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Distributed Gaussian Processes

Recommended reading:

Deisenroth & Ng (2015) [2]

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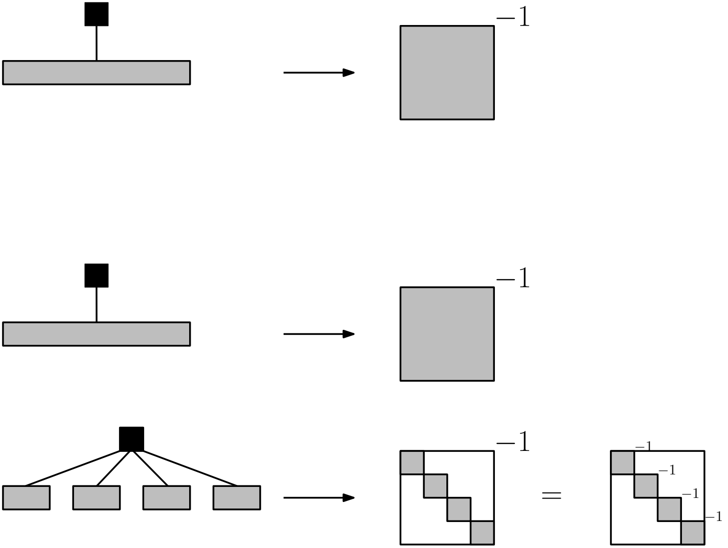
Large-Scale GPs via Distributed Inference



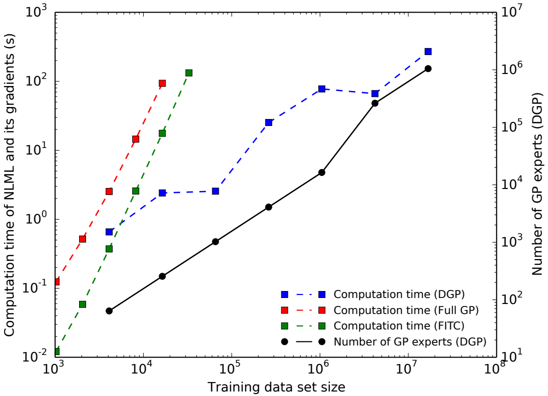
Training the Distributed GP

- Split data set of size N into M chunks of size P
- Independence of experts ⏩ Factorization of marginal likelihood:

$$\log p(\boldsymbol{y}|\boldsymbol{X}, \boldsymbol{\theta}) \approx \sum_{k=1}^{M} \log p_k(\boldsymbol{y}^{(k)}|\boldsymbol{X}^{(k)}, \boldsymbol{\theta})$$

- Distributed optimization and training straightforward
- Computational complexity: $\mathcal{O}(MP^3)$ [instead of $\mathcal{O}(N^3)$]
  But distributed over many machines
- Memory footprint: $\mathcal{O}(MP^2 + ND)$ [instead of $\mathcal{O}(N^2 + ND)$]

Empirical Training Time



- NLML is proportional to training time
- Full GP (16K training points) $\approx$ sparse GP (50K training points) $\approx$ distributed GP (16M training points)

▶▶ Push practical limit by order(s) of magnitude

Practical Training Times

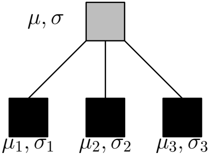
- Training* with $N = 10^6, D = 1$ on a laptop: $\approx$ 30 min
- Training* with $N = 5 \times 10^6, D = 8$ on a workstation: $\approx$ 4 hours

*: Maximize the marginal likelihood, stop when converged**

: Convergence often after 30–80 line searches*

***: Line search $\approx$ 2–3 evaluations of marginal likelihood and its gradient (usually $\mathcal{O}(N^3)$)

Predictions with the Distributed GP



- Prediction of each GP expert is Gaussian $\mathcal{N}(\mu_i, \sigma_i^2)$
- How to combine them to an overall prediction $\mathcal{N}(\mu, \sigma^2)$?

▸▸ Product-of-GP-experts

- PoE (product of experts) ▸▸ (Ng & Deisenroth, 2014)
- gPoE (generalized product of experts) ▸▸ (Cao & Fleet, 2014)
- BCM (Bayesian Committee Machine) ▸▸ (Tresp, 2000)
- rBCM (robust BCM) ▸▸ (Deisenroth & Ng, 2015)

Objectives

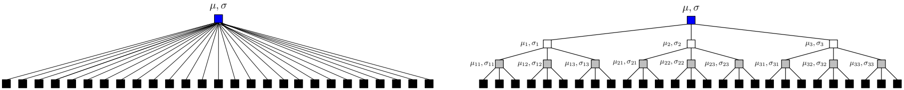
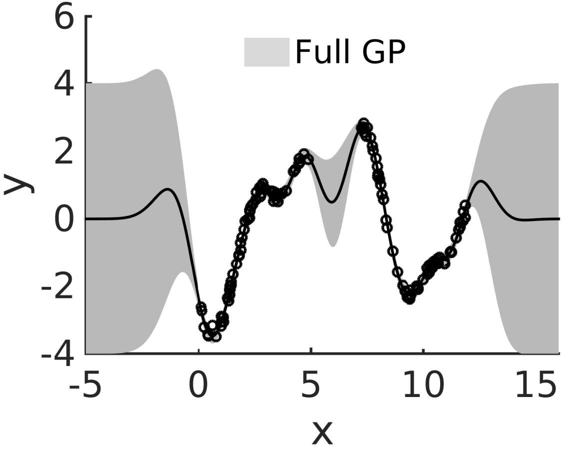


Figure: Two computational graphs

- Scale to large data sets ✓
- Good approximation of full GP ("ground truth")
- Predictions independent of computational graph

  ⏩ Runs on heterogeneous computing infrastructures (laptop, cluster, ...)
- Reasonable predictive variances

Running Example



- Investigate various product-of-experts models
  Same training procedure, but different mechanisms for predictions

Product of GP Experts

- Prediction model (independent predictors):

$$p(f_*|\boldsymbol{x}_*, \mathcal{D}) = \prod_{k=1}^{M} \overbrace{p_k(f_*|\boldsymbol{x}_*, \mathcal{D}^{(k)})}^{\text{GP expert}},$$

$$p_k(f_*|\boldsymbol{x}_*, \mathcal{D}^{(k)}) = \mathcal{N}\big(f_* \mid \mu_k(\boldsymbol{x}_*), \sigma_k^2(\boldsymbol{x}_*)\big)$$

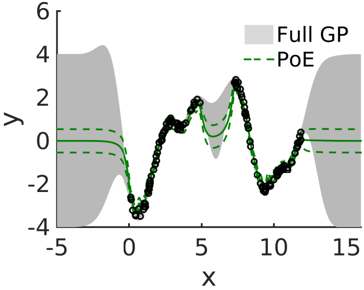
- Predictive precision (inverse variance) and mean:

$$(\sigma_*^{\text{poe}})^{-2} = \sum\nolimits_k \sigma_k^{-2}(\boldsymbol{x}_*)$$

$$\mu_*^{\text{poe}} = (\sigma_*^{\text{poe}})^2 \sum\nolimits_k \sigma_k^{-2}(\boldsymbol{x}_*)\mu_k(\boldsymbol{x}_*)$$

- Independent of the computational graph ✓

Product of GP Experts



- Unreasonable variances for $M > 1$:

$$(\sigma_*^{\text{poe}})^{-2} = \sum\nolimits_k \sigma_k^{-2}(\boldsymbol{x}_*)$$

- The more experts the more certain the prediction, even if every expert itself is very uncertain ✗ ⏩ Cannot fall back to the prior

Generalized Product of GP Experts (Cao & Fleet, 2014)

- Weight the responsiblity of each expert in PoE with β_k
- Prediction model (independent predictors):

$$p(f_*|\boldsymbol{x}_*, \mathcal{D}) = \prod_{k=1}^{M} p_k^{\beta_k}(f_*|\boldsymbol{x}_*, \mathcal{D}^{(k)})$$

$$p_k(f_*|\boldsymbol{x}_*, \mathcal{D}^{(k)}) = \mathcal{N}\big(f_* \mid \mu_k(\boldsymbol{x}_*),\, \sigma_k^2(\boldsymbol{x}_*)\big)$$

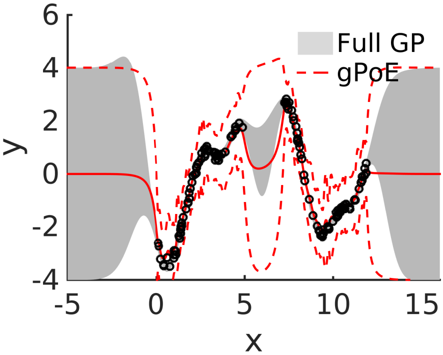
- Predictive precision and mean:

$$(\sigma_*^{\text{gpoe}})^{-2} = \sum\nolimits_k \beta_k \sigma_k^{-2}(\boldsymbol{x}_*)$$

$$\mu_*^{\text{gpoe}} = (\sigma_*^{\text{gpoe}})^2 \sum\nolimits_k \beta_k \sigma_k^{-2}(\boldsymbol{x}_*)\, \mu_k(\boldsymbol{x}_*)$$

- With $\sum_k \beta_k = 1$, the model can fall back to the prior ✓
  "Log-opinion pool" model (Heskes, 1998)
- Independent of computational graph for $\beta_k = 1/M$ ✓

Generalized Product of GP Experts (Cao & Fleet, 2014)



- Same mean as PoE
- Model no longer overconfident and falls back to prior ✓
- Very conservative variances ✗

Bayesian Committee Machine (Tresp, 2000)

- Apply Bayes' theorem when combining predictions (and not only for computing predictions)
- Prediction model ($\mathcal{D}^{(j)} \perp\!\!\!\perp \mathcal{D}^{(k)} | f_*$):

$$p(f_*|\boldsymbol{x}_*, \mathcal{D}) = \frac{\prod_{k=1}^{M} p_k(f_*|\boldsymbol{x}_*, \mathcal{D}^{(k)})}{p^{M-1}(f_*)}$$

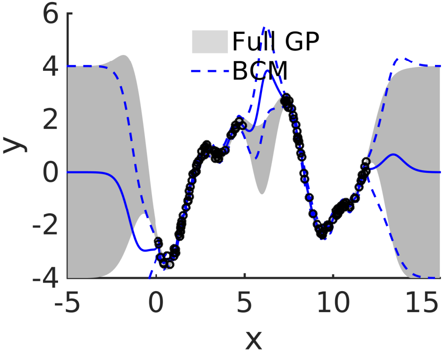
- Predictive precision and mean:

$$(\sigma_*^{\text{bcm}})^{-2} = \sum_{k=1}^{M} \sigma_k^{-2}(\boldsymbol{x}_*) - (M-1)\sigma_{**}^{-2}$$

$$\mu_*^{\text{bcm}} = (\sigma_*^{\text{bcm}})^2 \sum_{k=1}^{M} \sigma_k^{-2}(\boldsymbol{x}_*)\mu_k(\boldsymbol{x}_*)$$

- Product of GP experts, divided by $M-1$ times the prior
- Guaranteed to fall back to the prior outside data regime ✓
- Independent of computational graph ✓

Bayesian Committee Machine



- Variance estimates are about right ✓
- When leaving the data regime, the BCM can produce junk ✗

  ⏩ **Robustify**

Robust Bayesian Committee Machine

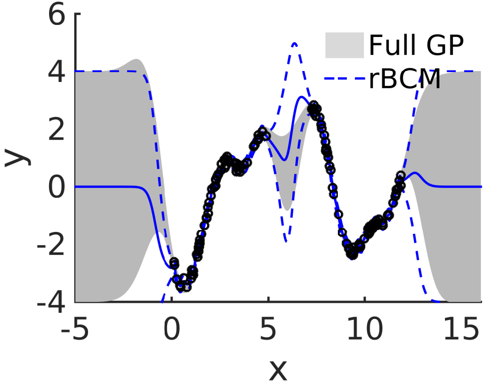
- Merge gPoE (weighting of experts) with the BCM (Bayes' theorem when combining predictions)
- Prediction model (conditional independence $\mathcal{D}^{(j)} \perp\!\!\!\perp \mathcal{D}^{(k)} | f_*$):

$$p(f_*|\boldsymbol{x}_*, \mathcal{D}) = \frac{\prod_{k=1}^{M} p_k^{\beta_k}(f_*|\boldsymbol{x}_*, \mathcal{D}^{(k)})}{p^{\sum_k \beta_k - 1}(f_*)}$$

- Predictive precision and mean:

$$(\sigma_*^{\text{rbcm}})^{-2} = \sum_{k=1}^{M} \beta_k \sigma_k^{-2}(\boldsymbol{x}_*) + (1 - \sum_{k=1}^{M} \beta_k) \sigma_{**}^{-2},$$
$$\mu_*^{\text{rbcm}} = (\sigma_*^{\text{rbcm}})^2 \sum_k \beta_k \sigma_k^{-2}(\boldsymbol{x}_*) \mu_k(\boldsymbol{x}_*)$$

Robust Bayesian Committee Machine



- Does not break down in case of weak experts ⏩ Robustified ✓
- Robust version of BCM ⏩ Reasonable predictions ✓
- Independent of computational graph (for all choices of β_k) ✓

Setting the Weighting β_k

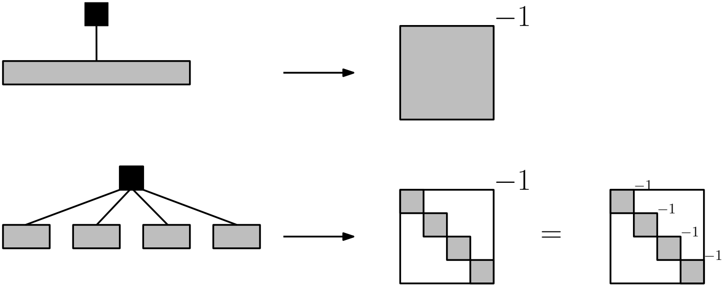
- The gPoE and the rBCM have a β_k parameter that assigns individual experts different weights when predicting:

$$p(f_*|\boldsymbol{x}_*, \mathcal{D}) = \prod_{k=1}^{M} p_k^{\beta_k}(f_*|\boldsymbol{x}_*, \mathcal{D}^{(k)})$$

$$p(f_*|\boldsymbol{x}_*, \mathcal{D}) = \frac{\prod_{k=1}^{M} p_k^{\beta_k}(f_*|\boldsymbol{x}_*, \mathcal{D}^{(k)})}{p^{\sum_k \beta_k - 1}(f_*)}$$

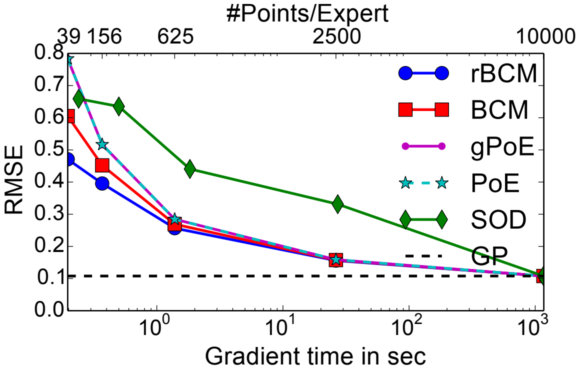
- Intuition: Set $\beta_k(\boldsymbol{x}_*)$ such that "informed" GP experts get more influence
- Use some distance/divergence between GP prior and GP posterior at test point $\boldsymbol{x}_*$
- Some options for β_k:
    - $\beta_k \propto \mathrm{KL}(\text{prior}||\text{posterior})$
    - $\beta_k \propto \mathrm{DiffEnt}(\text{prior}, \text{posterior})$

Splitting the Data



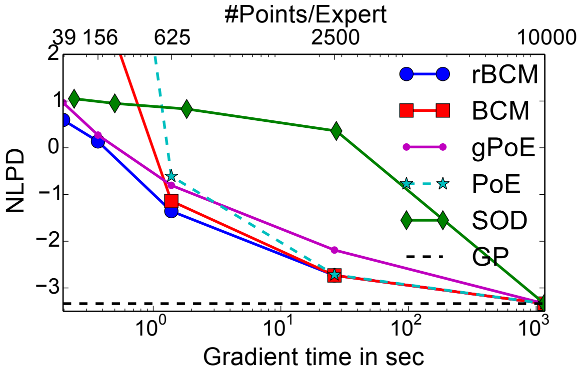
- Data sets should be of approximately the same size
- Random assignment of data points to experts
- Cluster inputs (e.g., k-means), assign clusters to experts

Empirical Approximation Error (1)



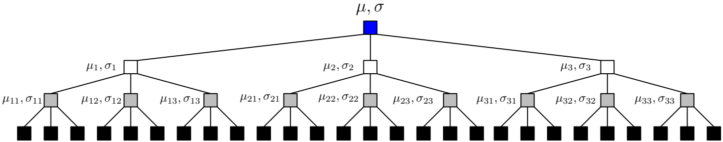
- Simulated robot arm data (10K training, 10K test)
- Hyper-parameters of ground-truth full GP
- RMSE as a function of the training time
- Subset of data (SOD) performs worse than any distributed GP
- rBCM performs best with “weak” GP experts

Empirical Approximation Error (2)



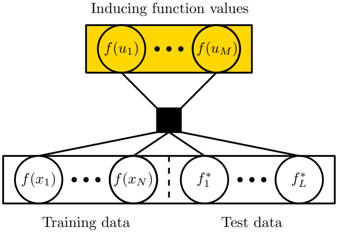
- NLPD as a function of the training time ▶▶ Mean and variance
- BCM and PoE are not robust for weak experts
- gPoE suffers from too conservative variances
- rBCM consistently outperforms other methods

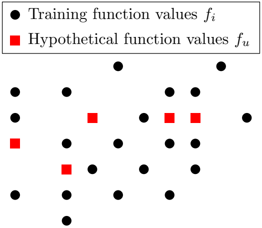
Summary: Distributed Gaussian Processes



- Scale Gaussian processes to large data (beyond 10^6)
- Model conceptually straightforward and easy to train
- Key: Distributed computation
- Currently tested with $N > 10^7$
- Scales to arbitrarily large data sets (with enough computing power)

Scaling GPs using Inducing Inputs





- Introduce inducing function values f_u
  ▶▶ "Hypothetical" function values
- All function values are still jointly Gaussian distributed (e.g., training, test and inducing function values)
- Compress information into inducing function values
- Selected references: [8–10, 5, 4, 12, 3]

References I

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Appendix

BCM: Derivation

Conditional Independence Assumption (BCM)

$\mathcal{D}^{(j)} \perp\!\!\!\perp \mathcal{D}^{(k)} | f_*$

$$
\begin{aligned}
p(f_*|\mathcal{D}^{(j)}, \mathcal{D}^{(k)}) &\propto p(\mathcal{D}^{(j)}, \mathcal{D}^{(k)}|f_*)p(f_*) \\
&\overset{\text{BCM}}{=} p(\mathcal{D}^{(j)}|f_*)\, p(\mathcal{D}^{(k)}|f_*)p(f_*) \\
&= \frac{p(\mathcal{D}^{(j)}, f_*)\, p(\mathcal{D}^{(k)}, f_*)}{p(f_*)} \\
&\propto \frac{p_k(f_*|\mathcal{D}^{(k)})p_j(f_*|\mathcal{D}^{(j)})}{p(f_*)}
\end{aligned}
$$