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Distributed Gaussian Processes for Large-Scale Probabilistic Regression

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Joint work with Jun Wei Ng

Workshop on Gaussian Process Approximations
Copenhagen, 21 May 2015

Scaling Gaussian Processes to Large Data Sets

Two orthogonal approaches

- Sparse Gaussian processes
  - ⏩ Use (smart) subset of data.
- Distributed Gaussian processes
  - ⏩ Use full data set, distribute computations

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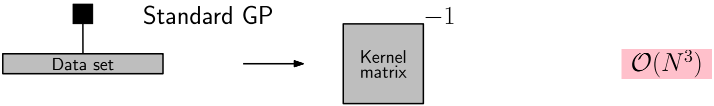
- Computational complexity: $\mathcal{O}(M^3)$ or $O(NM^2)$ for training
- Practical limit of the data set size is $N \in \mathcal{O}(10^6)$

Distributed Gaussian Processes



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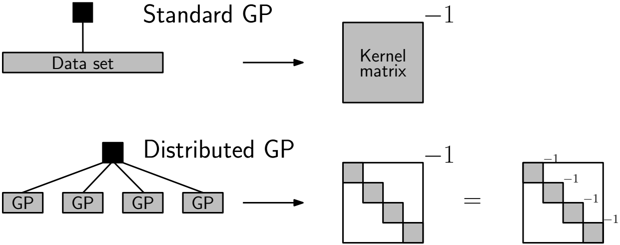
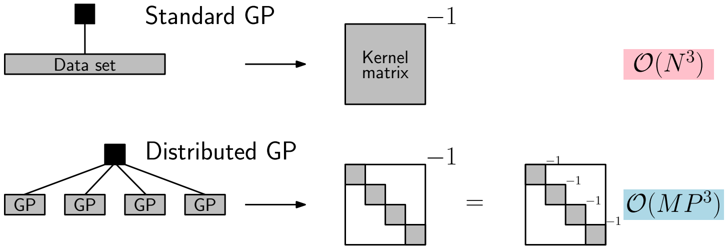


$\mathcal{O}(N^3)$

$\mathcal{O}(MP^3)$

- Randomly split the full data set into M chunks of size P

Distributed Gaussian Processes



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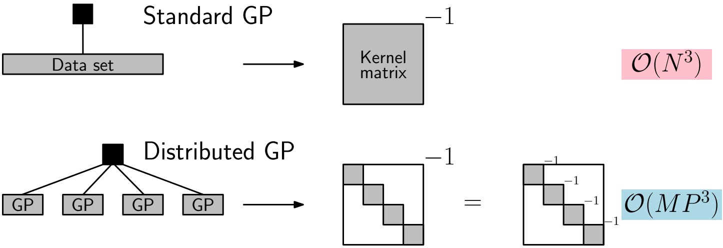

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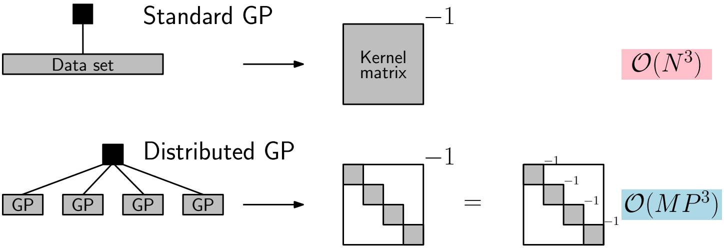

- Randomly split the full data set into M chunks of size P
- Place M independent GP experts on these small chunks
- Block-diagonal approximation of kernel matrix $\boldsymbol{K}$ (sim. to PIC)
- Combine independent computations to an overall result

Training the Distributed GP

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

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

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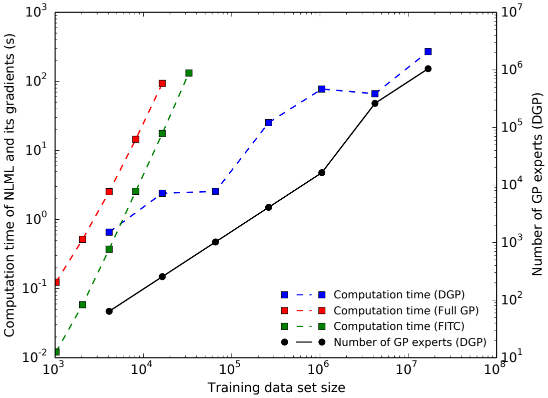
- Distributed optimization and training straightforward
- No inducing/variational parameters ⏩ Easy optimization
- Computational complexity: $\mathcal{O}(MP^3)$ [instead of $\mathcal{O}(N^3)$]
- Memory footprint: $\mathcal{O}(MP^2 + ND)$ [instead of $\mathcal{O}(N^2 + ND)$], potentially distributed across M computing nodes

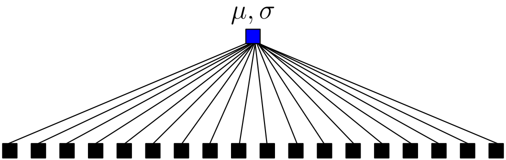
Scaling



- NLML is proportional to training time
- Full GP (16K training points) $\approx$ sparse GP (32K training points) $\approx$ distributed GP (16M training points)

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

Predictions with the Distributed GP



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- How to combine them to an overall prediction $\mathcal{N}(\mu, \sigma^2)$?

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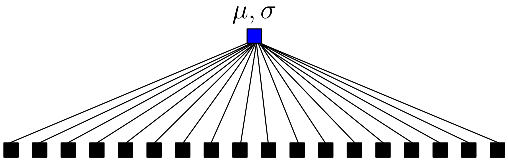

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▸▸ Product-of-GP-experts

- 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)

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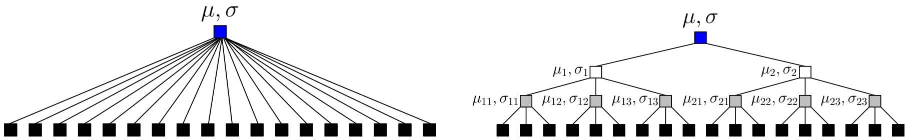

Figure: Two computational graphs

- Scale to large data sets ✓
- Good approximation of full GP ("ground truth")
- Predictions independent of computational graph
  ⏩ Heterogeneous computing infrastructures (laptop, cluster, ...)

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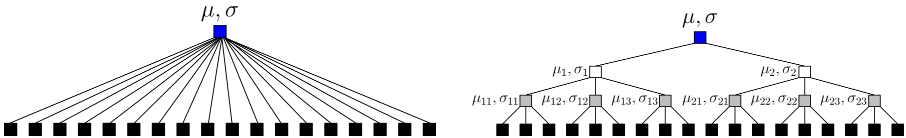
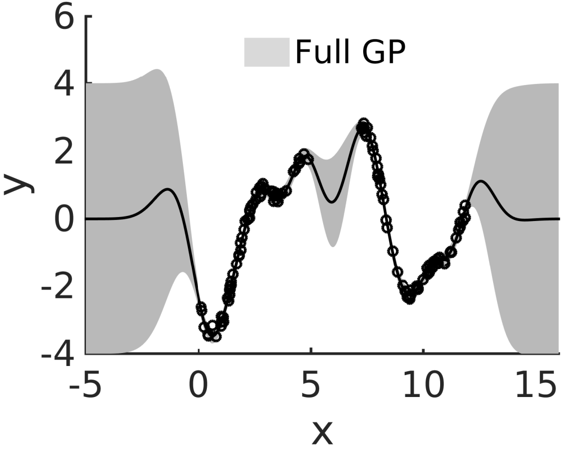


Figure: Two computational graphs

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

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

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

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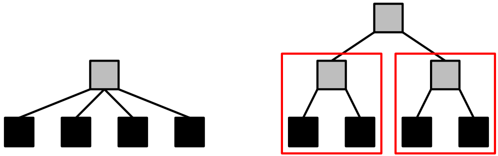
Computational Graph



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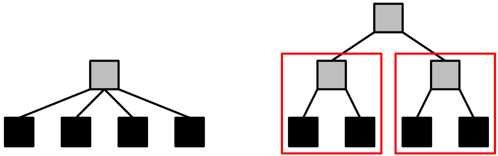

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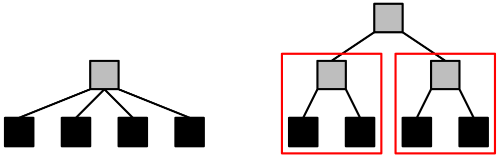

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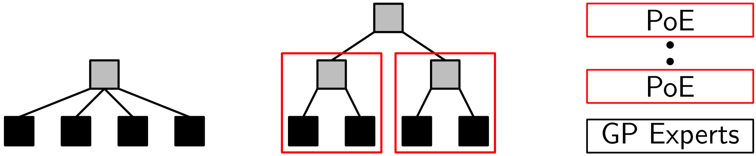
Computational Graph



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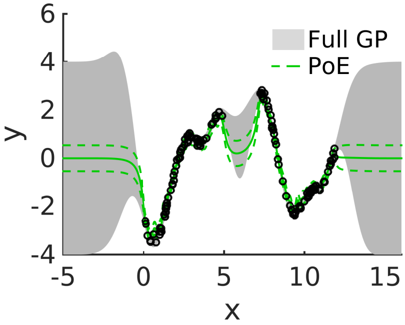
Product of GP Experts



- Unreasonable variances for $M > 1$:

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

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

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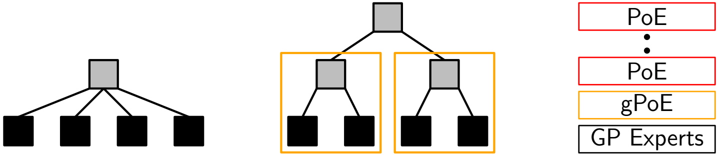
- With $\sum_k \beta_k = 1$, the model can fall back to the prior ✓

  ▸▸ Log-opinion pool model (e.g., Heskes, 1998)

Computational Graph



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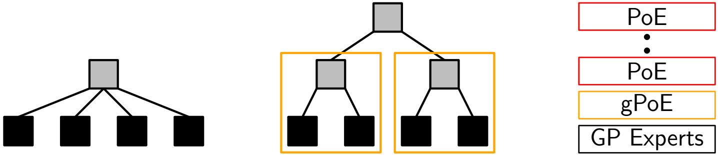

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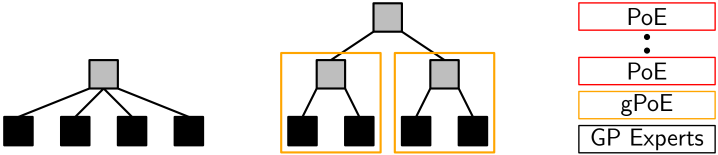

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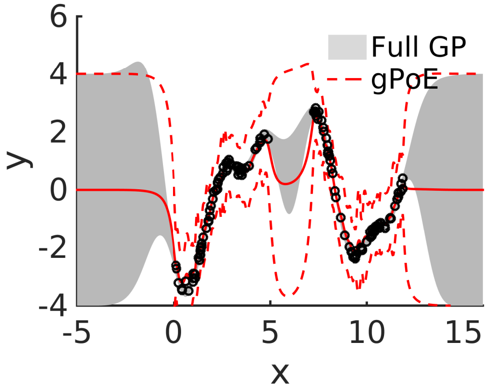
- Independent of computational graph if $\sum_{k,i} \beta_{k_i} = 1$ ✓
- A priori setting of β_{k_i} required ✗
  - ▸▸ $\beta_{k_i} = 1/M$ a priori (✓)

Generalized Product of GP Experts



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

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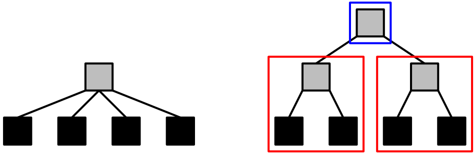
- Guaranteed to fall back to the prior outside data regime ✓

Computational Graph



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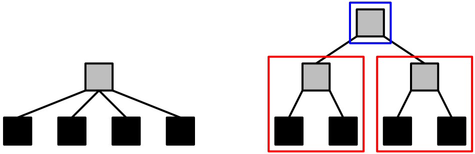

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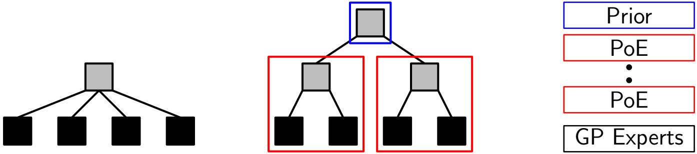

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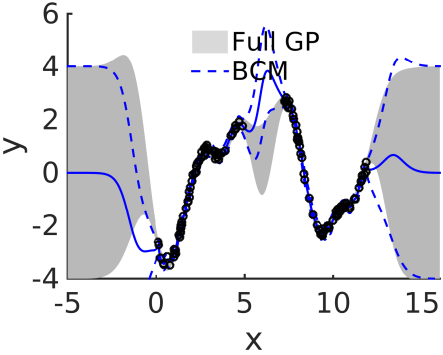
Bayesian Committee Machine



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

  ▸▸ **Robustify**

Robust Bayesian Committee Machine

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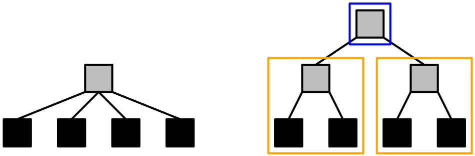
- Predictive precision and mean:

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

$$\mu_*^{\text{rbcm}} = (\sigma_*^{\text{rbcm}})^2 \sum_k \beta_k \sigma_k^{-2}(\boldsymbol{x}_*) \mu_k(\boldsymbol{x}_*)$$

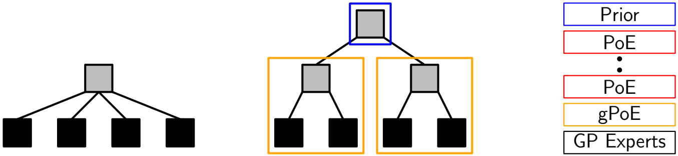
Computational Graph



Prediction:

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

Computational Graph

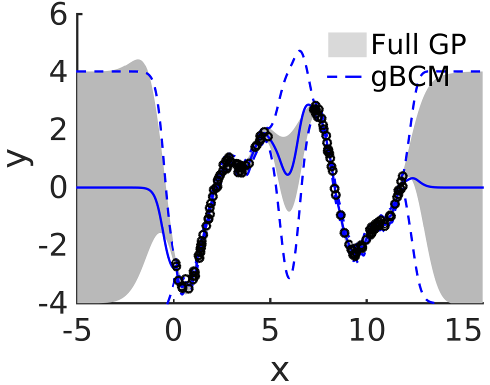


Prediction:

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

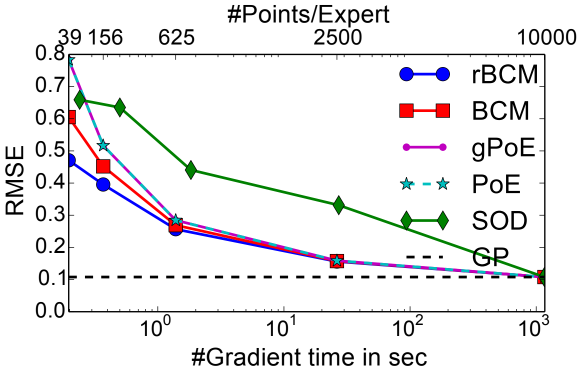
▸▸ Independent of computational graph, even with arbitrary β_k ✓

Robust Bayesian Committee Machine



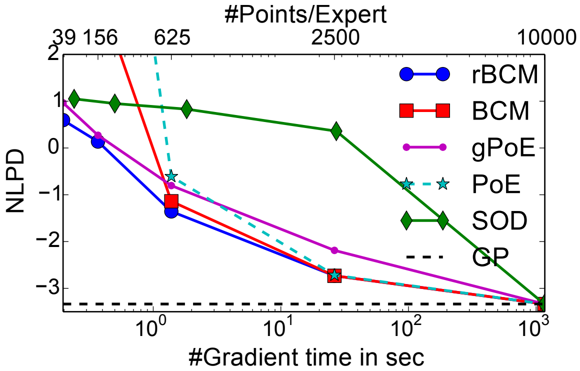
- Does not break down in case of weak experts ⏩ Robustified ✓
- Robust version of BCM ⏩ Reasonable predictions ✓
- Independent of computational graph (for all choices of β_k) ✓

Empirical Approximation Error



- Simulated robot arm data (10K training, 30K test)
- All models use hyper-parameters of ground-truth full GP
- RMSE as a function of the training time
- Sparse GP (SOD) performs worse than any distributed GP
- rBCM performs best with "weak" GP experts

Empirical Approximation Error (2)

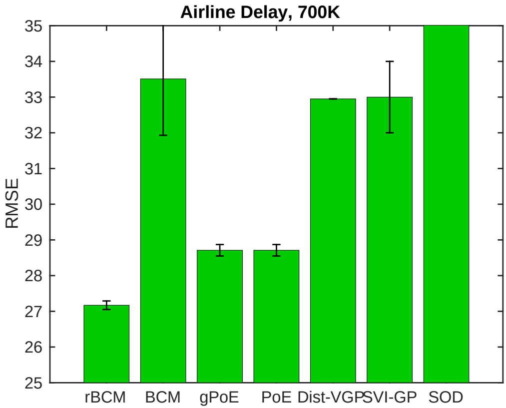


- NLPD as a function of the training time ⏩ Mean and variance
- BCM and PoE are not robust to weak experts
- gPoE suffers from too conservative variances
- rBCM consistently outperforms other methods

Large Data

- Predict US Airline Delays (01/2008–04/2008) of commercial flights
- Inputs: age of aircraft, flight distance, departure/arrival time, airtime, day of week, day of month, month,
- Training data: 700K, 2M, 5M. Test data: 100K

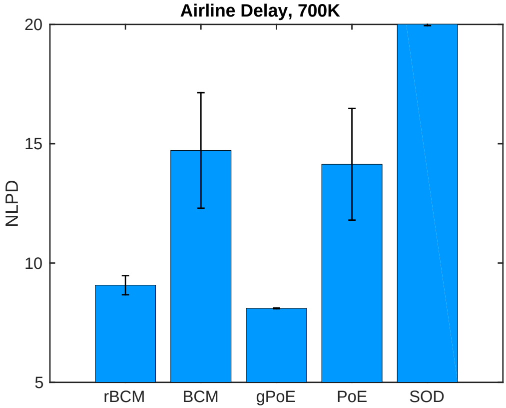
Training Data: 700K — RMSE



- (r)BCM and (g)PoE with 4096 GP experts
- Gradient time: 13 seconds (12 cores)
- Inducing inputs: Dist-VGP (Gal et al., 2014), SVI-GP (Hensman et al., 2013)

- rBCM performs best
- (g)PoE and BCM performs not worse sparse GPs

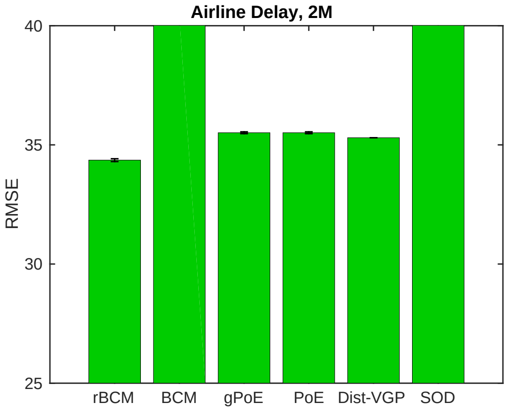
Training Data: 700K — NLPD



- (r)BCM and (g)PoE with 4096 GP experts
- Gradient time: 13 seconds (12 cores)
- No results reported for inducing input methods (Gal et al., 2014; Hensman et al., 2013)

- gPoE performs best, just ahead of rBCM

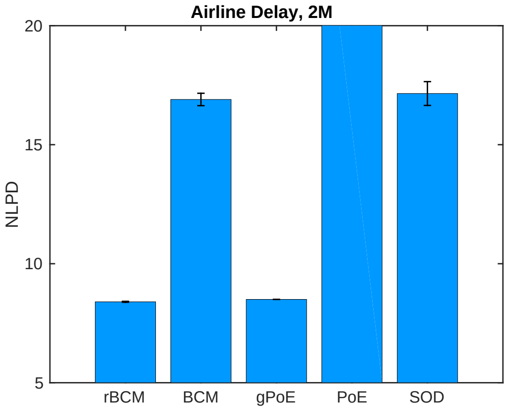
Training Data: 2M — RMSE



- (r)BCM and (g)PoE with 8192 GP experts
- Gradient time: 39 seconds (12 cores)
- Inducing inputs: Dist-VGP (Gal et al., 2014)

- rBCM performs best
- (g)PoE as good as best results reported for sparse methods
- BCM suffers from weak experts

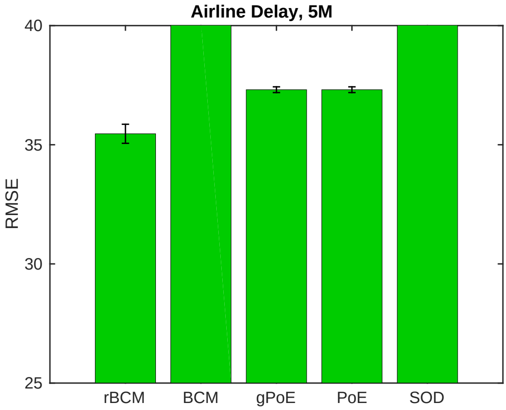
Training Data: 2M — NLPD



- (r)BCM and (g)PoE with 8192 GP experts
- Gradient time: 39 sec (12 cores)
- Inducing inputs: no results reported

- rBCM and gPoE perform best
- BCM suffers from weak experts
- PoE suffers from under-estimation of variances

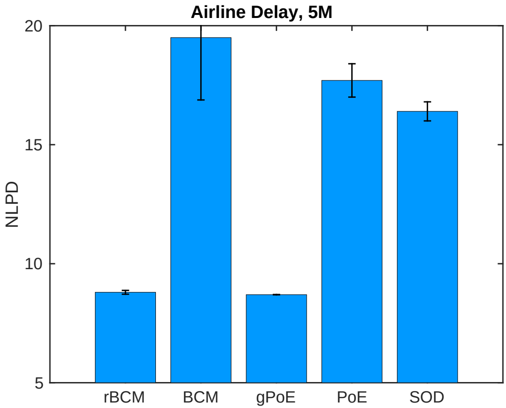
Training Data: 5M — RMSE



- (r)BCM and (g)PoE with 32768 GP experts
- Gradient time: 90 sec (12 cores)

- rBCM performs best
- (g)PoE produce good results
- BCM off the chart ▶▶ suffers from weak experts

Training Data: 5M — NLPD



- (r)BCM and (g)PoE with 32768 GP experts
- Gradient time: 90 sec (12 cores)

- rBCM and gPoE perform best
- PoE and BCM significantly worse

Overview Airline Delays

- RMSE: rBCM consistently performs best
- NLPD: rBCM and gPoE approximately the same
  ⏩ gPoE recovers because of conservative variance estimates
- BCM suffers from "wrong means", PoE suffers from overconfident estimates
- All models: Training time is acceptable
- All experiments (DGP) run on a laptop

Summary

- Distributed product-of-experts approaches to scaling Gaussian processes to large data sets
- Robust Bayesian Committee Machine
- Model conceptually straightforward and easy to train
  - ▸▸ Only kernel hyper-parameters need to be optimized
- Independent of computational graph
- Scales to arbitrarily large data sets (in principle)

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Thank you for your attention

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