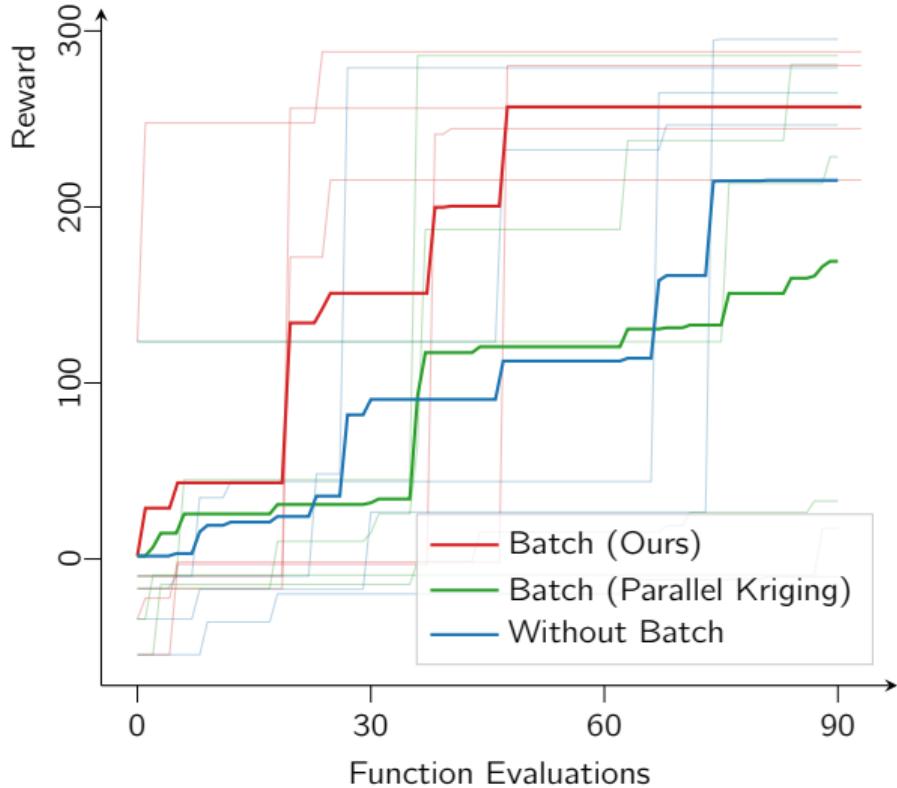
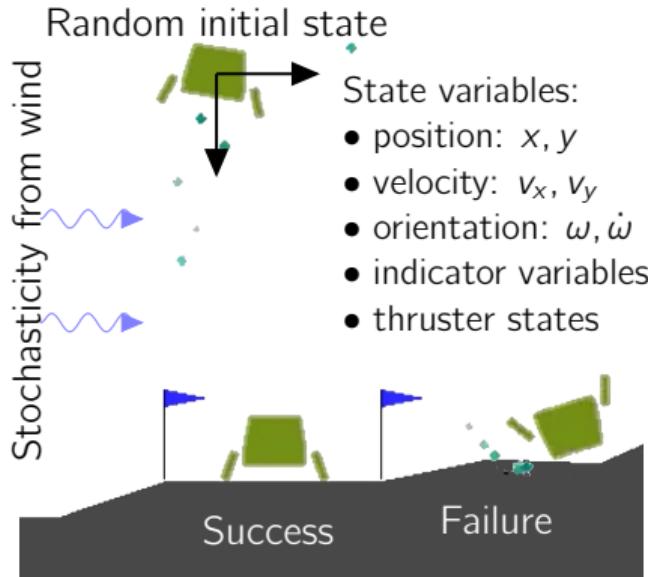
$$\boldsymbol{\alpha}_{\mathbf{u}} = \boldsymbol{\alpha}_{\mathbf{u}}^{\text{old}} + \boldsymbol{\alpha}_{\mathbf{u}}^{\text{new}} \quad \text{and} \quad \mathbf{B}_{\mathbf{u}} = \mathbf{B}_{\mathbf{u}}^{\text{old}} + \mathbf{B}_{\mathbf{u}}^{\text{new}}$$

- ▶ natural gradient descent on new batch to find  $\boldsymbol{\alpha}_{\mathbf{u}}^{\text{new}}$  and  $\mathbf{B}_{\mathbf{u}}^{\text{new}}$

# Continual learning



# Bayesian optimization with fantasizing



# Learning from the dual parameterization

- ▶ Dual parameters: derivatives of log likelihood  $\Leftrightarrow$  sensitivities w.r.t. data points
- + Cheap natural gradient updates
- + EP-like objective for hyperparameter learning
- + Good parameterization for sequential learning

## Find out more:

- 📄 *Improving Hyperparameter Learning under Approximate Inference in Gaussian Process Models.* Li, John, & Solin; ICML 2023. ([arXiv:2306.04201](https://arxiv.org/abs/2306.04201) - 📄 *Memory-Based Dual Gaussian Processes for Sequential Learning.* Chang, Verma, John, Solin, & Khan; ICML 2023. ([arXiv:2306.03566](https://arxiv.org/abs/2306.03566) - 📄 *Dual parameterization for dummies* (in preparation, coming to an arXiv near you)