

# Probabilistic Programming with Gaussian Process Memoization

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## Abstract

This paper describes the *Gaussian process memoizer*, a probabilistic programming technique that uses Gaussian processes to provide a statistical alternative to memorization. Memoizing a target procedure results in a “self-caching” wrapper that remembers previously computed values. Gaussian process memoization additionally produces a statistical emulator based on a Gaussian process whose predictions automatically improve whenever a new value of the target procedure becomes available. This paper also introduces an efficient implementation, named `gpmem`, that can use kernels given by a broad class of probabilistic programs. The flexibility of `gpmem` is illustrated via three applications: (i) GP regression with hierarchical hyper-parameter learning, (ii) Bayesian structure learning via compositional kernels generated by a probabilistic grammar, and (iii) a bandit formulation of Bayesian optimization with automatic inference and action selection. All applications share a single 85-line Python library and require fewer than 20 lines of probabilistic code each.

## GP Memoization: `gpmem`

### Gaussian Processes

$f(\mathbf{x})$  is the multivariate Gaussian  $f(\mathbf{x}) \sim \mathcal{N}(0, k(\mathbf{x}, \mathbf{x}))$ , where  $k(\mathbf{x}, \mathbf{x}') = \text{Cov}_f(f(\mathbf{x}), f(\mathbf{x}'))$  is the covariance function, a.k.a. kernel. The marginal likelihood can be expressed as:

$$p(f(\mathbf{x}) = \mathbf{y} | \mathbf{x}) = \int p(f(\mathbf{x}) = \mathbf{y} | f, \mathbf{x}) p(f|\mathbf{x}) df$$

### A Variation on Memoization

*GP memoization* produces two components:

$$f \rightarrow (f_{\text{compute}}, f_{\text{emu}})$$

- is a generalization of traditional memoization;
- changes semantics of a probabilistic program;
- $f_{\text{emu}}$  is a statistical emulator with GP prior;
- each time  $f_{\text{compute}}$  is called, an observation is incorporated into  $f_{\text{emu}}$  and predictions improve.

### Bayesian GP

We show how we can use `gpmem` to reproduce Neal’s Hierarchical Bayesian GP regression [2] for data with outliers.

Regression on data set  $D$

↑

Statistical emulation of  $f_{\text{restr}}(x) = \begin{cases} D[x], & \text{if } x \text{ is a data point} \\ \text{Error}, & \text{otherwise} \end{cases}$

```
// SETTING UP THE MODEL
assume alpha_sf = tag('hyperhyper, gamma(7, 1))
assume beta_sf = tag('hyperhyper, gamma(7, 1))
assume alpha_l = tag('hyperhyper, gamma(7, 1))
assume beta_l = tag('hyperhyper, gamma(7, 1))
// Parameters of the covariance function
assume log_sf = tag('hyper, log(gamma(alpha_sf, beta_sf)))
assume log_l = tag('hyper, log(gamma(alpha_l, beta_l)))
assume log_sigma = tag('hyper, log(uniform_continuous(0, 2)))

// The covariance function
assume se = make_squaredexp(log_sf, log_l)
assume wn = make_whitenoise(log_sigma)
assume composite_covariance = add_funcs(se, wn)

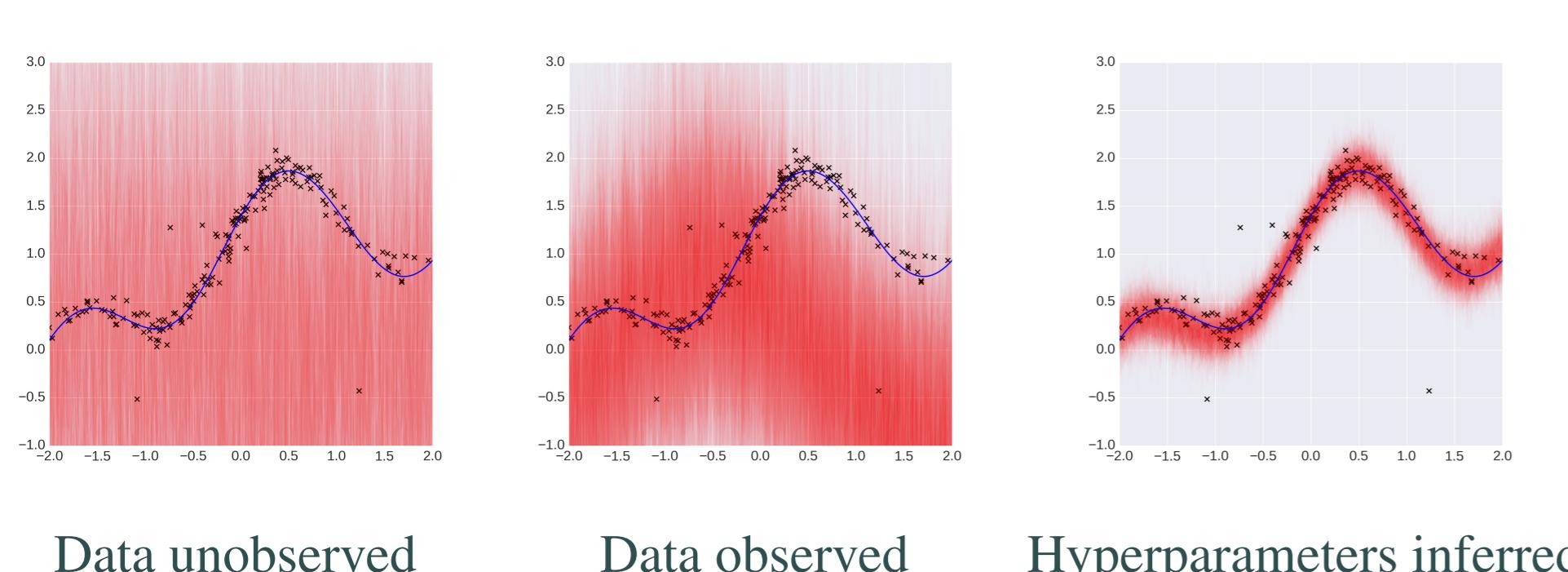
// PERFORMING INFERENCE
// Create a prober and emulator using gpmem
assume f_restr = get_neal_blackbox()
assume (f_compute, f_emu) = gpmem(f_restr, composite_covariance)

// Probe all data points
predict mapv(f_compute, get_neal_data_xs())

// Infer hypers and hyperhypers
infer repeat(100, do(
    mh('hyperhyper, one, 2),
    mh('hyper, one, 1)))
```

### Results

Ran the above program on data with outliers: noise  $\sigma = 1.0$  with probability 0.05, noise  $\sigma = 0.1$  otherwise.



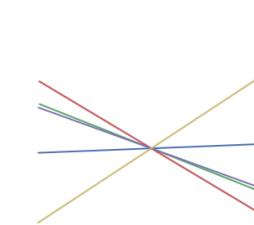
## GP Structure Learning

### Base Kernels

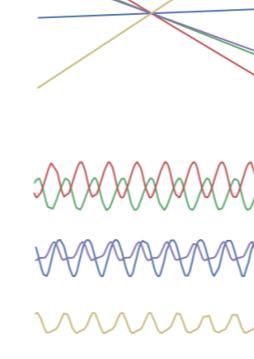
$$SE = \sigma^2 \exp\left(-\frac{(x-x')^2}{2\ell^2}\right)$$



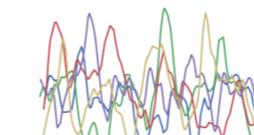
$$LIN = \theta(x x')$$



$$PER = \theta \exp\left(\frac{2 \sin^2(\pi(x-x')/\ell)}{\ell^2}\right)$$

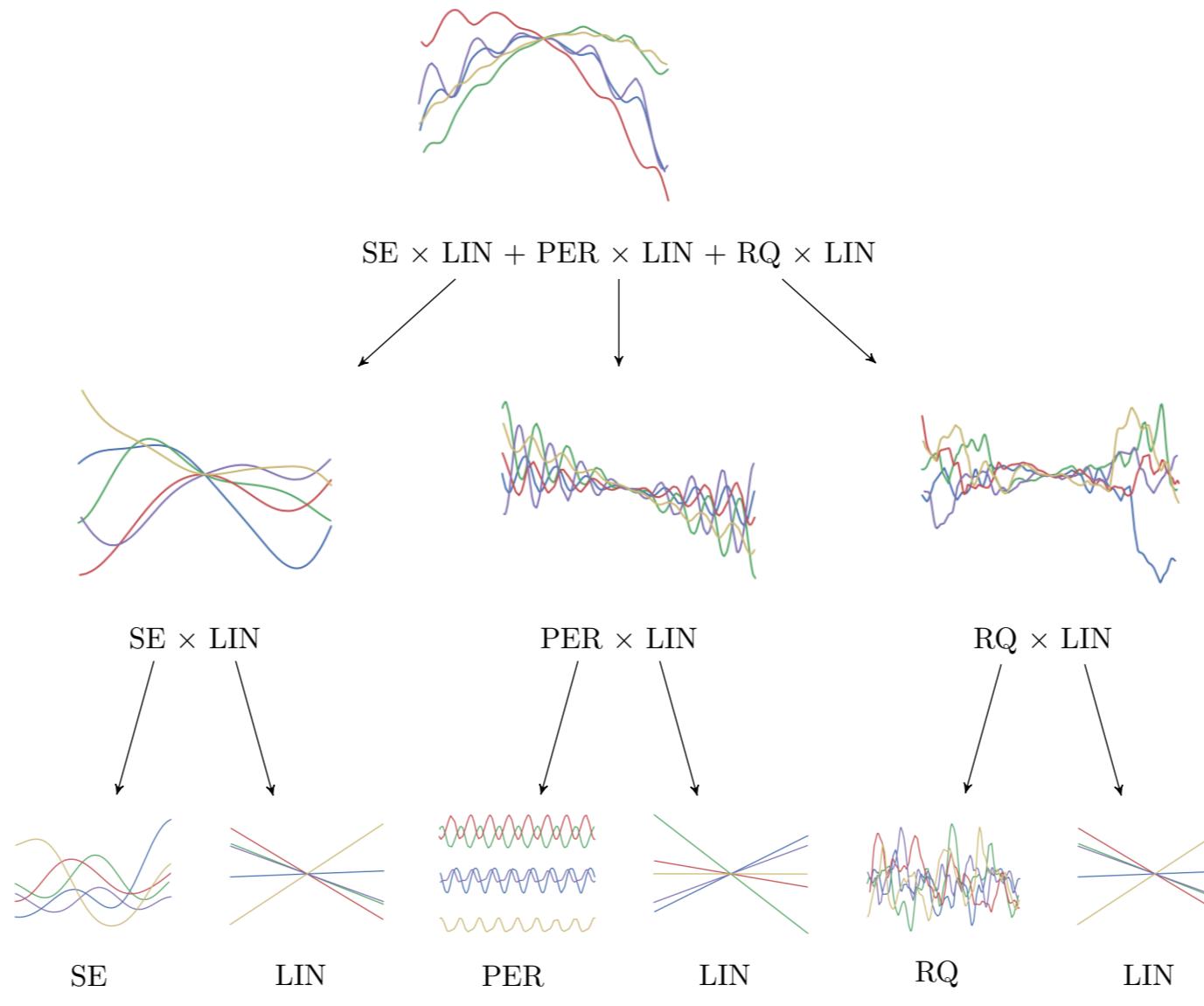


$$RQ = \theta \left(1 + \frac{(x-x')^2}{2\alpha\ell^2}\right)^{-\alpha}$$



### Kernel Composition

$$\mathbf{K}_{\text{new}} = \mathbf{K}_1 + \mathbf{K}_2 \quad \text{or} \quad \mathbf{K}_{\text{new}} = \mathbf{K}_1 \times \mathbf{K}_2$$



```
// GRAMMAR FOR KERNEL STRUCTURE
assume base_kernels = list(se, wn, lin, per, rq) // defined as above

// prior on the number of kernels
assume p_number_k = tag('number_kernels, uniform_structure(n))
assume s = tag('choice_subset, subset(base_kernels, p_number_k))

assume cov_compo = proc(l) {
    // kernel composition
    if (size(l) <= 1)
        then { first(l) }
    else { if (flip()) then { add_funcs(first(l), cov_compo(rest(l))) }
           else { mult_funcs(first(l), cov_compo(rest(l))) }
    }
}

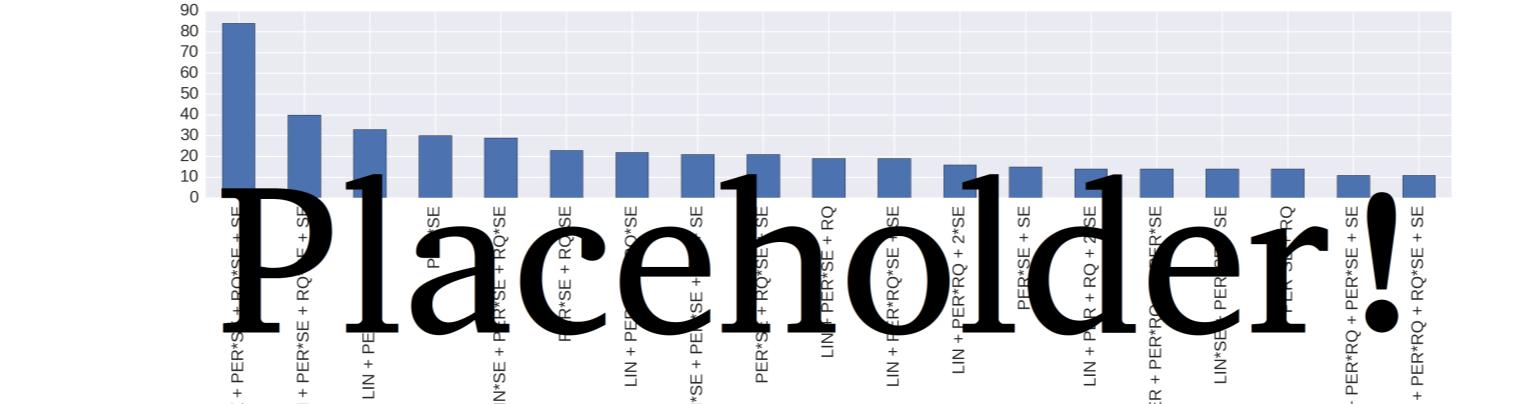
assume K = tag('composit, cov_compo(s))

assume (f_compute f_emu) = gpmem(f_restr, K)
predict mapv(f_compute(get_data_xs)) // probe all data points

// PERFORMING INFERENCE
infer repeat(2000, do(
    mh('number_kernel, one, 1),
    mh('choice_subset, one, 1),
    mh('composit, one, 1),
    mh('hyper, one, 10)))
```

### Results

500 samples drawn from the posterior on structure for the CO2 dataset used in the Automated Statistician Project [1]:



Posterior samples for curves for the airline dataset where  $SE \times LIN + PER \times LIN + RQ \times LIN$  is sampled from the structure grammar:

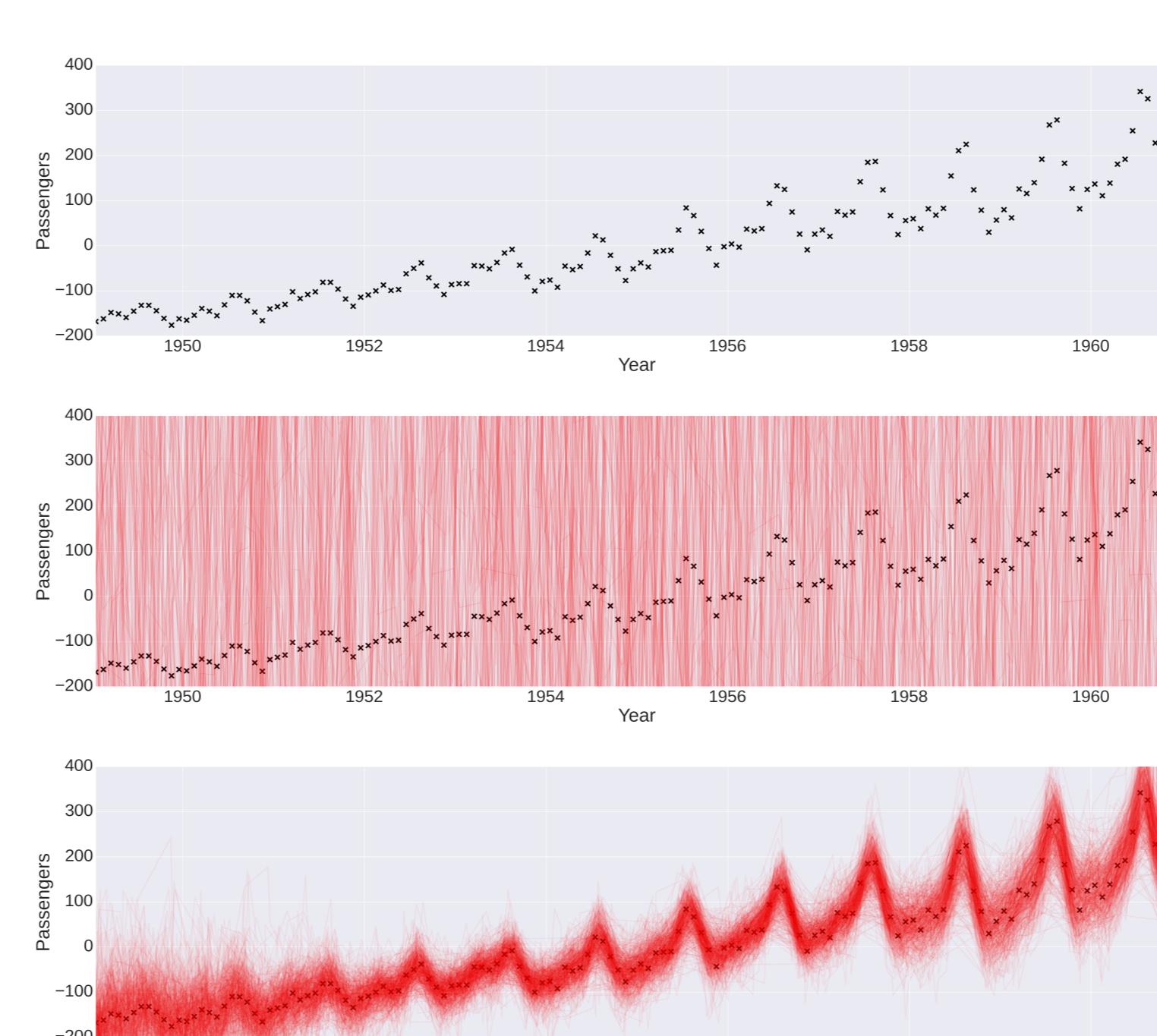


Figure 1: Top: raw data, monthly airline passengers. Middle, prior on functions. Bottom, posterior.

## Bayesian Optimization

### Thompson Sampling for Homogeneous Sequential Markov Decision Processes

Two phases, each takes one line of code:

1. Sample a context  $V_{\text{emu}} \sim P(V_{\text{emu}})$  using a Metropolis–Hastings sampler.
2. Probe the point  $x_{\text{next}} = \arg \max_x V_{\text{emu}}(x)$ .

```
assume log_sf = tag('hyper, log(uniform_continuous(0, 10)))
assume log_l = tag('hyper, log(uniform_continuous(0, 10)))
assume se = make_squaredexp(log_sf, log_l)
assume blackbox_f = get_bayesopt_blackbox()
assume (f_compute, f_emu) = gpmem(blackbox_f, se)

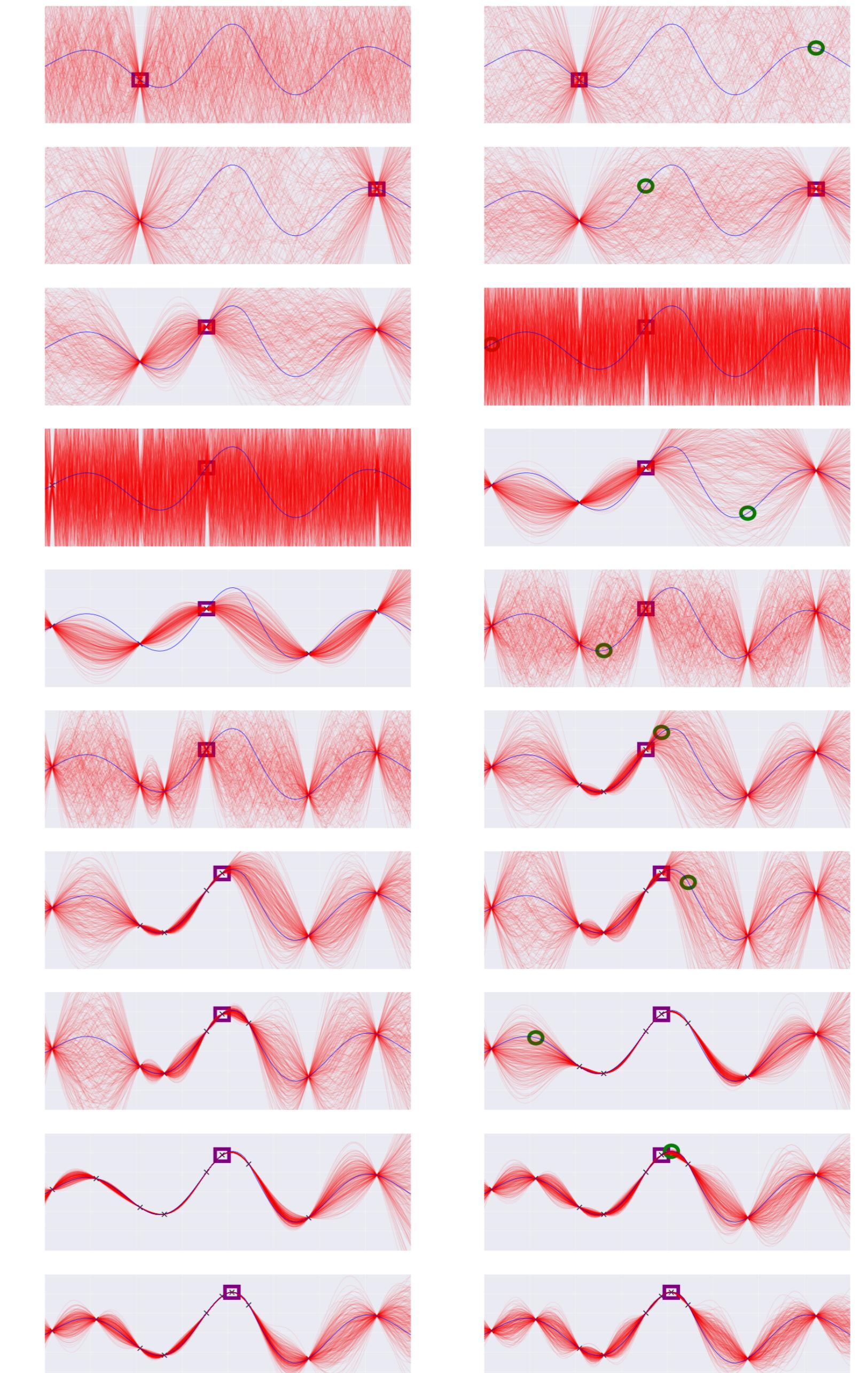
define get_uniform_candidate = proc(prev_xs) {
    uniform_continuous(-20, 20)
}

define mc_argmax = proc(func, prev_xs) {
    // Monte Carlo estimator for the argmax of func.
    run(do(
        candidate_xs <- mapv(proc(i) get_uniform_candidate(prev_xs)),
        linspace(0, 19, 20),
        candidate_ys <- mapv(func, candidate_xs),
        lookup(candidate_xs, argmax_of_array(candidate_ys)))
    )
}

define emulator_point_sample = proc(x) {
    run(sample(lookup(
        f_emu(array(x)),
        0)))
}

infer repeat(15, do(pass,
    // Phase 2: Call f_compute on the next probe point
    predict f_compute(
        mc_argmax(emulator_point_sample, '_'),
        // Phase 1: Hyperparameter inference
        mh('hyper, one, 50)))
```

### Results



- Blue: Unknown true value function  $V$
- Red: Current state of our statistical emulator  $V_{\text{emu}}$ , conditioned on previously probed values of  $V$
- Purple: Best probe point seen so far,  $x_{\text{best}}$
- Green: Next chosen probe point,  $x_{\text{next}}$
- Left: before hyperparameter inference; right: after hyperparameter inference

Probes tend to happen at points either where the value of  $V_{\text{emu}}$  is high, or where  $V_{\text{emu}}$  has high uncertainty.

## References

- [1] D. Duvenaud, J. R. Lloyd, R. Grosse, J. Tenenbaum, and Z. Ghahramani. Structure discovery in nonparametric regression through compositional kernel search. In *Proceedings of the 30th International Conference on Machine Learning (ICML-13)*, pages 1166–1174, 2013.
- [2] R. M. Neal. Monte carlo implementation of gaussian process models for bayesian regression and classification. *arXiv preprint physics/9701026*, 1997.