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# 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 provides 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 50-line Python library and require fewer than 20 lines of probabilistic code each.

## 1 Introduction

Probabilistic programming could be revolutionary for machine intelligence due to universal inference engines and the rapid prototyping for novel models (Ghahramani, 2015). This levitates the design and testing of new models as well as the incorporation of complex prior knowledge which currently is a difficult and time consuming task. Probabilistic programming languages aim to provide a formal language to specify probabilistic models in the style of computer programming and can represent any computable probability distribution as a program. In this work, we will introduce new features of Venture, a recently developed probabilistic programming language. We consider Venture the most compelling of the probabilistic programming languages because it is the first probabilistic programming language suitable for general purpose use (Mansinghka et al., 2014). Venture comes with scalable performance on hard problems and with a general purpose inference engine. The inference engine deploys Markov Chain Monte Carlo (MCMC) methods (for an introduction, see Andrieu et al. (2003)). MCMC lends itself to models with complex structures such as probabilistic programs or hierarchical Bayesian non-parametric models since they can provide a vehicle to express otherwise intractable integrals necessary for a fully Bayesian representation. MCMC is scalable, often distributable and also compositional. That is, one can arbitrarily chain MCMC kernels to infer over several hierarchically connected or nested models as they will emerge in probabilistic programming.

One very powerful model yet unseen in probabilistic programming languages are Gaussian Processes (GPs). GPs are gaining increasing attention for representing unknown functions by posterior probability distributions in various fields such as machine learning, signal processing, computer vision and bio-medical data analysis. Making GPs available in probabilistic programming is crucial to allow a language to solve a wide range of problems. Hard problems include but are not limited

054 to hierarchical prior construction (Neal, 1997), Bayesian Optimization Snoek et al. (2012) and sys-  
055 tems for inductive learning of symbolic expressions such as the one introduced in the Automated  
056 Statistician project Duvenaud et al. (2013); Lloyd et al. (2014). Learning such symbolic expressions  
057 is a hard problem that requires careful design of approximation techniques since standard inference  
058 method do not apply.

059 In the following, we will present `gpmem` as a novel probabilistic programming technique that solves  
060 such hard problems. `gpmem` introduces a statistical alternative to standard memoization. Our con-  
061 tribution is threefold:

- 063 • we introduce an efficient implementation of `gpmem` in form of a self-caching wrapper that  
064 remembers previously computed values;
- 065 • we illustrate the statistical emulator that `gpmem` produces and how it improves with every  
066 data-point that becomes available; and
- 067 • we show how one can solve hard problems of state-of-the-art machine learning related to  
068 GP using `gpmem` in a Bayesian fashion and with only a few lines of Venture code.

070 We evaluate the contribution on problems posed by the GP community using real world and syn-  
071 thetic data by assessing quality in terms of posterior distributions of symbolic outcome and in terms  
072 of the residuals produced by our probabilistic programs. The paper is structured as follows, we will  
073 first provide some background on memoization. We will explain programming in Venture and pro-  
074 vide a brief introduction to GPs. We introduce `gpmem` and its use in probabilistic programming and  
075 Bayesian modeling. Finally, we will show how we can apply `gpmem` on problems of causally struc-  
076 tured hierarchical priors for hyper-parameter inference, structure discovery for Gaussian Processes  
077 and Bayesian Optimization including experiments with real world and synthetic data.

## 078 2 Background

### 079 2.1 Memoization

080 Memoization is the practice of storing previously computed values of a function so that future calls  
081 with the same inputs can be evaluated by lookup rather than recomputation. Research on the Church  
082 language (Goodman et al., 2008) pointed out that although memoization does not change the se-  
083 mantics of a deterministic program, it does change that of a stochastic program. In fact, there is an  
084 infinite range of possible caching policies (specifications of when to use a stored value and when  
085 to recompute), each potentially having a different semantics. Any particular caching policy can  
086 be understood by random world semantics (Poole, 1993; Sato, 1995) over the stochastic program:  
087 each possible world corresponds to a mapping from function input sequence to function output se-  
088 quence (McAllester et al., 2008). In Venture, these possible worlds are first-class objects, known as  
089 *traces* (Mansinghka et al., 2014).

### 090 2.2 Venture

091 Venture is a compositional language for custom inference strategies that comes with a Scheme-  
092 like and a JavaScript-like front-end syntaxes. Its implementation is based on on three concepts:  
093 (i) *stochastic procedures* that specify and encapsulate random variables, analogously to conditional  
094 probability tables in a Bayesian network; (ii) *execution traces* that represent (partial) execution his-  
095 tories and track the conditional dependencies of the random variables occurring therein; and (iii)  
096 *scaffolds* that partition execution histories and factor global inference problems into sub-problems.  
097 These building blocks provide a powerful and concise way to represent probability distributions,  
098 including distributions with a dynamically determined and unbounded set of random variables. In  
099 this paper we will use only the four basic Venture directives: ASSUME, OBSERVE, SAMPLE and  
100 INFER.

- 104 • ASSUME induces a hypothesis space for (probabilistic) models including random variables  
105 by binding the result of a supplied expression to a supplied symbol.
- 106 • Whereas in Scheme an expression is evaluated within an environment, in Venture an ex-  
107 pression is evaluated within a (partial) trace of the model program. Thus, the value of an

108 expression within a model program is a random variable, whose randomness comes from  
 109 the distribution on possible execution traces of the program. The SAMPLE directive sam-  
 110 plesthe value of the supplied expression within the current model program.

- 111 • OBSERVE constrains the supplied expression to have the supplied value. In other words,  
 112 all samples taken after an OBSERVE are conditioned on the observed data.
- 113 • INFER uses the supplied inference program to mutate the execution trace. For a correct in-  
 114 ference program, this will result approximate sampling from the true posterior on execution  
 115 traces, conditioned on the model and constraints introduced by ASSUME and OBSERVE.  
 116 The posterior on any random variable can then be approximately sampled by calling SAM-  
 117 PLE to extract values from the trace.

119 INFER is commonly done using the Metropolis–Hastings algorithm (MH) (Metropolis et al., 1953).  
 120 Many of the most popular MCMC algorithms can be interpreted as special cases of MH (Andrieu  
 121 et al., 2003). We can outline the MH algorithm as follows. The following two-step process is  
 122 repeated as long as desired (say, for  $T$  steps): First we sample  $x^*$  from a proposal distribution  $q$ :

$$123 \quad x^* \sim q(x^* | x^t); \quad (1)$$

124 then we accept this proposal ( $x^{t+1} \leftarrow x^*$ ) with probability

$$125 \quad \alpha = \min \left\{ 1, \frac{p(x^*)q(x^t | x^*)}{p(x^t)q(x^* | x^t)} \right\}; \quad (2)$$

126 if the proposal is not accepted then we take  $x^{t+1} \leftarrow x^t$ .

127 Venture includes a built-in generic MH inference program which performs the above steps on any  
 128 specified set of random variables in the model program. In that inference program, probabilistic  
 129 execution traces play the role of  $x$  above.

### 132 2.3 Gaussian Processes

133 We now introduce GP related theory and notations. We work exclusively with two-variable regres-  
 134 sion problems. Let the data be pairs of real-valued scalars  $\{(x_i, y_i)\}_{i=1}^n$  (complete data will be de-  
 135 noted by column vectors  $\mathbf{x}, \mathbf{y}$ ). In regression, one tries to learn a functional relationship  $y_i = f(x_i)$ ,  
 136 where the function  $f$  is to be learned. GPs present a non-parametric way to express prior knowledge  
 137 on the space of possible functions  $f$ . Formally, a GP is an infinite-dimensional extension of the  
 138 multivariate Gaussian distribution. For any finite set of inputs  $\mathbf{x}$ , the marginal prior on  $f(\mathbf{x})$  is the  
 139 multivariate Gaussian

$$141 \quad f(\mathbf{x}) \sim \mathcal{GP}(m(\mathbf{x}), k(\mathbf{x}, \mathbf{x})),$$

142 where  $m(\mathbf{x}) = \mathbb{E}_f[f(\mathbf{x})]$  is the mean function and  $k(\mathbf{x}, \mathbf{x}') = \text{Cov}_f(f(\mathbf{x}), f(\mathbf{x}'))$  is the covariance  
 143 function, a.k.a. kernel.<sup>1</sup> In all examples below, our prior mean function  $m$  is identically zero; this is  
 144 the most common choice. The marginal likelihood can be expressed as:

$$145 \quad p(f(\mathbf{x}) = \mathbf{y} | \mathbf{x}) = \int p(f(\mathbf{x}) = \mathbf{y} | f, \mathbf{x}) p(f|\mathbf{x}) df \quad (3)$$

146 where here  $p(f|\mathbf{x}) = p(f) \sim \mathcal{GP}(m, k)$  since we assume no dependence of  $f$  on  $\mathbf{x}$ . We can sample  
 147 a vector of unseen data  $\mathbf{y}^* = f(\mathbf{x}^*)$  from the predictive posterior with

$$148 \quad \mathbf{y}^* \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma}), \quad (4)$$

149 a multivariate normal with mean vector

$$150 \quad \boldsymbol{\mu} = k(\mathbf{x}, \mathbf{x}^*) k(\mathbf{x}^*, \mathbf{x}^*)^{-1} \mathbf{y} \quad (5)$$

151 and covariance matrix

$$152 \quad \boldsymbol{\Sigma} = k(\mathbf{x}, \mathbf{x}) - k(\mathbf{x}, \mathbf{x}^*) k(\mathbf{x}^*, \mathbf{x}^*)^{-1} k(\mathbf{x}^*, \mathbf{x}). \quad (6)$$

153 Often one assumes the values  $\mathbf{y}$  are noisily measured, that is, one only sees the values of  $\mathbf{y}_{\text{noisy}} =$   
 154  $\mathbf{y} + \mathbf{w}$  where  $\mathbf{w}$  is Gaussian white noise with variance  $\sigma_{\text{noise}}^2$ . In that case, the log-likelihood is

$$155 \quad \log p(\mathbf{y}_{\text{noisy}} | \mathbf{x}) = -\frac{1}{2} \mathbf{y}^\top (\boldsymbol{\Sigma} + \sigma_{\text{noise}}^2 \mathbf{I})^{-1} \mathbf{y} - \frac{1}{2} \log |\boldsymbol{\Sigma} + \sigma_{\text{noise}}^2 \mathbf{I}| - \frac{n}{2} \log 2\pi \quad (7)$$

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160 <sup>1</sup> Note that  $m(\mathbf{x}) = (m(x_i))_{i=1}^n$  and  $k(\mathbf{x}, \mathbf{x}') = (k(x_i, x'_{i'}))_{1 \leq i \leq n, 1 \leq i' \leq n'}$ , where  $n'$  is the number of entries in  
 161  $\mathbf{x}'$ .

162 where  $n$  is the number of data points. Both log-likelihood and predictive posterior can be computed  
 163 efficiently in a Venture SP with an algorithm that resorts to Cholesky factorization(Rasmussen and  
 164 Williams, 2006, chap. 2) resulting in a computational complexity of  $\mathcal{O}(n^3)$  in the number of data  
 165 points.

166 The covariance function governs high-level properties of the observed data such as linearity, periodicity  
 167 and smoothness. The most widely used form of covariance function is the squared exponential:  
 168

$$k(x, x') = \sigma^2 \exp\left(-\frac{(x - x')^2}{2\ell^2}\right), \quad (8)$$

171 where  $\sigma$  and  $\ell$  are hyperparameters:  $\sigma$  is a scaling factor and  $\ell$  is the typical length-scale.  
 172

173 Adjusting hyperparameters results in a new covariance function with the same qualitative human-  
 174 interpretation; more drastically different covariance functions are achieved by changing the structure  
 175 of the covariance function. Note that covariance function structures are compositional: adding or  
 176 multiplying two valid covariance functions results in another valid covariance function. We suggest  
 177 (**TODO** cite or point to later in paper) that adding covariance structures  $k_1, k_2$  together,  
 178

$$k_3(x, x') = k_1(x, x') + k_2(x, x'), \quad (9)$$

179 corresponds to combining global structures, while multiplying covariance functions,  
 180

$$k_4(x, x') = k_1(x, x') \times k_2(x, x'), \quad (10)$$

181 corresponds to combining local structures. Note that both  $k_3$  and  $k_4$  are valid covariance function  
 182 structures.

### 184 3 Venture GPs

186 The Venture procedure `make-gp` takes as input a mean function and a covariance function, and  
 187 outputs a procedure for sampling from a Gaussian process. In effect, each call to this procedure  
 188 samples from (4) conditioned on the return values of all previous samples. `make-gp` allows us to  
 189 perform GP inference in Venture with only a few lines of code. We can concisely express a wide  
 190 variety of GPs: simple smoothing with fixed hyper-parameters, or a prior on hyper-parameters, or  
 191 a custom covariance function. Inference on hyper-parameters can be performed using Venture's  
 192 built-in MH operator or a custom inference strategy.

193 Venture code to create and sample from a GP with a smoothing kernel and hyperparameters  
 194 is shown in Listing 1. Throughout the paper, we will use the Scheme-like front-end syntax.

```
1 [ASSUME l (gamma 1 3)] ∈ {hyper-parameters}
2 [ASSUME sf (gamma 1 3)] ∈ {hyper-parameters}
3
4 k(x, x') := σ² exp(-\frac{(x - x')²}{2ℓ²})
5
6 [ASSUME f VentureFunction(k, σ, ℓ) ]
7 [ASSUME SE (apply-function make-se f l sf) ]
8 [ASSUME GP (make-gp zero SE) ]
9
10 [SAMPLE GP (array 1 2 3)] % Prior
11 [OBSERVE GP (array x[1] ... x[n]) (array y[1] ... y[n])] % Data
12 [SAMPLE GP (array 1 2 3)]
13 [INFER (MH {hyper-parameters} one 100) ]
14 [SAMPLE GP (array 1 2 3)] % Posterior
```

207 Listing 1: Bayesian GP Smoothing  
 208

209 The first two lines declare the hyper-parameters. We tag both of them to belong to the “scope”  
 210 `{hyper-parameters}`. These tags are supplied to the inference program (in this case, MH) to  
 211 specify on which random variables inference should be done. In this paper, we use MH inference  
 212 throughout. Scopes may be further subdivided into blocks, on which block proposals can be made.  
 213 In this paper we do not use block proposals; MH inference is done on one variable at a time.

215 The `ASSUME` directives describe the GP model: `sf` and `l` (corresponding to  $\sigma$  and  $\ell$ ) are drawn  
 216 from independent  $\Gamma(1, 3)$  distributions. The squared exponential covariance function can be defined

outside the Venture code in a conventional programming language (e.g. Python) and imported as a foreign SP. In that way, the user can define custom covariance functions using his or her language and libraries of choice, without having to port existing code into Venture’s modelling language. In the above, the factory function `f`, which produces a squared exponential function with the supplied hyperparameters, is imported from Python (we have omitted the Python code). In the next line `f` is used to produce a covariance function `SE`, whose (random) hyperparameters are `l` and `s f`. Finally, we declare `GP` to be a Gaussian process with mean zero and covariance function `SE`.

I don’t know what these two paragraphs mean –Ben

In the case where hyper-parameters are unknown they can be found deterministically by optimizing the marginal likelihood using a gradient based optimizer. Non-deterministic, Bayesian representations of this case are also known (Neal, 1997).

We have already implemented this in listing 1. We draw the hyper-parameters from a  $\Gamma$ -prior for a Bayesian treatment of hyper-parameters. This is simple using the build in stochastic procedure that simulates drawing samples from a gamma distribution. The program gives rise to a Bayesian representation of GPs, which we will explore in the following.

### 3.1 Gaussian process memoization: `gpmem`

**TODO** write

### 3.2 A Bayesian interpretation

#### 3.2.1 Data modelling as a special case of `gpmem`

From the standpoint of computation, a data set of the form  $\{(x_i, y_i)\}$  can be thought of as a function  $y = f_{\text{restr}}(x)$ , where  $f_{\text{restr}}$  is restricted to only allow evaluation at a specific set of inputs  $x$ . Modelling the data set with a GP then amounts to trying to learn a smooth function  $f_{\text{emu}}$  (“emu” stands for “emulator”) which extends  $f$  to its full domain. Indeed, if  $f_{\text{restr}}$  is a foreign procedure made available as a black-box to Venture, whose secret underlying source code is:

```

245 def f_restr(x):
246     if x in D:
247         return D[x]
248     else:
249         raise Exception('Illegal input')
  
```

Then the `OBSERVE` code in Listing 1 can be rewritten using `gpmem` as follows (where here the data set `D` has keys  $x[1], \dots, x[n]$ ):

```

252 [ASSUME (list f_compute f_emu) (gpmem f_restr)]
253 for i=1 to n:
254   [PREDICT (f_compute x[i])]
255   [INFER (MH {hyper-parameters} one 100)]
256   [SAMPLE (f_emu (array 1 2 3))]
  
```

This rewriting has at least two benefits: (i) readability (in some cases), and (ii) amenability to active learning. As to (i), the statistical code of creating a Gaussian process is replaced with a memoization-like idiom, which will be more familiar to programmers. As to (ii), when using `gpmem`, it is quite easy to decide incrementally which data point to sample next: for example, the loop from  $x[1]$  to  $x[n]$  could be replaced by a loop in which the next index  $i$  is chosen by a supplied decision rule. In this way, we could use `gpmem` to perform online learning using only a subset of the available data.

#### 3.2.2 The efficacy of learning hyperparameters

The probability of the hyper-parameters of a GP with assumptions as above and given covariance function structure  $\mathbf{K}$  can be described as:

$$P(\boldsymbol{\theta} | \mathbf{D}, \mathbf{K}) = \frac{P(\mathbf{D} | \boldsymbol{\theta}, \mathbf{K})P(\boldsymbol{\theta} | \mathbf{K})}{P(\mathbf{D} | \mathbf{K})}. \quad (11)$$

Let the  $\mathbf{K}$  be the sum of a smoothing and a white noise (WN) kernel. For this case, Neal suggested the problem of outliers in data as a use-case for a hierarchical Bayesian treatment of Gaussian processes (1997)<sup>2</sup>. The work suggests a hierarchical system of hyper-parameterization (Fig. 1a). Here, we draw hyper-parameters from a  $\Gamma$  distributions:

$$\ell^{(t)} \sim \Gamma(\alpha_1, \beta_1), \sigma^{(t)} \sim \Gamma(\alpha_2, \beta_2) \quad (12)$$

and in turn sample the  $\alpha$  and  $\beta$  from  $\Gamma$  distributions as well:

$$\alpha_1^{(t)} \sim \Gamma(\alpha_\alpha^1, \beta_\alpha^1), \alpha_2^{(t)} \sim \Gamma(\alpha_\alpha^2, \beta_\alpha^2), \dots \quad (13)$$

Assuming the covariance structure is an additive comprised of a smoothing and a white noise kernel, one can represent this kind of model using `gpmm` with only a few lines of code:

```

[ASSUME alpha (mem (lambda (i) (gamma 1 3 )))] ∈ {hyper-parameters-Γ}
[ASSUME beta (mem (lambda (i) (gamma 1 3 )))] ∈ {hyper-parameters-Γ}

[ASSUME l (gamma (alpha 1) (beta 1))] ∈ {hyper-parameters}
[ASSUME sf (gamma (alpha 2) (beta 2))] ∈ {hyper-parameters}
[ASSUME sigma (uniform 0 5)] ∈ {hyper-parameters} % Fig. 2
% above: structured prior, Fig. 1a

 $k_{SE}(x, x') := \theta^2 \exp\left(-\frac{(x-x')^2}{2\ell^2}\right)$ 
 $k_{WN}(x, x') := \sigma^2 \delta_{x,x'}$ 

[ASSUME kSE VentureFunction(kSE, θ, ℓ) ]
[ASSUME kWN VentureFunction(kWN, σ) ]

[ASSUME SE make-se (apply-function kSE l sf) ]
[ASSUME WN make-se (apply-function kWN sigma) ]

[ASSUME (list f_compute f_emu) (gpmem f_restr (function-plus SE WN) )]
[SAMPLE (f_emu (array 1 2 3))] % prior, Fig. 1b

for i=1 to n:
  [PREDICT (f_compute x[i])] % observing with a look-up function
  [SAMPLE (f_emu (array 1 2 3))] % after observation, Fig. 1c

[INFER (REPEAT 100
  (DO (MH {hyper-parameters} one 2)
    (MH {hyper-parameters-Γ} one 2)))
  [SAMPLE (f_emu (array 1 2 3))] % posterior, Fig. 1d

```

Listing 2: Hierarchical GP Smoothing

Neal provides a custom inference algorithm setting and evaluates it using the following synthetic data problem. Let  $f$  be the underlying function that generates the data:

$$f(x) = 0.3 + 0.4x + 0.5 \sin(2.7x) + \frac{1.1}{(1+x^2)} + \eta \quad \text{with } \eta \sim \mathcal{N}(0, \sigma) \quad (14)$$

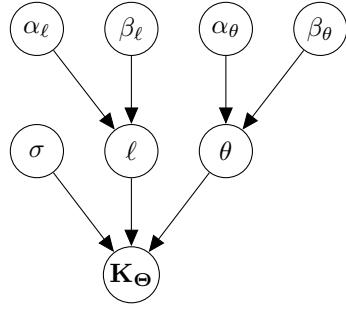
We synthetically generate outliers by setting  $\sigma = 0.1$  in 95% of the cases and to  $\sigma = 1$  in the remaining cases. `gpmem` can capture the true underlying function within only 100 MH steps on the hyper-parameters to get a good approximation for their posterior (see Fig. 1). Note that Neal devices an additional noise model and performs large number of Hybrid-Monte Carlo and Gibbs steps. We illustrate the hyper-parameter by showing the shift of the distribution on the noise parameter  $\sigma$  (Fig. 2). We see that `gpmem` learns the posterior distribution well, the posterior even exhibits a bimodal histogram when sampling  $\sigma$  100 times reflecting the two modes of data generation, that is normal noise and outliers<sup>3</sup>.

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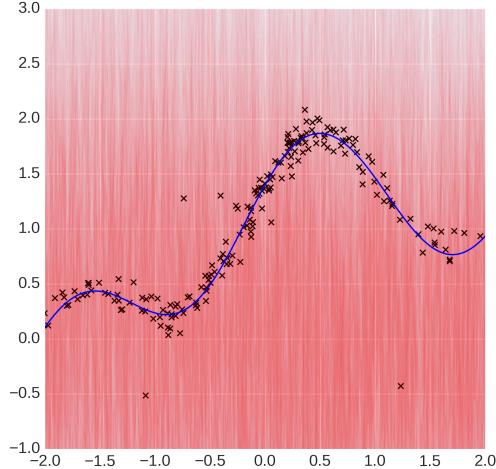
<sup>2</sup>In (Neal, 1997) the sum of an SE plus a constant kernel is used. We stick to the WN kernel for illustrative purposes.

<sup>3</sup>For this pedagogical example we have increased the probability for outliers in the data generation slightly from 0.05 to 0.2.

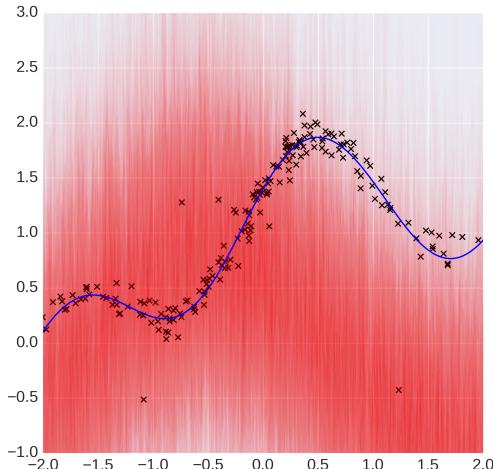
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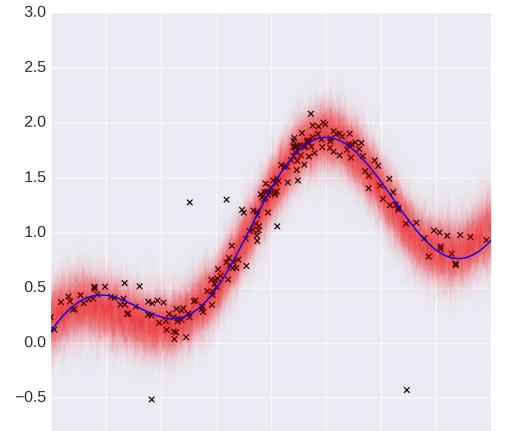
(a) Hierarchical Prior



(b) Prior Inference



(c) Observed



(d) Inferred

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Figure 1: (a) depicts the hierarchical structure of the hyper-parameter as constructed in the work by Neal as a Bayesian Network. (b)-(d) shows gpmem on Neal's example. We see that prior renders functions all over the place (a). After gpmem observes a some data-points an arbitrary smooth trend with a high level of noise is sampled. After running inference on the hierarchical system of hyper-parameters we see that the posterior reflects the actual curve well. Outliers are treated as such and do not confound the GP.

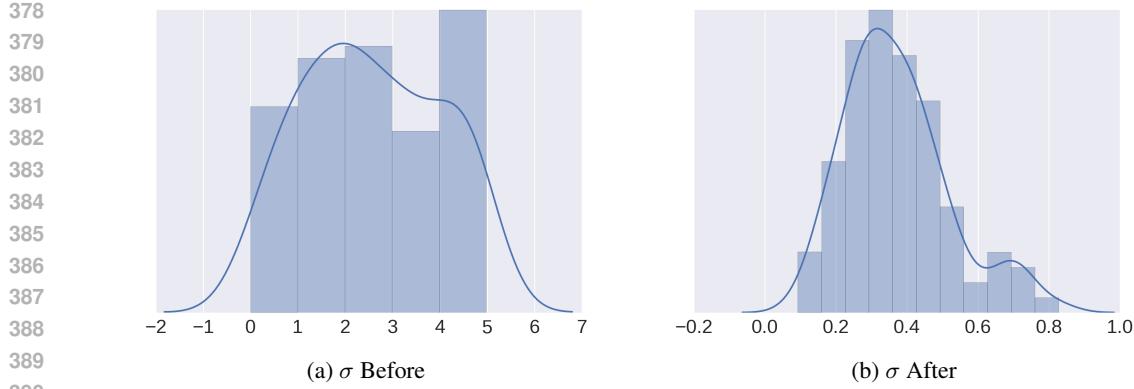


Figure 2: Hyper-parameter inference on the parameter of the noise kernel. We show 100 samples drawn from the distribution on  $\sigma$ . One can clearly recognise the shift from the uniform prior  $\mathcal{U}(0, 5)$  to a double peak distribution around the two modes - normal and outlier.

### 3.2.3 Broader applicability of gpmem

More generally, gpmem is relevant not just when a data set is available, but also whenever we have at hand a function  $f_{\text{restr}}$  which is expensive or impractical to evaluate many times. gpmem allows us to model  $f_{\text{restr}}$  with a GP-based emulator  $f_{\text{emu}}$ , and also to use  $f_{\text{emu}}$  during the learning process to choose, in an online manner, an effective set of probe points  $\{x_i\}$  on which to use our few evaluations of  $f_{\text{restr}}$ . This idea is illustrated in detail in Section 4. Before doing this, we will illustrate another benefit of having a probabilistic programming apparatus for GP modelling: the linguistically unified treatment of inference over structure and inference over parameters. This unification makes interleaved joint inference over structure and parameters very natural, and allows us to give a short, elegant description of what it means to “learn the covariance function,” both in prose and in code. Furthermore, the example in Section 3.3 below recovers the performance of current state-of-the-art GP-based models.

## 3.3 Structure Learning

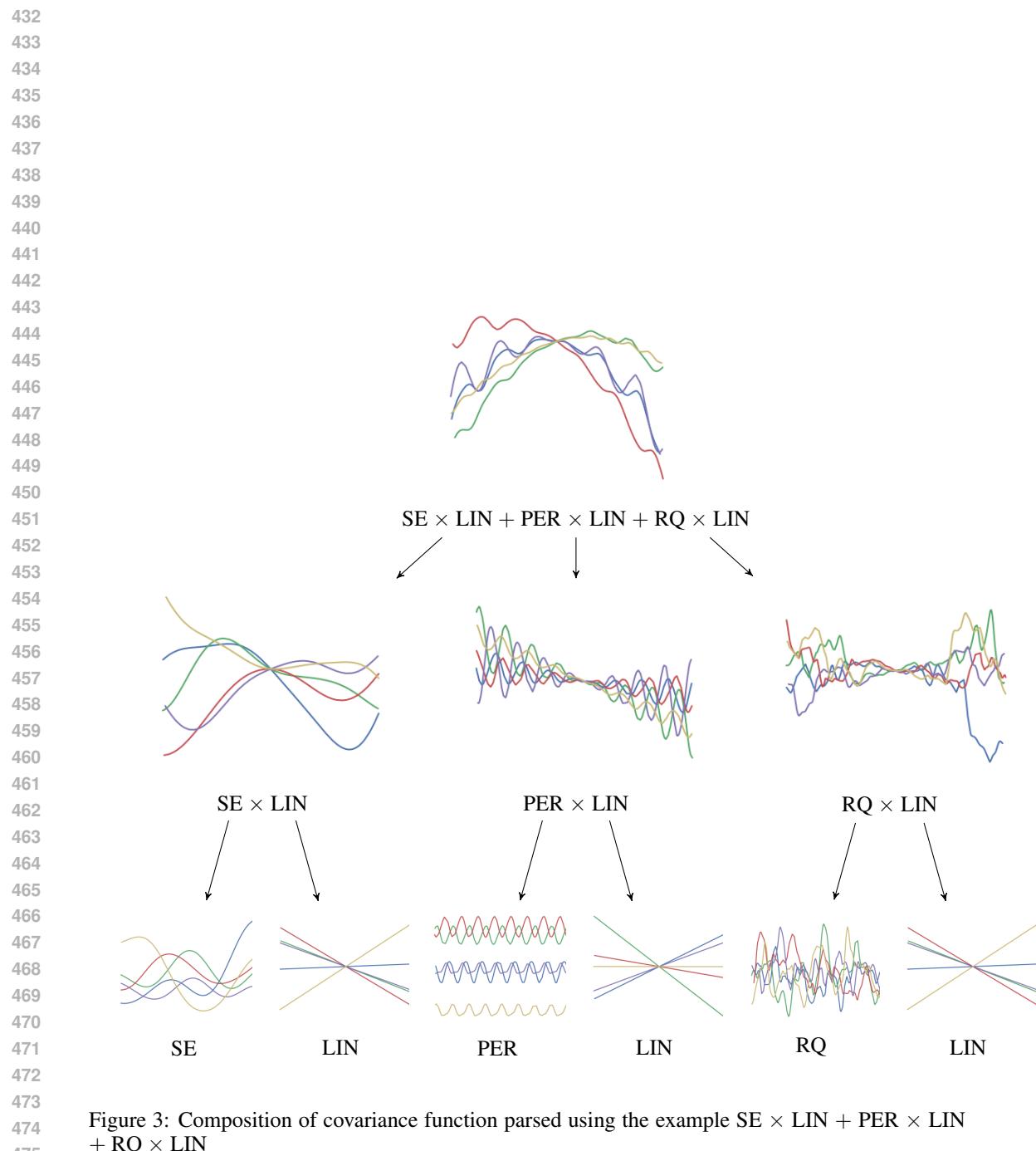
The space of possible kernel composition is infinite. Combining inference over this space with the problem of finding a good parameterization that could potentially explain the observed data best poses a hard problem. The natural language interpretation of the meaning of a kernel and its composition renders this a problem of symbolic computation. Duvenaud and colleagues note that a sum of kernels can be interpreted as logical OR operations and kernel multiplication as logical AND (2013). This is due to the kernel rendering two points similar if  $k_1$  OR  $k_2$  outputs a high value in the case of a sum. Respectively, multiplication of two kernels results in high values only if  $k_1$  AND  $k_2$  have high values (see Fig. 3 exemplifies how to interpret global vs. local aspects and its symbolic analog respectively). In the following, we will refer to covariance functions that are not composite as base covariance functions.

Knowledge about the composite nature of covariance functions is not new, however, until recently, the choice and the composition of covariance functions were done ad-hoc. The Automated Statistician Project came up with an approximate search over the possible space of kernel structures (Duvenaud et al., 2013; Lloyd et al., 2014). However, a fully Bayesian treatment of this was not done before. The case where the covariance structure is not given is even more interesting. Our probabilistic programming based MCMC framework approximates the following intractable integrals of the expectation for the prediction:

$$\mathbb{E}[y^* | x^*, \mathbf{D}, \mathbf{K}] = \iint f(x^*, \boldsymbol{\theta}, \mathbf{K}) P(\boldsymbol{\theta} | \mathbf{D}, \mathbf{K}) P(\mathbf{K} | \Omega, s, n) d\boldsymbol{\theta} d\mathbf{K}. \quad (15)$$

This is done by sampling from the posterior probability distribution of the hyper-parameters and the possible kernel:

$$y^* \approx \frac{1}{T} \sum_{t=1}^T f(x^* | \boldsymbol{\theta}^{(t)}, \mathbf{K}^{(t)}). \quad (16)$$



473                    Figure 3: Composition of covariance function parsed using the example  $SE \times LIN + PER \times LIN$   
 474                    +  $RQ \times LIN$   
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 478  
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 481  
 482  
 483  
 484  
 485

486 In order to provide the sampling of the kernel, we introduce a stochastic process to the SP that  
 487 simulates the grammar for algebraic expressions of covariance function algebra:  
 488

$$500 \quad \mathbf{K}^{(t)} \sim P(\mathbf{K} | \boldsymbol{\Omega}, s, n) \quad (17)$$

512 Here, we start with a set of possible kernels and draw a random subset. For this subset of size  $n$ , we  
 513 sample a set of possible operators that operate on the base kernels.

514 The marginal probability of a kernel structure which allows us to sample is characterized by the  
 515 probability of a uniformly chosen subset of the set of  $n$  possible covariance functions times the  
 516 probability of sampling a global or a local structure which is given by a binomial distribution:  
 517

$$518 \quad P(\mathbf{K} | \boldsymbol{\Omega}, s, n) = P(\boldsymbol{\Omega} | s, n) \times P(s | n) \times P(n), \quad (18)$$

519 with

$$521 \quad P(\boldsymbol{\Omega} | s, n) = \binom{n}{r} p_{+\times}^k (1 - p_{+\times})^{n-k} \quad (19)$$

522 and

$$523 \quad P(s | n) = \frac{n!}{|s|!} \quad (20)$$

525 where  $P(n)$  is a prior on the number of base kernels used which can sample from a discrete uniform  
 526 distribution. This will strongly prefer simple covariance structures with few base kernels since  
 527 individual base kernels are more likely to be sampled in this case due to (20). Alternatively, we  
 528 can approximate a uniform prior over structures by weighting  $P(n)$  towards higher numbers. It is  
 529 possible to also assign a prior for the probability to sample global or local structures, however, we  
 530 have assigned complete uncertainty to this with the probability of a flip  $p = 0.5$ .

531 Many equivalent covariance structures can be sampled due to covariance function algebra and equiv-  
 532 alent representations with different parameterization (Lloyd et al., 2014). Certain covariance func-  
 533 tions can differ in terms of the hyper-parameterization but can be absorbed into a single covariance  
 534 function with a different parameterization. To inspect the posterior of these equivalent structures  
 535 we convert each kernel expression into a sum of products and subsequently simplify. Rules for this  
 536 simplification can be found in appendix B.

537 For reproducing results from the Automated Statistician Project in a Bayesian fashion we first define  
 538 a prior on the hypothesis space. Note that, as in the implementation of the Automated Statistician,  
 539 we upper-bound the complexity of the space of covariance functions we want to explore. We also  
 put vague priors on hyper-parameters.

```

540
541 [ASSUME base_kernels (list K1,K2,...,Kn) ] % defined as above
542 [ASSUME pn (uniform_structure n)] % prior on the number of kernels
543 [ASSUME SK (subset base_kernels pn) ] % sampling a subset of size n
544 [ASSUME composition (lambda (l) % kernel composition
545           (if (lte (size l) 1)
546               (first l)
547               (if (flip)
548                   (func_plus (first l) (cov_compo (rest l)))
549                   (func_times (first l) (cov_compo (rest l))))
550               )
551           )
552       )
553 [ASSUME K (composition SK) ]
554
555 [ASSUME (list f_compute f_emu) (gpmem f_restr K )]
556
557 for i=1 to n:
558   [PREDICT (f_compute x[i])] % observing with a look-up function
559
560 [INFER (REPEAT 2000 (DO
561           (MH pn one 1)
562           (MH SK one 1)
563           (MH K* one 1)
564           (MH {hyper-parameters} one 10)) ]

```

Listing 3: Venture Code for Bayesian GP Structure Learning

We defined the space of covariance structures in a way allowing us to reproduce results for covariance function structure learning as in the Automated Statistician. This lead to coherent results, for example for the airline data set describing monthly totals of international airline passengers (Box et al., 1997, according to Duvenaud et al., 2013). We will elaborate the result using a sample from the posterior (Fig. 4). The sample is identical with the highest scoring result reported in previous work using a search-and-score method (Duvenaud et al., 2013) for the CO<sub>2</sub> data set (see Rasmussen and Williams, 2006 for a description) and the predictive capability is comparable. However, the components factor in a different way due to different parameterization of the individual base kernels.

We further investigated the quality of our stochastic processes by running a leave one out cross-validation to gain confidence on the posterior. This resulted in 545 independent runs of the Markov chain that produced a coherent posterior: our Bayesian interpretation of GP structure and GPs produced a posterior of structures that is in line with previous results on this data set ( Duvenaud et al., 2013; see Fig. 5).

We ran similar evaluation on the airline data set resulting in a similar structure to what was previously reporte (Fig. 6, residuals and log-score along the Markov chain see Fig. 7).

We found the final sample of multiple runs to be most informative. This kind of Markov Chain seems to produce samples that are highly auto-correlated.

Given two additive components  $\mathbf{K} = \mathbf{K}_a + \mathbf{K}_b$ , one can compute the marginal of a global component of a composite kernel structure (Benavoli and Mangili, 2015) with a gaussian posterior  $\mathcal{N}(f_a | \hat{\mu}_a, \hat{\mathbf{K}}_a)$  where:

$$\hat{\mu}_a = \mathbf{K}_a(\mathbf{x}, \mathbf{x}^*) \mathbf{K}(\mathbf{x}^*, \mathbf{x}^*)^{-1} \mathbf{y} \quad (21)$$

and covariance matrix

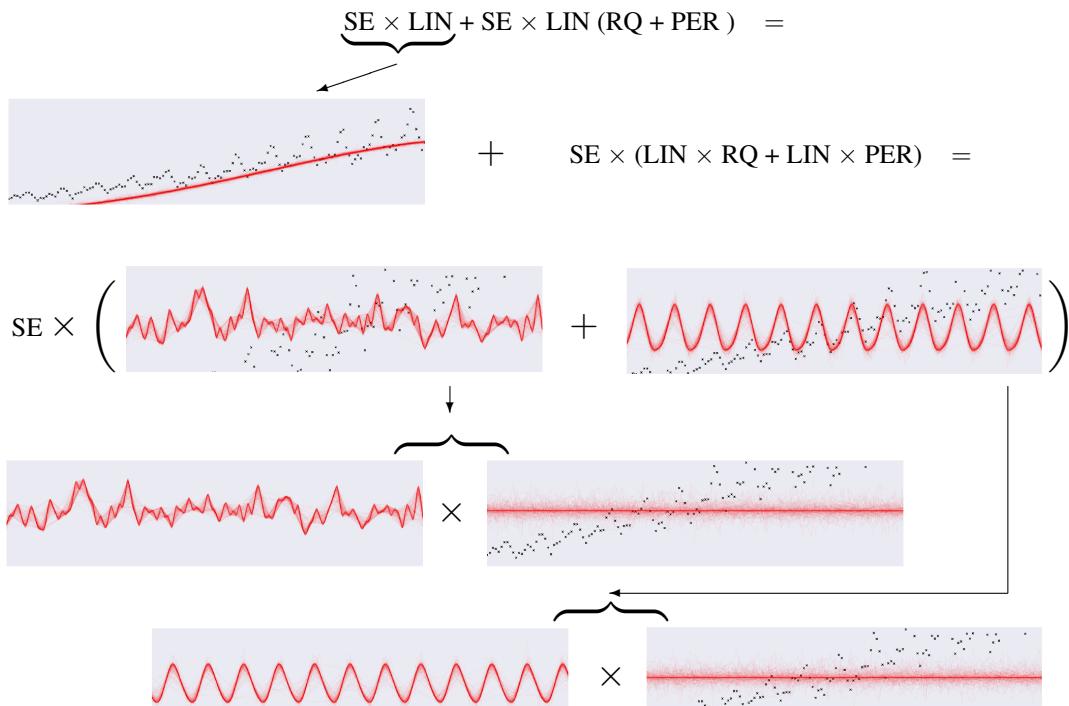
$$\hat{\mathbf{K}}_a = \mathbf{K}_a(\mathbf{x}, \mathbf{x}) - \mathbf{K}_a(\mathbf{x}, \mathbf{x}^*) \mathbf{K}(\mathbf{x}^*, \mathbf{x}^*)^{-1} \mathbf{K}_a(\mathbf{x}^*, \mathbf{x}). \quad (22)$$

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(a) The predictive posterior using the full grammar structure.

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(b) Compositional Structure

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Figure 4: a) We see the predictive posterior as a result 1000 nested MH steps on the airline data set. b) depicts a decomposition of this posterior for the structures sampled by Venture. RQ is the rational quadratic covariance function. The first line shows the global trend and denotes the rest of the structure that is shown above. In the second line, the see the periodic component on the right hand side. The left hand side denotes short term deviations both multiplied by a smoothing kernel. The third and fourth lines denote how we reach the second line: both periodic and rational quadratic covariance functions are multiplied by a linear covariance function with slope zero.

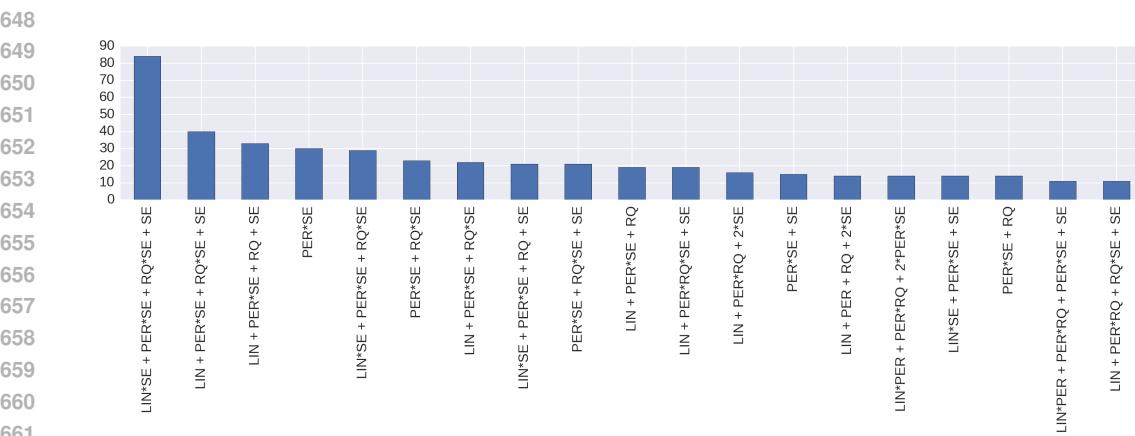


Figure 5: Posterior on structure of the CO<sub>2</sub> data. We have cut the tail of the distribution for space reasons since the number of possible structures is large. We see the final sample of the each of the 545 chains with 2000 nested steps each. Note that Duvenaud et al. (2013) report LIN × SE + PER × SE + RQ × SE.

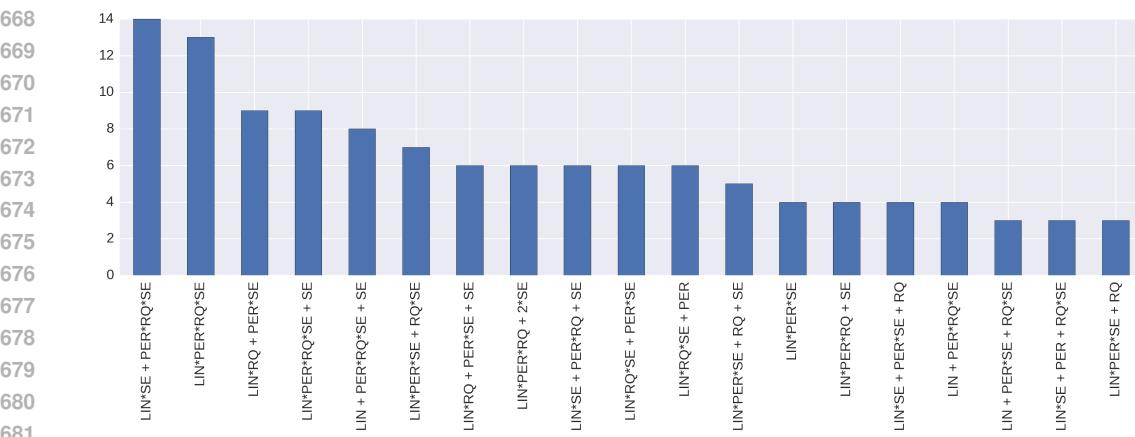


Figure 6: Posterior on structure of airline data set. We have cut the tail of the distribution for space reasons since the number of possible structures is large. We see the final sample of the each of the 144 chains with 2000 nested steps each. Note that Duvenaud et al. (2013) report  $\text{LIN} \times \text{SE} + (\text{PER} + \text{RQ}) \times \text{SE} \times \text{LIN}$

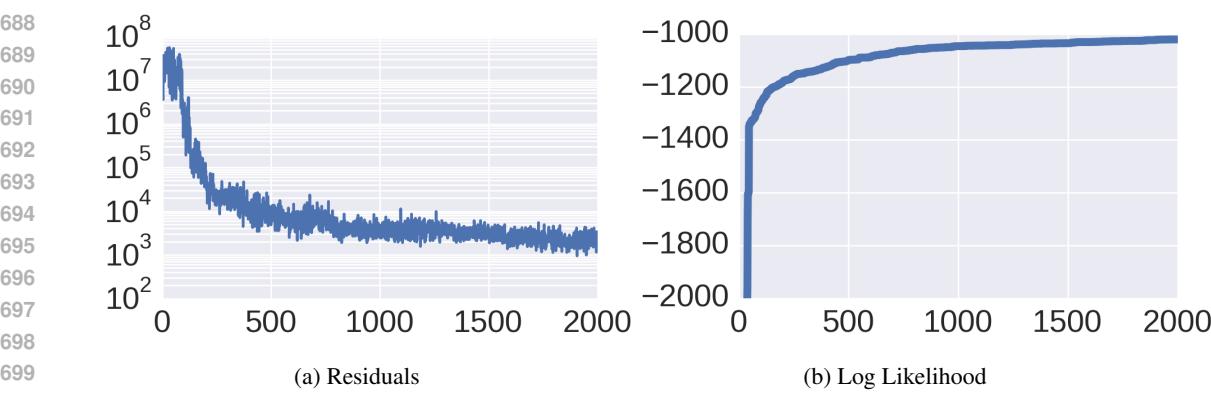


Figure 7: 2000 steps along the Markov Chain.

702           **4 Bayesian Optimization**  
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705       Bayesian optimization casts the problem of finding the global maximum of an unknown function as  
706       a hierarchical decision problem (Ghahramani, 2015). Evaluating the actual function may be very  
707       expensive, either in computation time or in some other resource. For one example, when searching  
708       for the best configuration for the learning algorithm of a large convolutional neural network, a large  
709       amount of computational work is required to evaluate a candidate configuration, and the space of  
710       possible configurations is high-dimensional. Another common example, alluded to in Section 3.2.3,  
711       is data acquisition: for machine learning problems in which a large body of data is available, it is  
712       often desirable to choose the right queries to produce a data set on which learning will be most  
713       effective. In continuous settings, many Bayesian optimization methods employ GPs (e.g. Snoek  
714       et al., 2012).

715       We have implemented a version of Thompson sampling using GPs in Venture. Thompson sam-  
716       pling Thompson (1933) is a widely-used Bayesian framework for solving exploration-exploitation  
717       problems. Our implementation has two notable features: (i) the ability to search over a broader  
718       space of contexts than the parametric families that are typically used, and (ii) the parsimony of the  
719       resulting probabilistic program.

720           **4.1 Thompson sampling framework**  
721

722       We now lay out the setup of Thompson sampling for Markov decision processes (MDPs). An agent  
723       is to take a sequence of actions  $a_1, a_2, \dots$  from a (possibly infinite) set of possible actions  $\mathcal{A}$ . After  
724       each action, a reward  $r \in \mathbb{R}$  is received, according to an unknown conditional distribution  $P_{\text{true}}(r|a)$ .  
725       The agent's goal is to maximize the total reward received for all actions. In Thompson sampling,  
726       the Bayesian agent accomplishes this by placing a prior distribution  $P(\theta)$  on the possible "contexts"  
727        $\theta \in \Theta$ . Here a context is a believed model of the conditional distributions  $\{P(r|a)\}_{a \in \mathcal{A}}$ , or at least,  
728       a believed statistic of these conditional distributions which is sufficient for deciding an action  $a$ .  
729       One example of such a sufficient statistic is the conditional mean  $V(a|\theta) = \mathbb{E}[r|a, \theta]$ , which can be  
730       thought of as a value function. Thompson sampling thus has the following steps, repeated as long  
731       as desired:

- 732       1. Sample a context  $\theta \sim P(\theta)$ .  
733  
734       2. Choose an action  $a \in \mathcal{A}$  which (approximately) maximizes  $V(a|\theta) = \mathbb{E}[r|a, \theta]$ .  
735  
736       3. Let  $r_{\text{true}}$  be the reward received for action  $a$ . Update the believed distribution on  $\theta$ , i.e.,  
737        $P(\theta) \leftarrow P_{\text{new}}(\theta)$  where  $P_{\text{new}}(\theta) = P(\theta | a \mapsto r_{\text{true}})$ .

738  
739       Note that when  $\mathbb{E}[r|a, \theta]$  (under the sampled value of  $\theta$  for some points  $a$ ) is far from the true value  
740        $\mathbb{E}_{P_{\text{true}}}[r|a]$ , the chosen action  $a$  may be far from optimal, but the information gained by probing  
741       action  $a$  will improve the belief  $\theta$ . This amounts to "exploration." When  $\mathbb{E}[r|a, \theta]$  is close to the  
742       true value except at points  $a$  for which  $\mathbb{E}[r|a, \theta]$  is low, exploration will be less likely to occur, but  
743       the chosen actions  $a$  will tend to receive high rewards. This amounts to "exploitation." Roughly  
744       speaking, exploration will happen until the context  $\theta$  is reasonably sure that the unexplored actions  
745       are probably not optimal, at which time the sampler will exploit by choosing actions in regions it  
746       knows to have high value.

747       Typically, when Thompson sampling is implemented, the search over contexts  $\theta \in \Theta$  is limited  
748       by the choice of representation. In traditional programming environments,  $\theta$  often consists of a few  
749       numerical parameters for a family of distributions of a fixed functional form. With work, a mixture of  
750       a few functional forms is possible; but without probabilistic programming machinery, implementing  
751       a rich context space  $\Theta$  would be an unworkably large technical burden. In a probabilistic programming  
752       language, however, the representation of heterogeneously structured or infinite-dimensional context  
753       spaces is quite natural. Any computable model of the conditional distributions  $\{P(r|a)\}_{a \in \mathcal{A}}$  can be  
754       represented as a stochastic procedure  $(\lambda(a) \dots)$ . Thus, for computational Thompson sampling, the  
755       most general context space  $\hat{\Theta}$  is the space of program texts. Any other context space  $\Theta$  has a natural  
embedding as a subset of  $\hat{\Theta}$ .

756    **4.2 Thompson sampling in Venture**

758 Because Venture supports sampling and inference on (stochastic-)procedure-valued random vari-  
 759 ables (and the generative models which produce those procedures), Venture can capture arbitrary  
 760 context spaces as described above. To demonstrate, we have implemented Thompson sampling  
 761 in Venture in which the contexts  $\theta$  are Gaussian processes over the action space  $\mathcal{A} = \mathbb{R}$ . That  
 762 is,  $\theta = (\mu, K)$ , where the mean  $\mu$  is a computable function  $\mathcal{A} \rightarrow \mathbb{R}$  and the covariance  $K$  is  
 763 a computable (symmetric, positive-semidefinite) function  $\mathcal{A} \times \mathcal{A} \rightarrow \mathbb{R}$ . This represents a Gaus-  
 764 sian process  $\{R_a\}_{a \in \mathcal{A}}$ , where  $R_a$  represents the reward for action  $a$ . Computationally, we rep-  
 765 resent a context not as a pair of infinite lookup tables for  $\mu$  and  $K$ , but as a finite data structure  
 766  $\theta = (K_{\text{prior}}, \sigma, \ell, \mathbf{a}_{\text{past}}, \mathbf{r}_{\text{past}})$ , where

- 767    •  $K_{\text{prior}} = K_{\text{prior}, \sigma, \ell}$  is a procedure, with parameters  $\sigma, \ell$ , to be used as the prior covariance  
 768    function:  $K_{\text{prior}}(a, a') = \sigma^2 \exp\left(-\frac{(a-a')^2}{2\ell^2}\right)$
- 769    •  $\sigma$  and  $\ell$  are (hyper)parameters for  $K_{\text{prior}}$
- 770    •  $\mathbf{a}_{\text{past}} = (a_i)_{i=1}^n$  are the previously probed actions
- 771    •  $\mathbf{r}_{\text{past}} = (r_i)_{i=1}^n$  are the corresponding rewards

774 To simplify the treatment, we take prior mean  $\mu_{\text{prior}} \equiv 0$ . The mean and covariance for  $\theta$  are then  
 775 gotten by the usual conditioning formula:

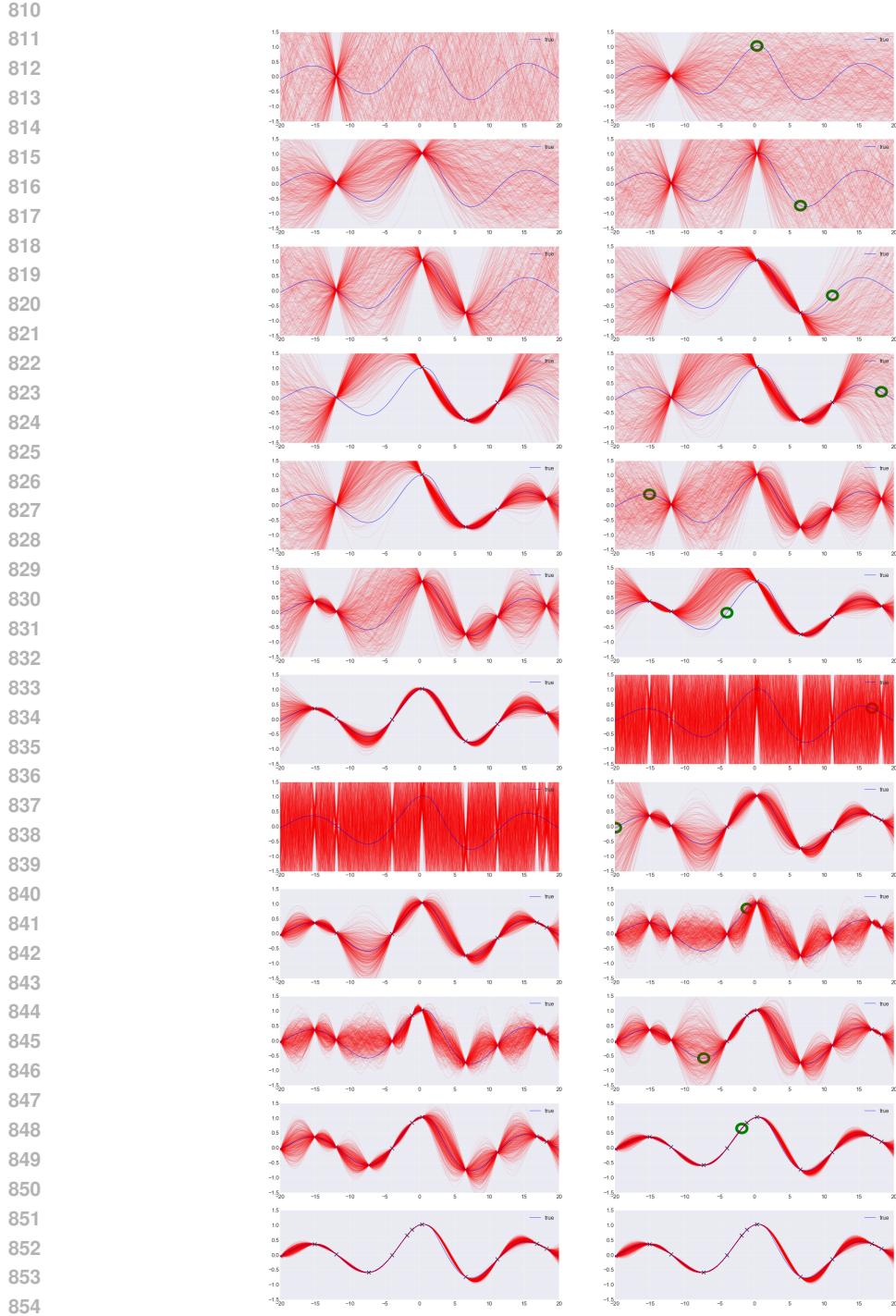
$$\begin{aligned} 776 \quad \mu(\mathbf{a}) &= \mu(\mathbf{a} \mid \mathbf{a}_{\text{past}}, \mathbf{r}_{\text{past}}) \\ 777 &= K_{\text{prior}}(\mathbf{a}, \mathbf{a}_{\text{past}}) K_{\text{prior}}(\mathbf{a}_{\text{past}}, \mathbf{a}_{\text{past}})^{-1} \mathbf{r}_{\text{past}} \\ 778 \quad K(\mathbf{a}, \mathbf{a}) &= K(\mathbf{a}, \mathbf{a} \mid \mathbf{a}_{\text{past}}, \mathbf{r}_{\text{past}}) \\ 779 &= K_{\text{prior}}(\mathbf{a}, \mathbf{a}) - K_{\text{prior}}(\mathbf{a}, \mathbf{a}_{\text{past}}) K_{\text{prior}}(\mathbf{a}_{\text{past}}, \mathbf{a}_{\text{past}})^{-1} K_{\text{prior}}(\mathbf{a}_{\text{past}}, \mathbf{a}). \end{aligned}$$

782 Note that even in this simple example, the context space  $\Theta$  is not a finite-dimensional parametric  
 783 family, since the vectors  $\mathbf{a}_{\text{past}}$  and  $\mathbf{r}_{\text{past}}$  grow as more samples are taken.  $\Theta$  is, however, quite easily  
 784 representable as a computational procedure together with parameters and past samples, as we do in  
 785 the representation  $\theta = (K_{\text{prior}}, \sigma, \ell, \mathbf{a}_{\text{past}}, \mathbf{r}_{\text{past}})$ .

786    **4.3 Implementation with gpmem**

787 As a demonstration, we use Thompson sampling to optimize an unknown function  $V(x)$  (the value  
 788 function) using gpmem. (TODO we should not assume  $V$  is deterministic, it would be easy enough  
 789 to make it random or have it give noisy samples.) We assume  $V$  is made available to Venture as a  
 790 black-box. The code for optimizing  $V$  is given in Listing 4. For step 3 of Thompson sampling, the  
 791 Bayesian update, we not only condition on the new data (the chosen action  $a$  and the received reward  
 792  $r$ ), but also perform inference on the hyperparameters  $\sigma, \ell$  using a Metropolis–Hastings sampler.  
 793 These two inference steps take 1 line of code: 0 lines to condition on the new data (as this is done  
 794 automatically by gpmem), and 1 line to call Venture’s built-in MH operator. The results are shown  
 795 in Figure 8. We can see from the figure that, roughly speaking, each successive probe point  $a$  is  
 796 chosen either because the current model  $V_{\text{emu}}$  thinks it will have a high reward, or because the value  
 797 of  $V_{\text{emu}}(a)$  has high uncertainty. In the latter case, probing at  $a$  decreases this uncertainty and, due to  
 798 the smoothing kernel, also decreases the uncertainty at points near  $a$ . We thus see that our Thompson  
 799 sampler simultaneously learns the value function and optimizes it.

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855 Figure 8: Dynamics of Thompson sampling in Venture. The blue curve is the true function  $V$ , and  
856 the red region is a blending of 100 samples of the curve generated (jointly) by a GP-based emulator  
857  $V_{\text{emu}}$ . The left and right columns show the state of  $V_{\text{emu}}$  before and after hyperparameter inference  
858 is run on the new data, respectively. (We can see, for example, that after the seventh probe point,  
859 the Metropolis–Hastings sampler chose a “crazy” set of hyperparameters, which was corrected at  
860 the next inference step.) In the right column, the next chosen probe point is circled in green. Each  
861 successive probe point  $a$  is the (stochastic) maximum of  $V_{\text{emu}}$ , sampled pointwise and conditioned  
862 on the values of the previously probed points. Note that probes tend to happen at points either where  
863 the value of  $V_{\text{emu}}$  is high, or where  $V_{\text{emu}}$  has high uncertainty.

```

864 1 [ASSUME sigma (sigma-prior) ]
865 2 [ASSUME l (l-prior) ]
866 3 [ASSUME K (make-squared-exponential sigma l) ]
867 4 [ASSUME (list V_compute V_emu) (gpmem V K) ]
868 5 [ASSUME V_emu_pointwise (lambda (a) (first (V_emu (array a))))) ]
869 6 [ASSUME mc_sampler (uniform_sampler -20 20) ]
870 7
871 8 for i=1 to 15:
872 9   [PREDICT (V_compute (mc_argmax V_emu_pointwise mc_sampler)) ]
873 10  [INFER (MH 'hypers one 50) ]
874 11
875 12 [INFER (extract_stats V_emu) ]

```

Listing 4: Code for Bayesian optimization using `gpmem`. In the loop, `V_compute` is called to probe the value of `V` at a new argument. The new argument, `(mc_argmax V_emu_pointwise mc_sampler)`, is a Monte Carlo estimate of the maximum pointwise sample of `V_emu` (itself a stochastic quantity), with the Monte Carlo samples being drawn in this case uniformly between  $-20$  and  $20$ . After each new call to `V_compute`, the Metropolis–Hastings algorithm is used to perform inference on the hyperparameters of the covariance function in the GP model in light of the new conditioning data. Once enough calls to `V_compute` have been made (in our case we stopped at 15 calls), we can inspect the full list of probed  $(a, r)$  pairs with `extract_stats`. The answer to our maximization problem is simply the pair having the highest  $r$ ; but our algorithm also learns more potentially useful information.

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## 5 Conclusion

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We have shown Venture GPs. We have introduced novel stochastic processes for a probabilistic programming language. We showed how flexible non-parametric models can be treated in Venture in only a few lines of code. We evaluated our contribution on a range of hard problems for state-of-the-art Bayesian non-parametrics. Venture GPs showed competitive performance in all of them.

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## Appendix

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### A Covariance Functions

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896

SE and WN are defined in the text above, for completeness we will introduce the covariance:

897

898

$$k_{LIN}(x, x') = \theta(x x') \quad (23)$$

899

900

$$k_{PER}(x, x') = \theta \exp \left( \frac{2 \sin^2(\pi(x - x')/p)}{\ell^2} \right) \quad (24)$$

901

902

$$k_{RQ}(x, x') = \theta \left( 1 + \frac{(x - x')^2}{2\alpha\ell^2} \right)^{-\alpha} \quad (25)$$

903

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906

### B Covariance Simplification

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1 SE $\times$ SE	$\rightarrow$ SE
2 {SE, PER, C, WN} $\times$ WN	$\rightarrow$ WN
3 LIN + LIN	$\rightarrow$ LIN
4 {SE, PER, C, WN, LIN} $\times$ C	$\rightarrow$ {SE, PER, C, WN, LIN}

914

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Listing 5: Grammar to simplify expressions

$$\theta(xx') = \theta_1(xx') + \theta_2(xx') \quad (26)$$

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919

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