Open Problems in GP Approximation and Benchmarking

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The Promises of Gaussian Processes

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1. Good uncertainty estimates, from infinite basis functions

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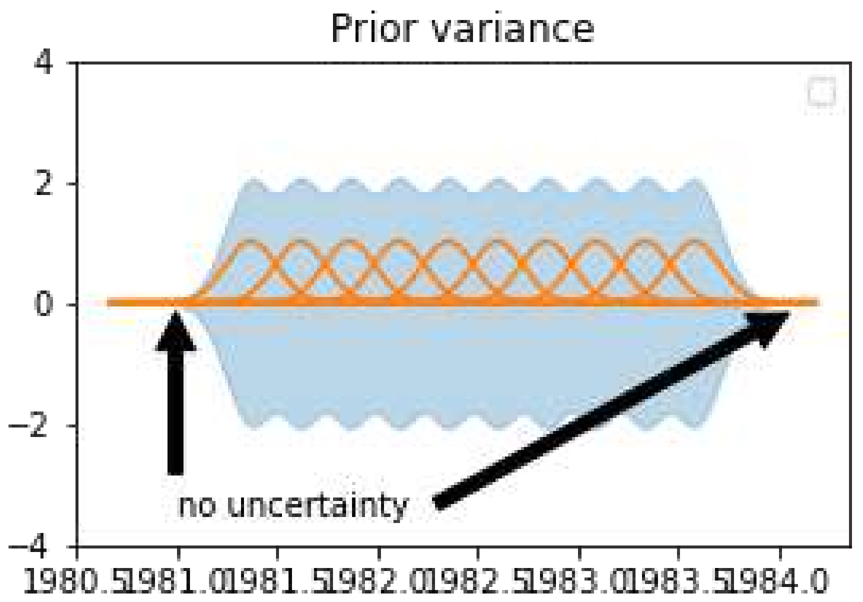

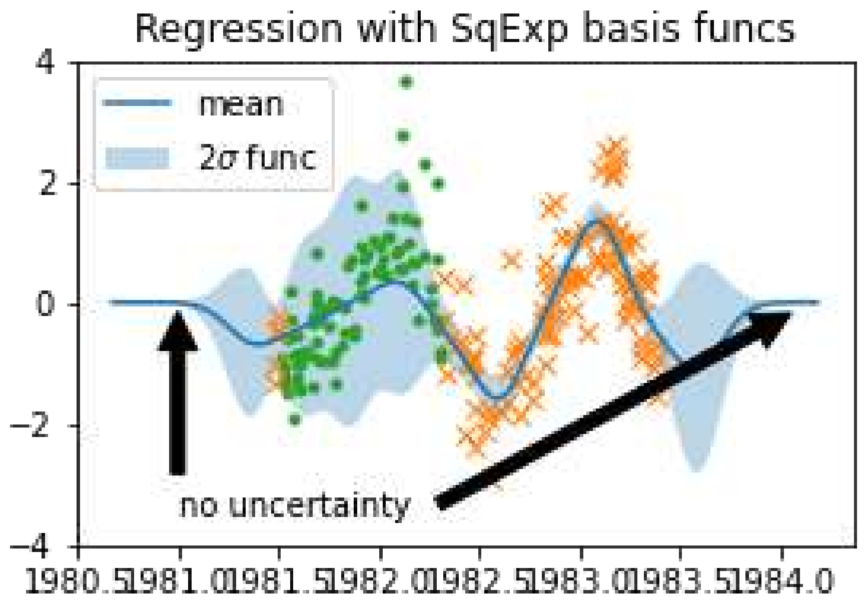

The Promises of Gaussian Processes

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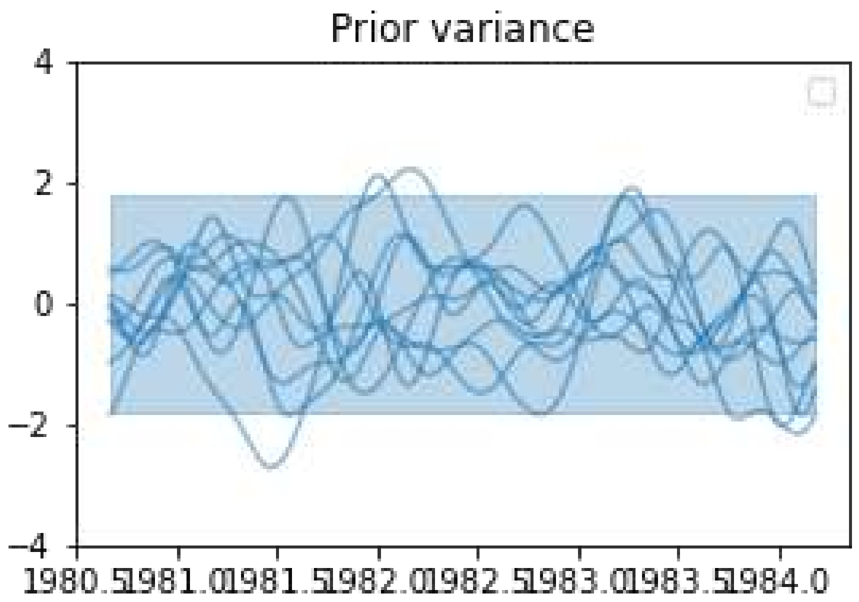

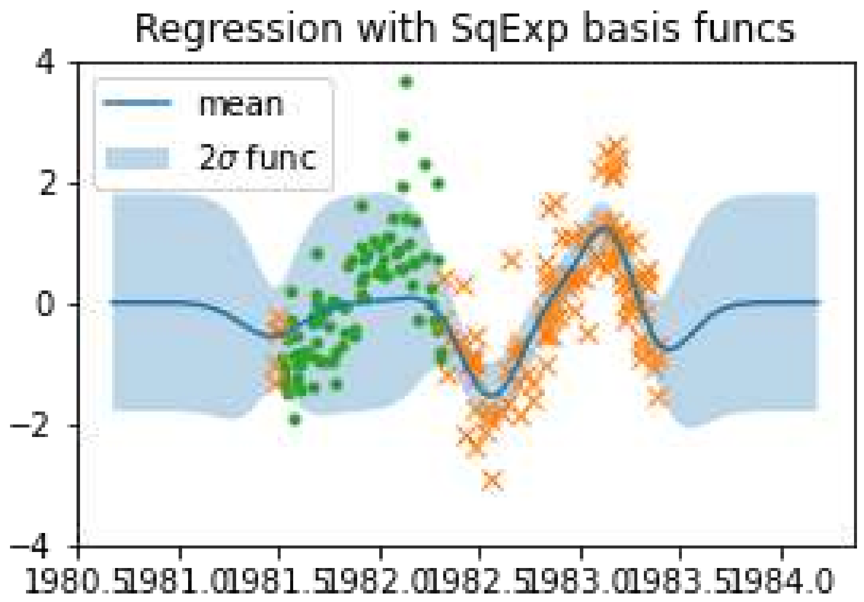

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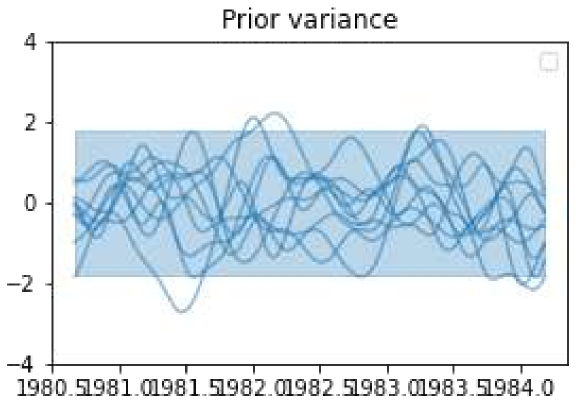
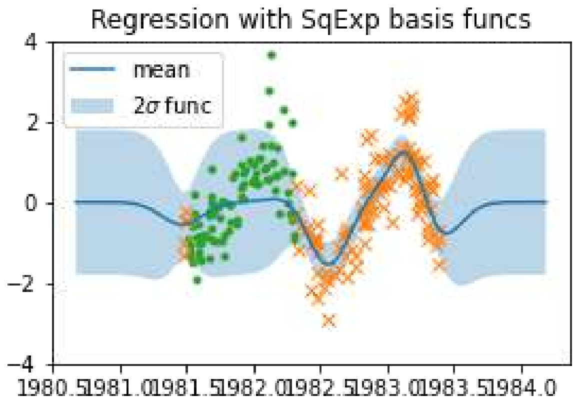


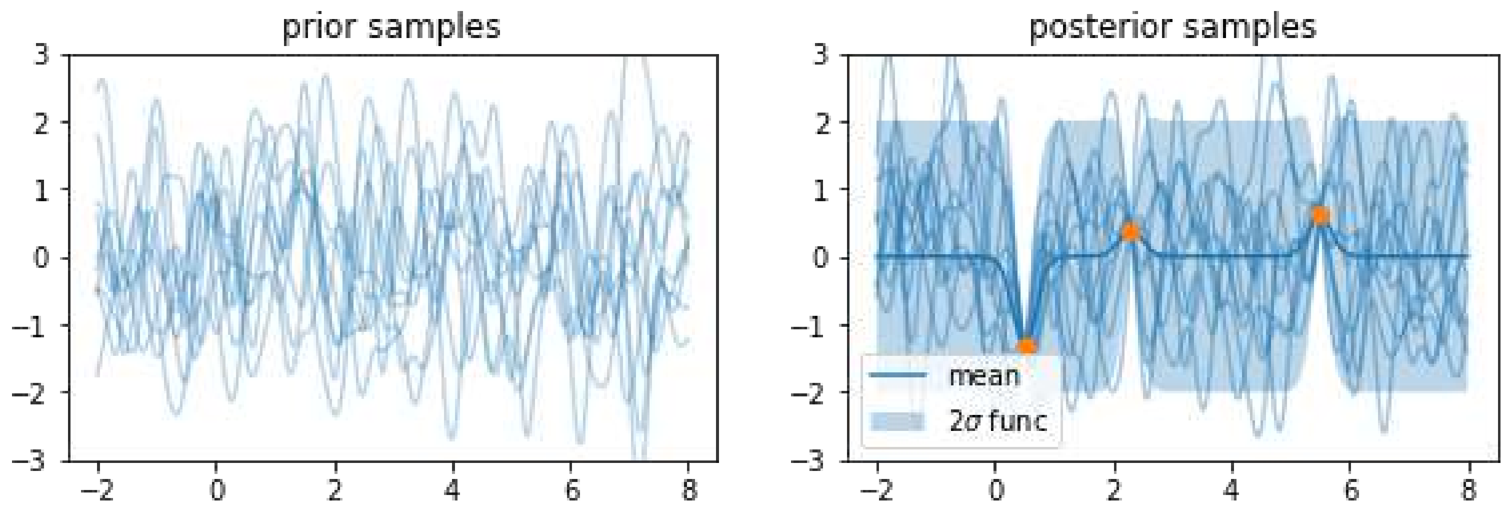


$$p(y^*|x^*, (\boldsymbol{y}, X), (\theta, \sigma)) = \mathcal{N}\Big(y^*; \quad k^\theta_{*X}\left(K^\theta_{XX} + \sigma^2\right)^{-1}\boldsymbol{y}$$

$$k^\theta_{**} - k^\theta_{*X}\left(K^\theta_{XX} + \sigma^2\right)^{-1}k^\theta_{X*}\Big)$$

The Promises of Gaussian Processes

Which kernel should we use?



The Promises of Gaussian Processes

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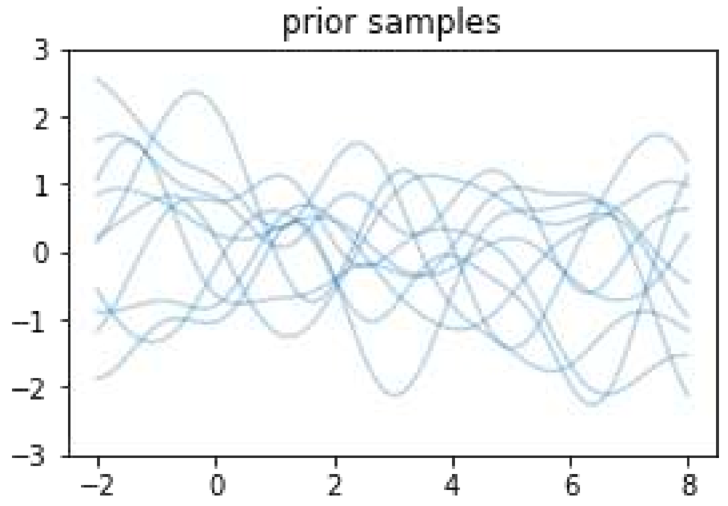

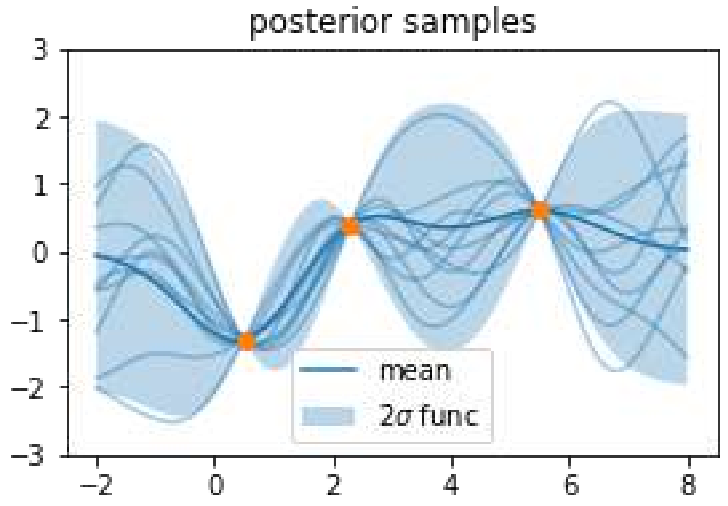

The Promises of Gaussian Processes

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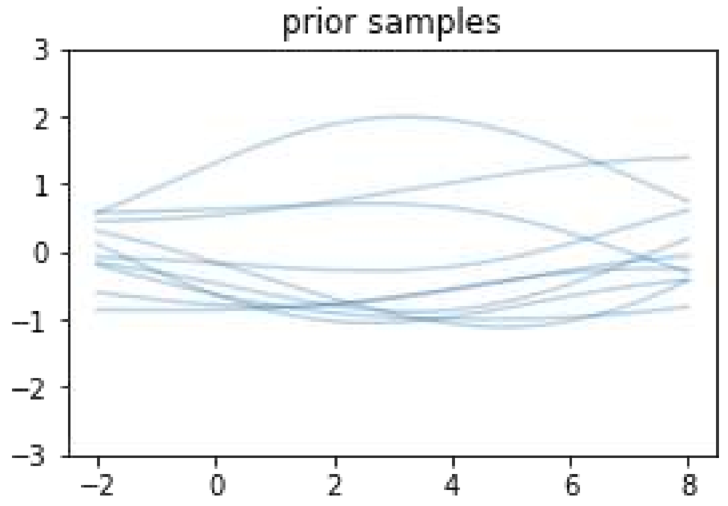
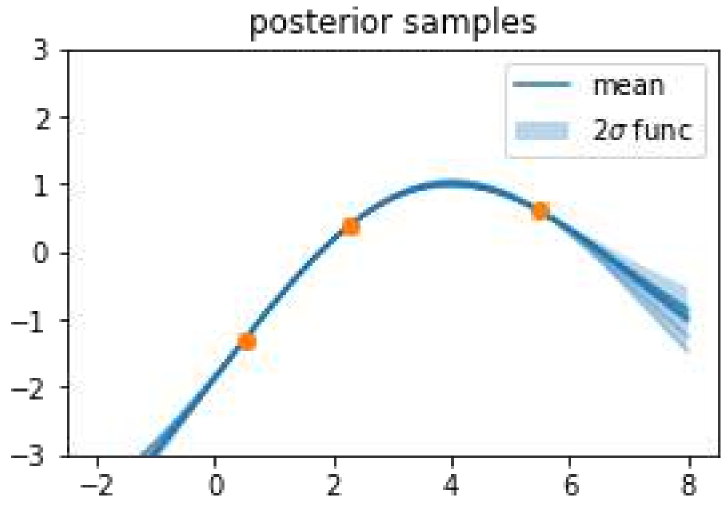




The Promises of Gaussian Processes

2. Automatic hyperparameter tuning

$$\underset{\theta,\sigma}{\operatorname{argmax}} \log p(\boldsymbol{y}|X,(\theta,\sigma)) = \underset{\theta,\sigma}{\operatorname{argmax}} \log \mathcal{N}\left(\boldsymbol{y};0,K_{XX}^{\theta}+\sigma^2 I\right)$$

The Promises of Gaussian Processes

Can even discover sophisticated structure in data!

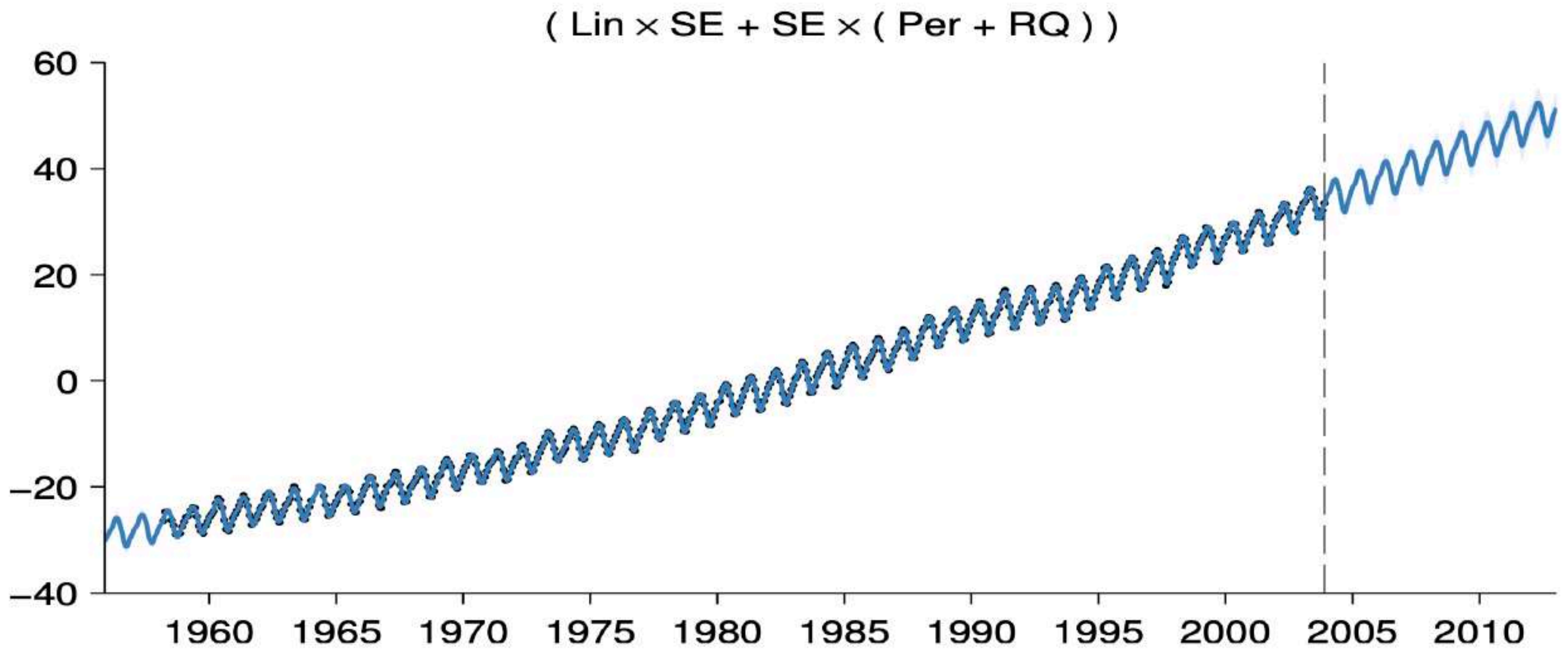


Figure 1: “Automatic Statistician” (Duvenaud et al., 2013)

The Promises of Gaussian Processes

Can even discover sophisticated structure in data!

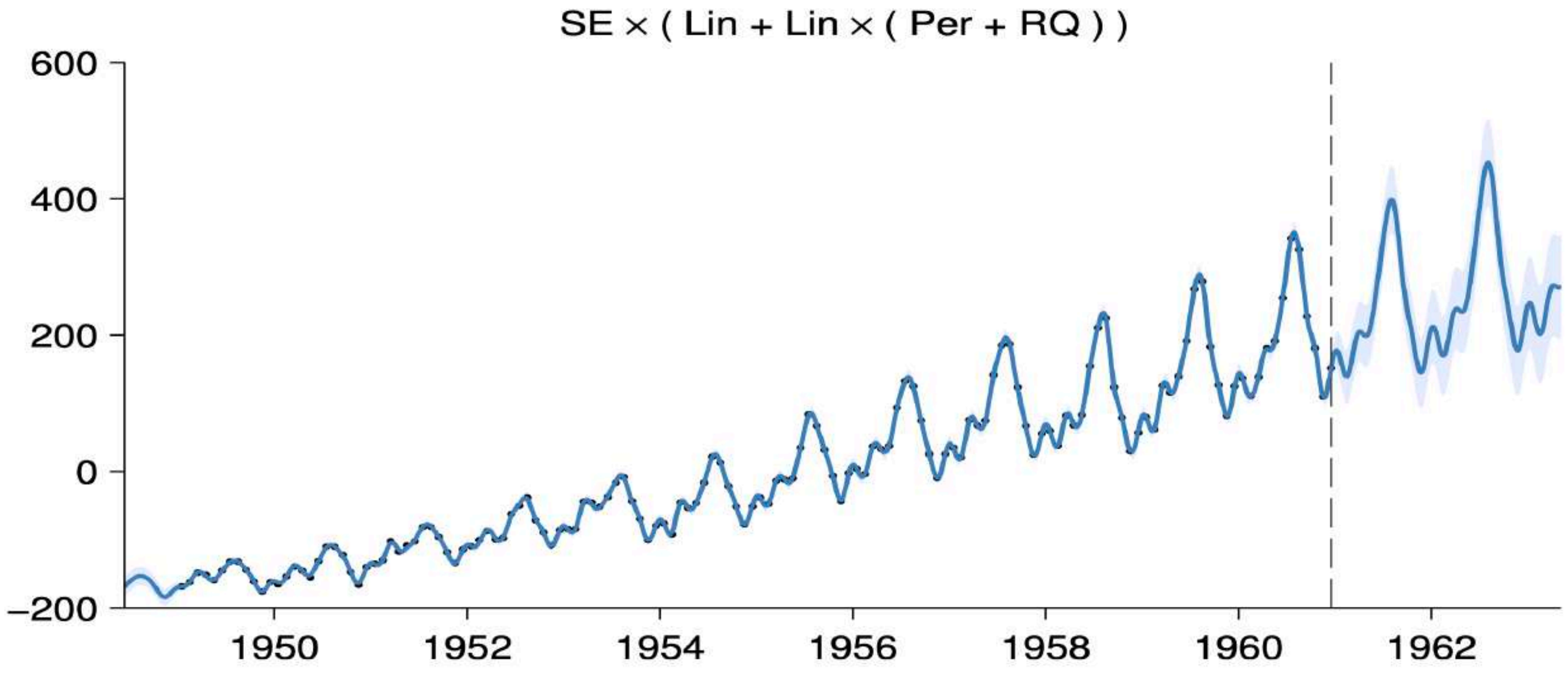


Figure 2: “Automatic Statistician” (Duvenaud et al., 2013)

The Promises of Gaussian Processes

1. Good uncertainty estimates

   from infinite basis functions.

2. Automatic hyperparameter / kernel selection

   from Bayesian model selection.

GPs should be robust, no-nonsense tools!

Practitioners benefit from:

- trustworthy predictions, due to uncertainty,
- ease-of-use, due to automatic tuning to dataset.

GPs are a **silent workhorse** in data science & stats!

What should I do if my dataset has 100,000 datapoints?

Decades of Progress in GP Approximations

- **Eigenfunction approximation**: Zhu et al. (1997), Ferrari-Trecate et al. (1998)
- **Finite basis functions**: Silverman (1985), Smola & Schölkopf (2000)
- **Inducing points**: Csató & Opper (2002), Seeger et al. (2003), Snelson & Ghahramani (2005), Titsias (2009)
- **Conjugate gradients**: Gibbs & MacKay (1996), Davies (2015), Wang et al. (2019)
- **Grid structures**: Saatçi (2011), Nickson et al. (2015), Wilson & Nickisch (2015)

… and many many more.

? What should I do if my dataset has 100,000 datapoints?

Practitioner expects:

- `gp_predict(X, Y)` ⇒ `gp_predict_approx(X, Y)`
- accurate predictions, similar behaviour to full GP
- … maybe `gp_predict_approx(X, Y, prediction_sacrifice="1%")`

Practitioner gets:

- “Well, which approximation do you want to use?” Too much choice!
- We need *fewer* answers to this question, not more!
- `gp_predict_approx_variational(X, Y, num_inducing=100, inducing_locations=???, jitter=1e-6, min_lengthscale=1e-3)`

⚠ **We don’t currently provide a black-box answer on how to approximate**

🎯 **Goal: Near-exact approximation, without thinking too hard**

So how do current approximations match up to this?

Example: Variational Inducing Points (Titsias, 2009)

Approximation parameters:

- Number of inducing points
- How to pick the inducing points
- Jitter value, for numerical stability

⚠ **Relies on manual tuning**

- Can't know correct M ahead of time for a new dataset
- Different advice on IP locations
- Jitter to make algorithm run

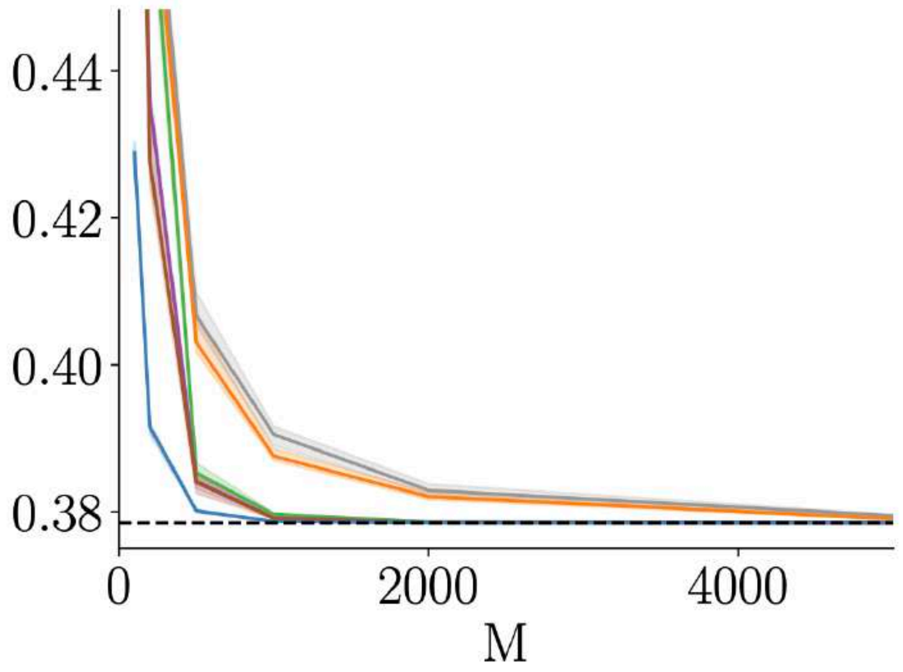


Figure 3: RMSE for `elevators` dataset

Example: Conjugate Gradients (Wang et al., 2019)

Approximation parameters:

- Number of probe vectors
- Lower noise limits
- CG termination criterion
- …

⚠ Relies on Manual Tuning

Getting parameters wrong leads to underperformance, or even bad divergence.

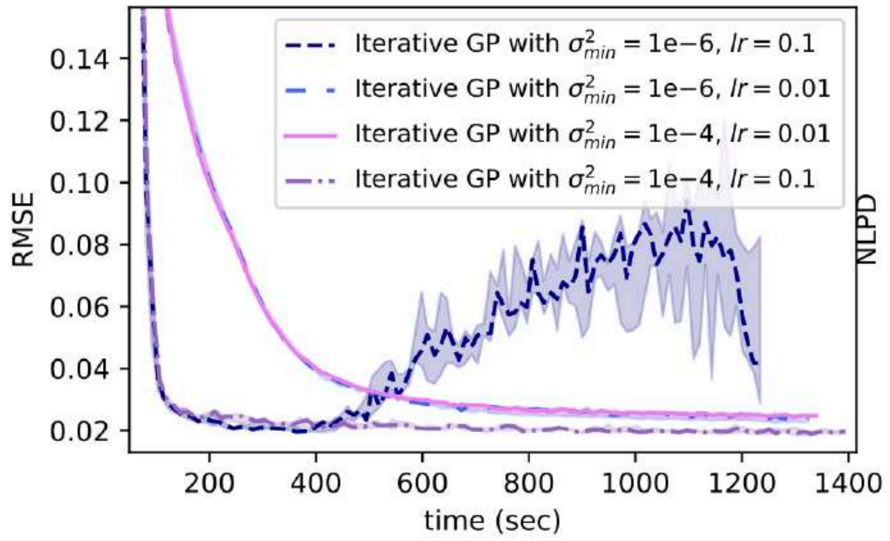


Figure 4: RMSE for `bike` dataset. Noise-free dataset, so full GP gets 0.000 RMSE.

⚠ **Methods work in the paper, but current default approximation parameters don’t work well for all datasets**

“I tried <approximation method>,

but the results were bad

… so GPs must be bad. ”

Decades of Progress in GP Approximations

… have brought us

- many methods, but little clarity on which one to use, and when
- approximations that need *tuning*, negating promise #2!

⚠ Approximate GPs should be robust, no-nonsense tools!

GPs are a **silent workhorse** in data science & stats!

… but approximate scalable GPs are not!

Decades of Progress in GP Approximations

… have also brought us
scalable methods, that are extremely accurate, *when tuned correctly*.

Case study:
Variational Inducing Points (Titsias, 2009)
vs
Conjugate Gradients (Davies, 2015; Gibbs & MacKay, 1996; Wang et al., 2019)

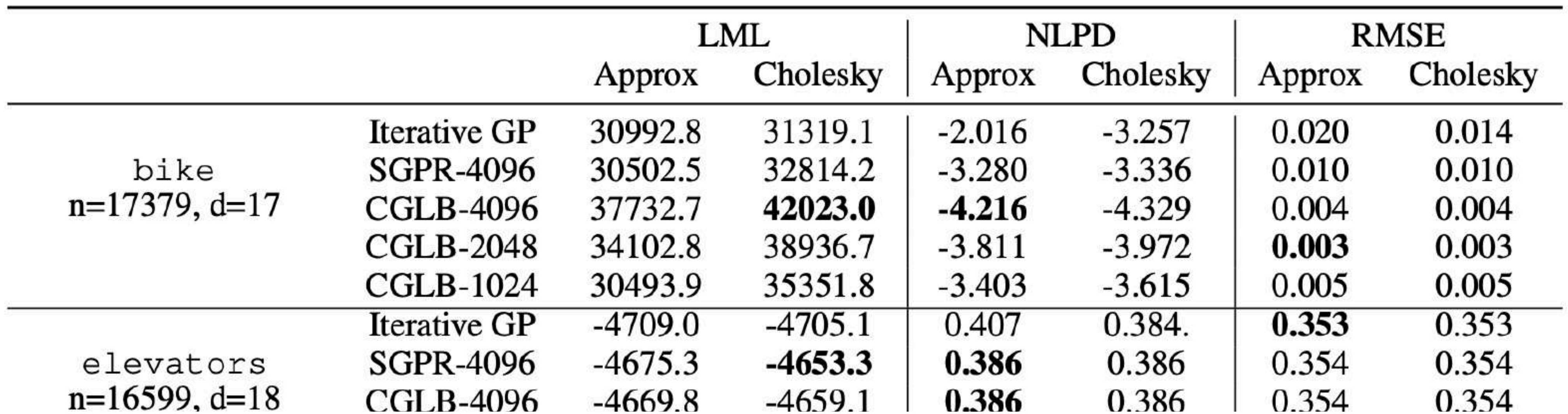
? So which method is better?

Keeping in mind: both are arbitrarily accurate, if tuned correctly.

Common Benchmarking

Some self-criticism (Artemev et al., 2021), but common practice.

- Pick a few datasets
- Run various approximations, possibly with various tuning parameters
- Measure predictive performance, present in a table, **bold** == publish.



		LML		NLPD		RMSE	
		Approx	Cholesky	Approx	Cholesky	Approx	Cholesky
bike n=17379, d=17	Iterative GP	30992.8	31319.1	-2.016	-3.257	0.020	0.014
	SGPR-4096	30502.5	32814.2	-3.280	-3.336	0.010	0.010
	CGLB-4096	37732.7	**42023.0**	**-4.216**	-4.329	0.004	0.004
	CGLB-2048	34102.8	38936.7	-3.811	-3.972	**0.003**	0.003
	CGLB-1024	30493.9	35351.8	-3.403	-3.615	0.005	0.005
elevators n=16599, d=18	Iterative GP	-4709.0	-4705.1	0.407	0.384.	**0.353**	0.353
	SGPR-4096	-4675.3	**-4653.3**	**0.386**	0.386	0.354	0.354
	CGLB-4096	-4669.8	-4659.1	**0.386**	0.386	0.354	0.354

Benchmarking Problems

⚠ **All these methods *can be* arbitrarily accurate**

All convergent approximations, if tuned correctly, should give **exactly the same** results.

$\Rightarrow$ **Any** performance difference, is **purely** down to tuning approximation parameters!

- So we are **not** measuring intrinsic quality of the approximation.
- Instead, we measure the quality of our tuning of the **approximation parameter**.
- Time-quality trade-off is only thing that matters, but not tested!

How Approximations should Work

Currently, approximations work by:

- making a choice for the approximation parameters,
- and then *measuring* the resulting performance.

We should develop methods which

- take a desired tolerance on predictive performance,
- the method runs until this guarantee is satisfied,
- **we measure how *long* it takes to reach this**.

How we should be Benchmarking

If approximations worked in this way, benchmarking would be easier too.

Measure time until accuracy target is reached

	Method 1	Method 2	Method 3
Dataset #1	11s	102s	3600s
Dataset #2	2345s	3134s	3714s
Dataset #3	142s	10s	343s

Table 1: Time until with 10% of optimal predictive accuracy

For this benchmarking to make sense, methods need to converge to the right answer!

Goal: Near-exact approximation, without thinking too hard

- Compute time is compared to human intervention.
- Methods should be set up such that more time makes them get continuously better, without human intervention.

How can we make methods convergent?

Making Variational Inducing Points Convergent

We know that as $M \to N$, we converge to the true posterior (Burt et al., 2019; 2020).

- To remove *all* tuning, we need to steadily increase the number of inducing points during training.
- Slow due to many repeated training runs, but does remove all tuning!
- Much closer to how method is used in practice!
- This cost **should** be measured in benchmarking!

⚠ **This is a difficult and a pain!**

Takes lots of effort, but this is the problem we are faced with.

Approximation and Model Specification are Dependent

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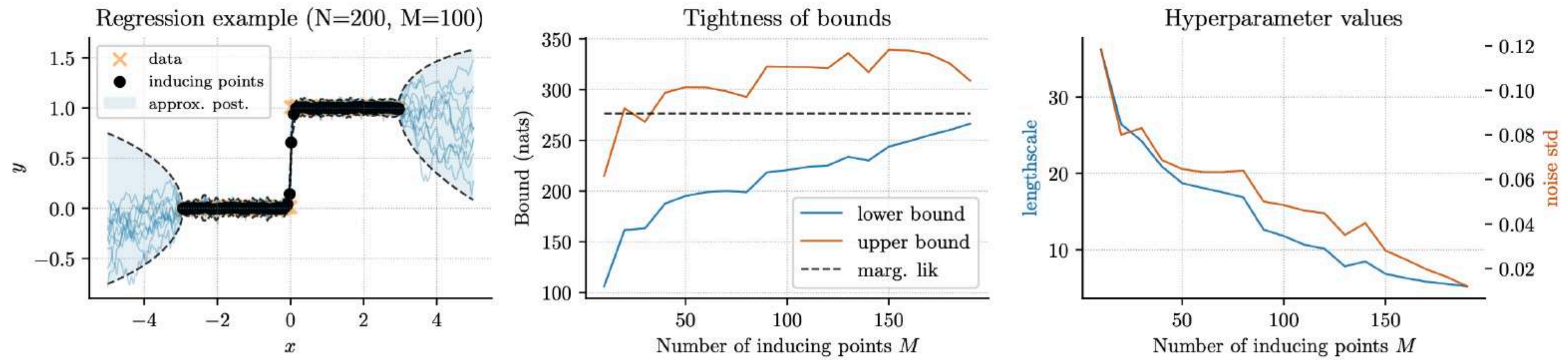
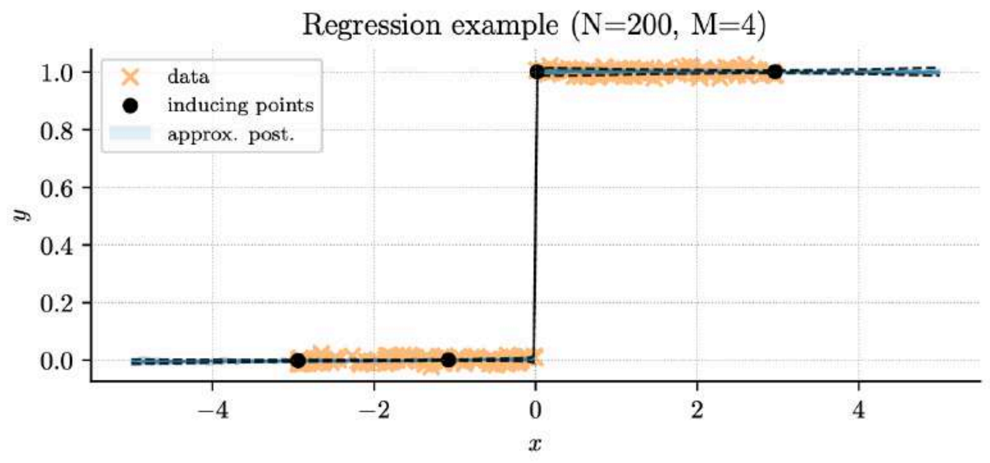
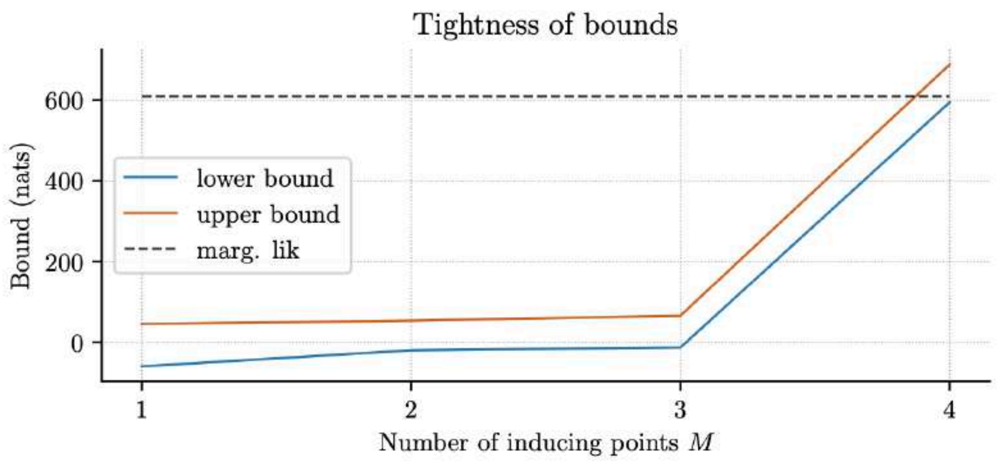
Approximations will behave strangely, if the true GP they are approximating behave strangely.



Approximation and Model Specification are Dependent

But this is fixed if model misspecification is removed!





⚠ **Kernel search and approximation are related problems**

… and should probably be studied together.

Conclusion

Conclusion

Good approximations to GPs already exist… if you tune them correctly

🎯 **Next frontier: Make approximations *transparent* to the user!**

Procedures should converge to exact solution as they run longer.

💡 **Benchmark the time it takes to reach a level of acccuracy**

⚠ **Kernel search and approximation are related problems**

… and should probably be studied together.

For more: *Recommendations for Baselines and Benchmarking Approx GPs* (Ober et al., 2024)

Outlook

Lots of interesting problems are still open:

- **Mathematical**: Can we find *proofs* on how to scale approximation tuning parameters to *guarantee* convergence to an exact solution?
- **Statistical**: How do we solve the statistical and computational problems *together*?
- **Software**: How do we build tools that practitioners can easily use to solve their prediction problems? (Huge current bottleneck!)

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