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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

- 082 • standard memoization
- 083 • memoization as described in (Goodman et al., 2008)

### 085 2.2 Venture

087 Venture is a compositional language for custom inference strategies that comes with a Scheme- and  
 088 Java-Script-like front-end syntax. Its implementation is based on on three concepts. (i) stochas-  
 089 tic procedure interfaces that specify and encapsulate random variables, analogously to conditional  
 090 probability tables in a Bayesian network; (ii) probabilistic execution traces that represent execution  
 091 histories and capture conditional dependencies; and (iii) scaffolds that partition execution histories  
 092 and factor global inference problems into sub-problems. These building blocks provide a powerful  
 093 way to represent probability distributions; some of which cannot be expressed with density func-  
 094 tions. For the purpose of this work the most important Venture directives that operate on these  
 095 building blocks to understand are ASSUME, OBSERVE, SAMPLE and INFER. ASSUME induces  
 096 a hypothesis space for (probabilistic) models including random variables by binding the result of an  
 097 expression to a symbol. SAMPLE simulates a model expression and returns a value. OBSERVE  
 098 adds constraints to model expressions. INFER instructions incorporate observations and cause Ven-  
 099 ture to find a hypothesis that is probable given the data.

100 INFER is most commonly done by deploying the Metropolis-Hastings algorithm (MH) (Metropolis  
 101 et al., 1953). Many algorithms used in the MCMC world can be interpreted as special cases of  
 102 MH (Andrieu et al., 2003). We can outline the MH algorithm as follows. For  $T$  steps we sample  $x^*$   
 103 from a proposal distribution  $q$ :

$$x^* \sim q(x^* | x^{(t)}) \quad (1)$$

104 which we accept ( $x^{t+1} \leftarrow x^*$ ) with ratio:

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

105 106 107 Venture implements an MH transition operator for probabilistic execution traces.

108    **2.3 Gaussian Processes**  
 109

110 In the following, we will introduce GP related theory and notations. We will exclusively work on  
 111 two variable regression problems. Let the data be real-valued scalars  $\{x_i, y_i\}_{i=1}^n$  (complete data will  
 112 be denoted by column vectors  $\mathbf{x}, \mathbf{y}$ ). GPs present a non-parametric way to express prior knowledge  
 113 on the space of possible functions  $f$  that we assume to have generated the data.  $f$  is assumed latent  
 114 and the GP prior is given by a multivariate Gaussian  $f(\mathbf{x}) \sim \mathcal{GP}(m(\mathbf{x}), k(x_i, x'_i))$ , where  $m(\mathbf{x})$  is  
 115 a function of the mean of all functions that map to  $y_i$  at  $x_i$  and  $k(x_i, x'_i)$  is a kernel or covariance  
 116 function that summarizes the covariance of all functions that map to  $y_i$  at  $x_i$ . We can absorb the  
 117 mean function into the covariance function so without loss of generality we can set the mean to  
 118 zero. The marginal likelihood can be expressed as:

$$119 \quad p(\mathbf{y}|\mathbf{x}) = \int p(\mathbf{y}|\mathbf{f}, \mathbf{x}) p(\mathbf{f}|\mathbf{x}) d\mathbf{f} \quad (3)$$

120 where the prior is Gaussian  $\mathbf{f}|\mathbf{x} \sim \mathcal{N}(0, k(\mathbf{x}, \mathbf{x}'))$ . We can sample a vector of unseen data from the  
 121 predictive posterior with

$$122 \quad \mathbf{y}^* \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma}) \quad (4)$$

123 for a zero mean prior GP with a posterior mean of:

$$124 \quad \boldsymbol{\mu} = \mathbf{K}(\mathbf{x}, \mathbf{x}^*) \mathbf{K}(\mathbf{x}^*, \mathbf{x}^*)^{-1} \mathbf{y} \quad (5)$$

125 and covariance

$$126 \quad \boldsymbol{\Sigma} = \mathbf{K}(\mathbf{x}, \mathbf{x}) + \mathbf{K}(\mathbf{x}, \mathbf{x}^*) \mathbf{K}(\mathbf{x}^*, \mathbf{x}^*)^{-1} \mathbf{K}(\mathbf{x}^*, \mathbf{x}). \quad (6)$$

127  $\mathbf{K}$  is a covariance function. The log-likelihood is defined as:

$$128 \quad \log P(\mathbf{y} | \mathbf{X}) = -\frac{1}{2}\mathbf{y}^\top (\mathbf{K} + \sigma^2 \mathbf{I})^{-1} \mathbf{y} - \frac{1}{2} \log |\mathbf{K} + \sigma^2 \mathbf{I}| - \frac{n}{2} \log 2\pi \quad (7)$$

129 with  $n$  being the number of data-points and sigma the independent observation noise. Both log-  
 130 likelihood and predictive posterior can be computed efficiently in a Venture SP with an algorithm  
 131 that resorts to Cholesky factorization(Rasmussen and Williams, 2006, chap. 2) resulting in a com-  
 132 putational complexity of  $\mathcal{O}(n^3)$  in the number of data-points.

133 The covariance function covers general high-level properties of the observed data such as linear-  
 134 ity, periodicity and smoothness. The most widely used type of covariance function is the squared  
 135 exponential covariance function:

$$136 \quad k(x, x') = \sigma^2 \exp\left(-\frac{(x - x')^2}{2\ell^2}\right) \quad (8)$$

137 where  $\sigma$  and  $\ell$  are hyper-parameters.  $\sigma$  is a scaling factor and  $\ell$  is the typical length-scale. Smaller  
 138 variations can be achieved by adapting these hyper-parameters.

139 Larger variations are achieved by changing the type of the covariance function structure. Note that  
 140 covariance function structures are compositional. We can add covariance functions if we want to  
 141 model globally valid structures

$$142 \quad k_3(x, x') = k_1(x, x') + k_2(x, x') \quad (9)$$

143 and we can multiply covariance functions if the data is best explained by local structure

$$144 \quad k_4(x, x') = k_1(x, x') \times k_2(x, x'); \quad (10)$$

145 both,  $k_3$  and  $k_4$  are valid covariance function structures.

146    **3 Venture GPs**  
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148 Given a stochastic process that implements the GP algebra above we can imple-  
 149 ment a GP sampler (4) to perform GP inference in a few lines of code. We  
 150 can express simple GP smoothing with fixed hyper-parameters or a prior on hyper-  
 151 parameters and perform MH on it while allowing users to custom design covari-

```

1  ance functions. Throughout the paper, we will use the Scheme-like front-end syntax.
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163
164 [ASSUME l (gamma 1 3)] ∈ {hyper-parameters}
165 [ASSUME sf (gamma 1 3)] ∈ {hyper-parameters}
166
167  $k(x, x') := \sigma^2 \exp\left(-\frac{(x-x')^2}{2\ell^2}\right)$ 
168
169 [ASSUME f VentureFunction(k, σ, ℓ) ]
170 [ASSUME SE make-se (apply-function f l sf) ]
171 [ASSUME (make-gp 0 SE) ]
172
173 [SAMPLE GP (array 1 2 3)] % Prior
174 [OBSERVE GP D]
175 [SAMPLE GP (array 1 2 3)]
176 [INFER (MH {hyper-parameters} one 100) ]
177 [SAMPLE GP (array 1 2 3)] % Posterior

```

Listing 1: Bayesian GP Smoothing

The first two lines depict the hyper-parameters. We tag both of them to belong to the set  $\{\text{hyper-parameters}\}$ . Every member of this set belongs to the same inference scope. This scope controls the application of the inference procedure used. In this paper, we use MH throughout. Each scope is further subdivided into blocks that allow to do block-proposals. In the following we omit the block notation for readability, since we always choose the block of a certain scope at random.

The ASSUME directives describe the assumptions we make for the GP model, we assume the hyper-parameters  $l$  and  $sf$  (corresponding to  $\ell, \sigma$ ) to be 1 and 2. The squared exponential covariance function can be defined outside the Venture code with foreign conventional programming languages, e.g. Python. In that way, the user can define custom covariance functions without being restricted to the most common ones. We then integrate the foreign function into Venture as VentureFunction. In the next line this function is associated with the hyper-parameters. Finally, we assume a Gaussian Process SP with a zero mean and the previously assumed squared exponential covariance function.

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 A Bayesian interpretation

#### 3.1.1 GP 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:

```

210 def f_restr(x):
211     if x in D:
212         return D[x]
213     else:
214         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  $x[1], \dots, x[n]$ ):

```

216 [ASSUME (list f_compute f_emu) (gpmem f_restr) ]
217 for i=1 to n:
218   [PREDICT (f_compute x[i])]
219   [INFER (MH {hyper-parameters} one 100) ]
220   [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.

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### 231   **3.1.2 The efficacy of learning hyperparameters**

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

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$$239 \quad P(\boldsymbol{\theta} | \mathbf{D}, \mathbf{K}) = \frac{P(\mathbf{D} | \boldsymbol{\theta}, \mathbf{K})P(\boldsymbol{\theta} | \mathbf{K})}{P(\mathbf{D} | \mathbf{K})}. \quad (11)$$

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

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$$252 \quad \ell^{(t)} \sim \Gamma(\alpha_1, \beta_1), \sigma^{(t)} \sim \Gamma(\alpha_2, \beta_2) \quad (12)$$

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

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$$262 \quad \alpha_1^{(t)} \sim \Gamma(\alpha_\alpha^1, \beta_\alpha^1), \alpha_2^{(t)} \sim \Gamma(\alpha_\alpha^2, \beta_\alpha^2), \dots \quad (13)$$

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269   <sup>1</sup>In (Neal, 1997) the sum of an SE plus a constant kernel is used. We stick to the WN kernel for illustrative  
purposes.

```

270 Assuming the covariance structure is an additive comprised of a smoothing and a white noise
271 kernel, one can represent this kind of model using gpmem with only a few lines of code:
272
1 [ASSUME alpha (mem (lambda (i) (gamma 1 3 )))] ∈ {hyper-parameters-Γ}
2 [ASSUME beta (mem (lambda (i) (gamma 1 3 )))] ∈ {hyper-parameters-Γ}
273
3
274
4 [ASSUME l (gamma (alpha 1) (beta 1))] ∈ {hyper-parameters}
5 [ASSUME sf (gamma (alpha 2) (beta 2))] ∈ {hyper-parameters}
6 [ASSUME sigma (uniform 0 5 )] ∈ {hyper-parameters}
275 % above: structured prior, Fig. 1a
276
7
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9  $k_1(x, x') := \theta^2 \exp\left(-\frac{(x-x')^2}{2\ell^2}\right)$ 
10  $k_2(x, x') := \sigma^2 \delta_{x,x'}$ 
279
11
280
12 [ASSUME k1 VentureFunction(k1, θ, ℓ) ]
281 [ASSUME k2 VentureFunction(k2, σ) ]
282
283
13
284 [ASSUME SE make-se (apply-function k1 l sf) ]
285 [ASSUME WN make-se (apply-function k1 sigma) ]
286
287
14
288 [ASSUME (list f_compute f_emu) (gpmem f_restr (function-plus SE WN) )]
289 [SAMPLE (f_emu (array 1 2 3))] % prior, Fig. 1b
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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>2</sup>.

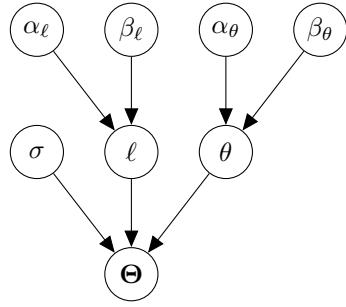
### 3.1.3 Broader applicability of gpmem

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.

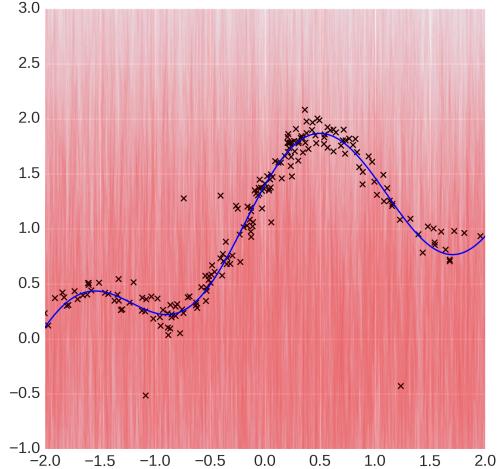
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<sup>2</sup>For this pedagogical example we have increased the probability for outliers in the data generation slightly from 0.05 to 0.2

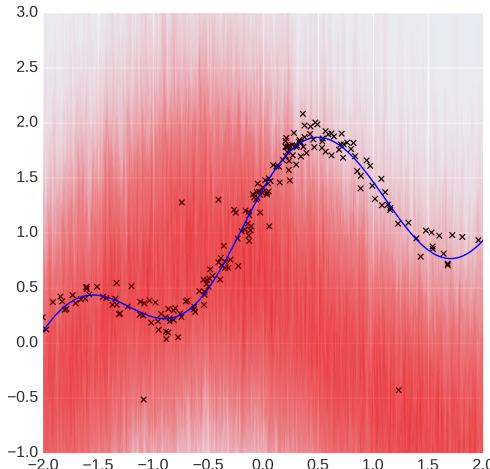
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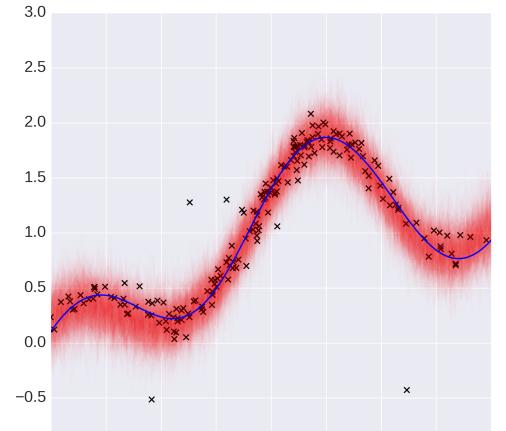
(a) Hierarchical Prior



(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 a Venture GP 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.

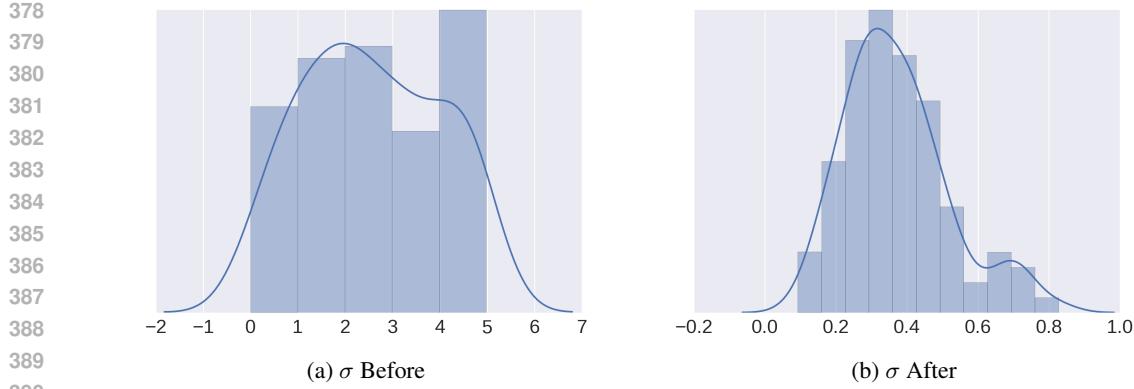


Figure 2: Hyper-parameter inference on the parameter of the noise kernel. We show 100 samples drawn from the distribution on  $\sigma$ . One can clearly recognise the shift from the uniform prior  $\mathcal{U}(0, 5)$  to a double peak distribution around the two modes - normal and outlier.

Furthermore, the example in Section 3.2 below recovers the performance of current state-of-the-art GP-based models.

### 3.2 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 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 kernel results in high values only if  $k_1$  AND  $k_2$  have high values (see Fig. 3 for examples 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. Note that this form of composition can be easily expressed in Venture, for example if one wishes to add a linear and a periodic kernel:

```

1 [ASSUME l (gamma 1 3)]
2 [ASSUME sf (gamma 1 2)]
3 [ASSUME a (gamma 2 2)]
4
5  $k_{LIN}(x, x') := \sigma_1^2(x - \ell)(x' - \ell)$ 
6  $k_{PER}(x, x') := \sigma_2^2 \exp(-\frac{2\sin^2(\pi(x-x')/p)}{\ell^2})$ 
7
8 [ASSUME fLIN VentureFunction(kLIN, σ1) ]
9 [ASSUME fPER VentureFunction(kPER, σ2, ℓ, p) ]
10 [ASSUME LIN (make-LIN (apply-function fLIN a)) ]
11 [ASSUME PER (make-PER (apply-function fPER 1 sf)) ]
12 [ASSUME (make-gp 0 (function-times LIN PER)) ]

```

Listing 3: LIN  $\times$  PER

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:

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

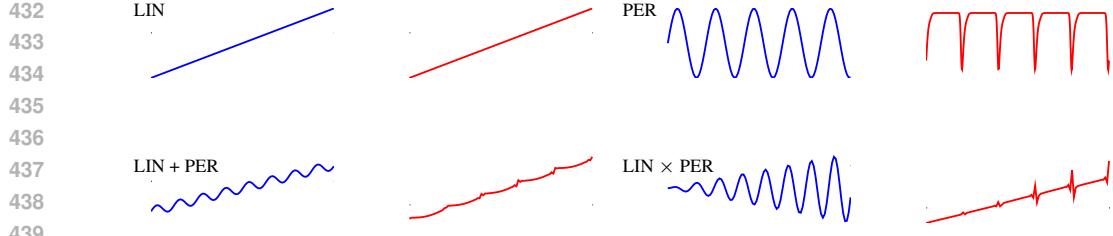


Figure 3: Composition of covariance functions (blue, left) and samples from the distribution of curves they can produce (red, right).

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

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

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

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

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

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

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

with

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

and

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

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

Many equivalent covariance structures can be sampled due to covariance function algebra and equivalent representations with different parameterization (Lloyd et al., 2014). Certain covariance functions can differ in terms of the hyper-parameterization but can be absorbed into a single covariance function with a different parameterization. To inspect the posterior of these equivalent structures we convert each kernel expression into a sum of products and subsequently simplify expressions using the following grammar:

<sup>1</sup>	SE × SE	→ SE
<sup>2</sup>	{SE, PER, C, WN} × WN	→ WN
<sup>3</sup>	LIN + LIN	→ LIN
<sup>4</sup>	{SE, PER, C, WN, LIN} × C	→ {SE, PER, C, WN, LIN}

Listing 4: Grammar to simplify expressions

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

```

486 1 [ASSUME base_kernels (list K1,K2,...,Kn) ] % defined as above
487 2 [ASSUME pn (uniform_structure n)] % prior on the number of kernels
488 3 [ASSUME SK (subset base_kernels pn) ] % sampling a subset of size n
489 4 [ASSUME composition (lambda (l) % kernel composition
490 5           (if (lte (size l) 1)
491 6             (first l)
492 7               (if (flip)
493 8                 (func_plus (first l) (cov_compo (rest l)))
494 9                 (func_times (first l) (cov_compo (rest l)))
495 10            )
496 11         )
497 12     )
498 13
499 14 [ASSUME K (composition SK) ]
500 15
501 16 [ASSUME (list f_compute f_emu) (gpmem f_restr K )]
502 17
503 18 for i=1 to n:
504 19   [PREDICT (f_compute x[i])] % observing with a look-up function
505 20
506 21 [INFER (REPEAT 2000 (DO
507 22   (MH pn one 1)
508 23   (MH SK one 1)
509 24   (MH K* one 1)
510 25   (MH {hyper-parameters} one 10))]
```

Listing 5: 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. 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 () 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. 8).

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).

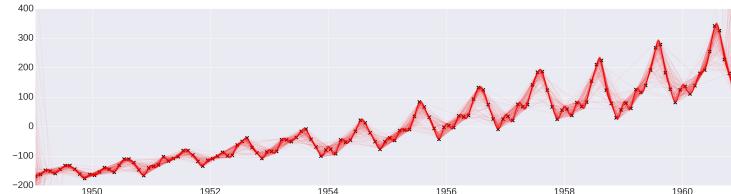
We found the final sample of multiple runs to be most informative. This kind of Markov Chain seems to produce samples that are highly auto-correlated.

## 4 Bayesian Optimization

Bayesian Optimization poses the problem of finding the global maximum of an unknown function as a hierarchical decision problem (Ghahramani, 2015). Evaluating the actual function can be very expensive. For example, finding the best configuration for the learning algorithm of a large convolutional neural network implies expensive function evaluations to compare a potentially infinite number of configurations. Another common example is the example of data acquisition. For problems with large amounts of data available it may be interesting to chose certain informative data-points to evaluate a model on. In continuous domains, many Bayesian Optimization methods deploy GPs (e.g. Snoek et al., 2012).

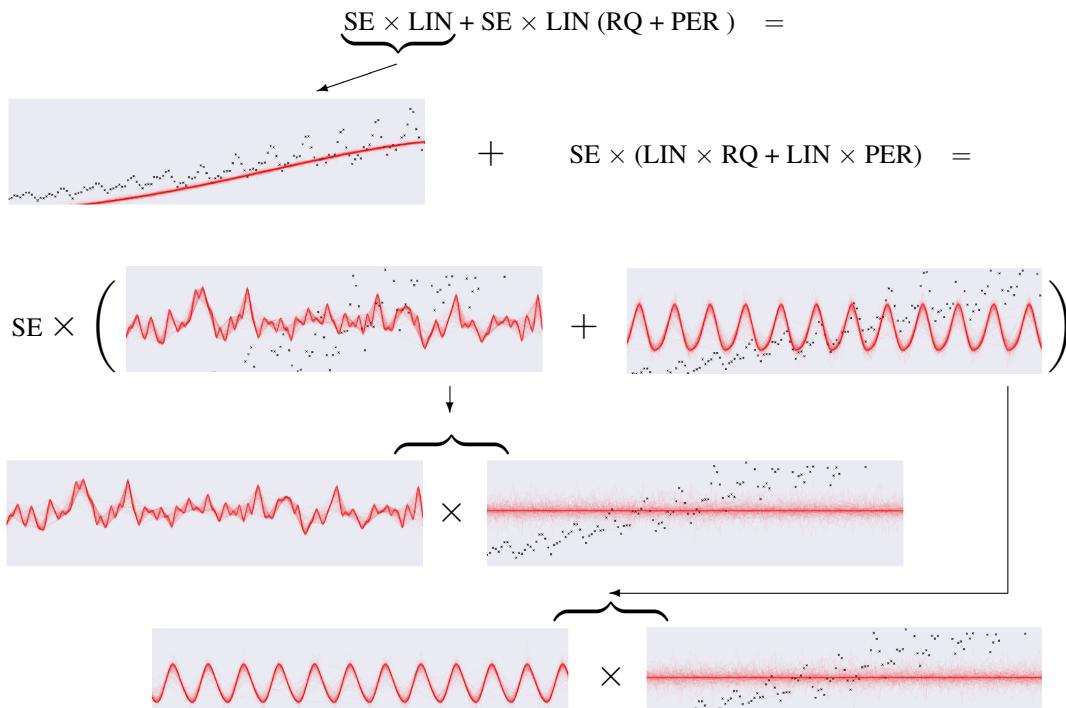
The hierarchical nature of Bayesian Optimization makes it an ideal application for GPs in Venture. The following Bayesian Optimization scheme is closely related to Thompson Sampling Thompson (1933), a general framework to solve exploration-exploitation problems. In our case, “exploration”

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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.

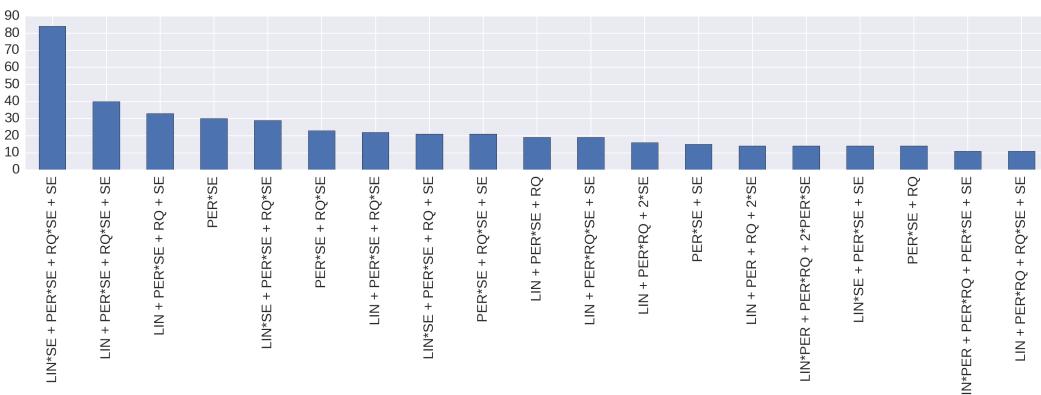


Figure 5: Posterior on structure of the CO<sub>2</sub> data. We have cut the tail of the distribution for space reasons since the number of possible structures is large. We see the final sample of the each of the 545 chains with 2000 nested steps each. Note that Duvenaud et al. (2013) report LIN × SE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

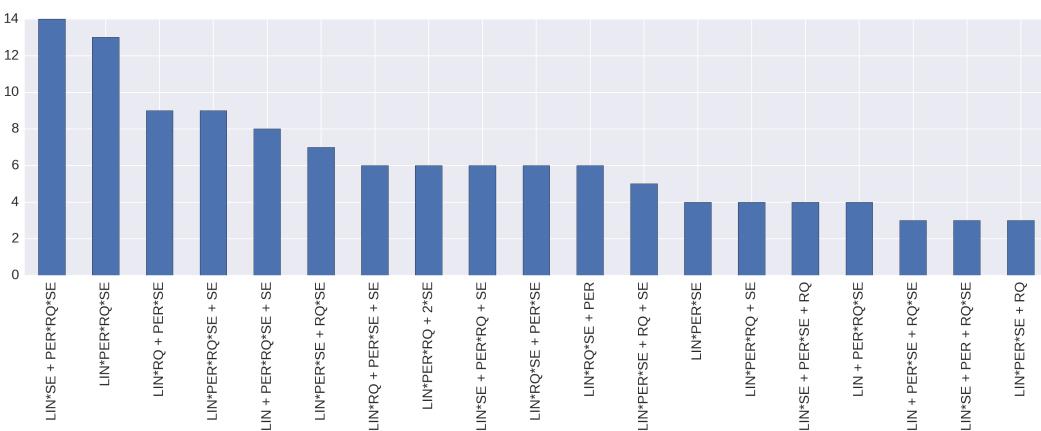


Figure 6: Posterior on structure of airline data set. We have cut the tail of the distribution for space reasons since the number of possible structures is large. We see the final sample of the each of the 144 chains with 2000 nested steps each. Note that Duvenaud et al. (2013) report LIN × SE + (PER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

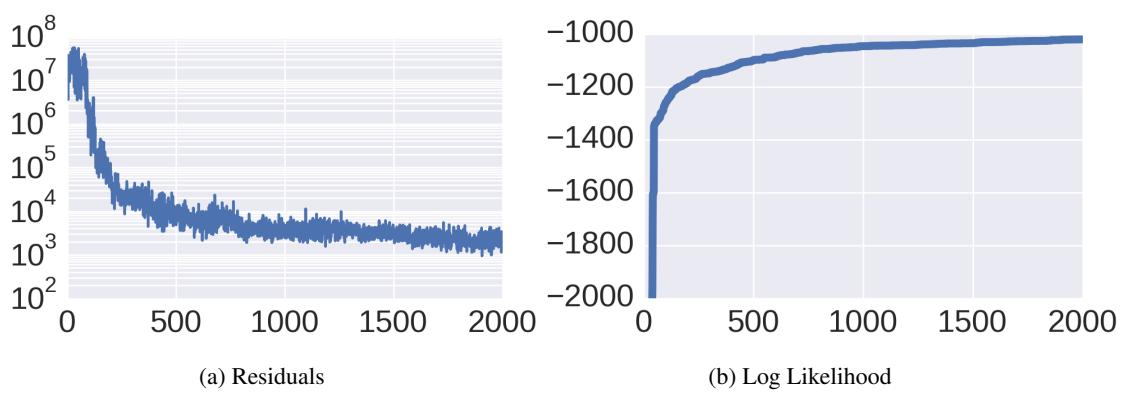
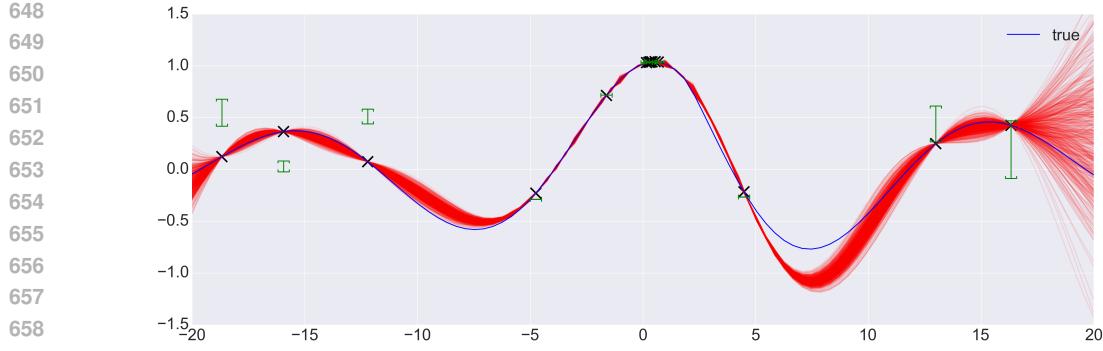


Figure 7: 2000 steps along the Markov Chain.



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660 Figure 8: Bayesian Optimization. Each successive probe point  $x$  is the (stochastic) maximum of a  
661 GP-based emulator conditioned on the values of the previously probed points. In the figure, each  
662 probe point  $x$  is marked with an  $\times$ , and a vertical green bar is drawn showing the mean  $\pm$  one  
663 standard deviation of the “leave-one-out” distribution—the distribution that would arise from the  
664 same covariance function if all marked points *except*  $x$  had been probed. Note that there are many  
665 probe points near the true maximum, and the uncertainty is quite low. Also note that probed points  
666 far away from the true maximum tend to be points at which the uncertainty is high.  
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669 is probing the true value of the function  $f$  by performing an expensive computation, and “exploitation-  
670” is using samples from a GP-based model (conditioned on the previously computed true values  
671 of  $f$ ) to approximate the values of  $f$  at new points; the cost of doing so will depend on the applica-  
672 tion. In the terminology of gpmem (see Section 3.1.1), the function  $f_{\text{restr}}$  is  $f$ , and the exploration-  
673 exploitation trade-off is: given a point  $x$ , should we evaluate  $f_{\text{restr}}$  directly, thus resulting in a more  
674 accurate value and more training data for the emulator  $f_{\text{emu}}$ , or should we just sample  $f_{\text{emu}}$  for a  
675 good-enough approximation? The answer will of course depend on the application, but also note  
676 that judicious choice of when to do each will result in more useful training data for the GP model.  
677

```
678 [ASSUME hypers ...]
679 [ASSUME se (make-squared-exponential hypers)]
680 [ASSUME (list f_compute f_emu) (gpmem f se)]
681 [ASSUME f_emu_pointwise (lambda (x) (first (f_emu (array x))))]
682 [ASSUME mc_sampler (uniform_sampler -20 20)]
683
684 for i=1 to 15:
685   [PREDICT (f_compute (mc_argmax f_emu_pointwise mc_sampler))]
686   [INFER (MH 'hypers one 50)
687 [INFER (collect_stats f_emu)]
```

688 Listing 6: Code for Bayesian optimization using gpmem. The procedure  $f_{\text{compute}}$  computes  
689  $f$  directly, thus improving the GP model  $f_{\text{emu}}$ . ( $f_{\text{emu}}_{\text{pointwise}}$  is simply a shortcut for  
690 sampling the GP model at a single point;  $f_{\text{emu}}$  is more general, allowing joint samples to be  
691 taken at any set of points.) In the loop,  $f_{\text{compute}}$  is called to compute the value of  $f$  at a new  
692 argument. The new argument,  $(\text{mc\_argmax } f_{\text{emu}}_{\text{pointwise}} \text{ mc\_sampler})$ , is a Monte  
693 Carlo estimate of the maximum pointwise sample of  $f_{\text{emu}}$  (itself a stochastic quantity), with  
694 the Monte Carlo samples being drawn in this case uniformly between  $-20$  and  $20$ . After each  
695 new call to  $f_{\text{compute}}$ , the Metropolis–Hastings algorithm is used to perform inference on the  
696 hyperparameters of the covariance function in the GP model in light of the new conditioning data.  
697 Once enough calls to  $f_{\text{compute}}$  have been made (in our case we stopped at 15 calls), we can  
698 inspect the full list of probed  $(x, y)$  pairs with  $\text{extract\_stats}$ . The answer to our maximization  
699 problem is simply the maximum  $y$ ; but our algorithm also learns more potentially useful information.  
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702     **5 Conclusion**  
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704     We have shown Venture GPs. We have introduced novel stochastic processes for a probabilistic  
705     programming language. We showed how flexible non-parametric models can be treated in Venture  
706     in only a few lines of code. We evaluated our contribution on a range of hard problems for state-of-  
707     the-art Bayesian non-parametrics. Venture GPs showed competitive performance in all of them.  
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