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

1 Introduction

Gaussian processes are widely used tools in statistics (Barry, 1986), machine learning (Neal, 1995; Williams and Barber, 1998; Kuss and Rasmussen, 2005; Rasmussen and Williams, 2006; Damianou and Lawrence, 2013), robotics (Ferris et al., 2006), computer vision (Kemmler et al., 2013), and scientific computation (Kennedy and O'Hagan, 2001; Schneider et al., 2008; Kwan et al., 2013). They are also central to probabilistic numerics, an emerging effort to develop more computationally efficient numerical procedures, and to Bayesian optimization, a family of meta-optimization techniques that are widely used to tune parameters for deep learning algorithms (Snoek et al., 2012; Gelbart et al., 2014). They have even seen use in artificial intelligence; for example, they provide the key technology behind a project that produces qualitative natural language descriptions of time series (Duvenaud et al., 2013; Lloyd et al., 2014).

This paper describes Gaussian process memoization, a technique for integrating Gaussian processes into a probabilistic programming language, and demonstrates its utility by re-implementing and extending state-of-the-art applications of the GP. Memoization, typically implemented by a procedure called `mem()`, is a classic higher-order programming technique in which a procedure is augmented with an input-output cache that is checked each time before the function is invoked. This prevents unnecessary recomputation, potentially saving time at the cost of increased storage requirements. Gaussian process memoization, implemented by the `gpmem()` procedure, generalizes this idea to include a statistical emulator that uses previously computed values as data in a statistical model that can cheaply forecast probable outputs. The covariance function for the Gaussian process is also allowed to be an arbitrary probabilistic program.

This paper presents three applications of gpmem: (i) a replication of (Neal, 1997) results on outlier rejection via hyper-parameter inference; (ii) a fully Bayesian extension to the Automated Statistician project; and (iii) an implementation of Bayesian optimization via Thompson sampling. The first application can in principle be replicated in several other probabilistic languages embedding the proposal that is described in this paper. The remaining two applications rely on distinctive capabilities of Venture: support for fully Bayesian structure learning and language constructs for inference programming. All applications share a single 50-line Python library and require fewer than 20 lines of probabilistic code each.

2 Gaussian Processes Memoization

Let the data be pairs of real-valued scalars $\{(x_i, y_i)\}_{i=1}^n$ (complete data will be denoted by column vectors $\mathbf{x}$, $\mathbf{y}$). Gaussian Process (GP)s present a non-parametric way to express prior knowledge on the space of possible functions f modeling a regression relationship. Formally, a GP is an infinite-dimensional extension of the multivariate Gaussian distribution. Often one assumes the values $\mathbf{y}$ are noisily measured, that is, one only sees the values of $\mathbf{y}_{\text{noisy}} = \mathbf{y} + \mathbf{w}$ where $\mathbf{w}$ is Gaussian white noise with variance σ^2_{noise}. In that case, the log-likelihood of a GP is

$$\log p\left(\mathbf{y}_{\text{noisy}} \mid \mathbf{x}\right) = -\frac{1}{2}\mathbf{y}^\top(\mathbf{\Sigma} + \sigma^2_{\text{noise}}\mathbf{I})^{-1}\mathbf{y} - \frac{1}{2}\log\left|\mathbf{\Sigma} + \sigma^2_{\text{noise}}\mathbf{I}\right| - \frac{n}{2}\log 2\pi \tag{1}$$

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

The covariance function (or kernel) of a GP governs high-level properties of the observed data such as linearity, periodicity and smoothness. It comes with few free parameters that we call hyper-parameters. Adjusting these results in minor changes, for example with regards to when two data points are treated similar. More drastically different covariance functions are achieved by changing the structure of the covariance function itself. Note that covariance function structures are compositional: adding or multiplying two valid covariance functions results in another valid covariance function.

Venture includes the primitive `make_gp`, which takes as arguments a unary function `mean` and a binary (symmetric, positive-semidefinite) function `cov` and produces a function `g` distributed as a Gaussian process with the supplied mean and covariance. For example, a function $\mathsf{g} \sim \mathcal{GP}(0, \text{SE})$, where SE is a squared-exponential covariance

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

with $\sigma = 1$ and $\ell = 1$, can be instantiated as follows:

```
assume zero = make_const_func( 0.0)
assume se = make_squaredexp( 1.0, 1.0)
assume g  = make_gp( zero, se)
```

There are two ways two view `g` as a "random function." In the first view, the `assume` directive that instantiates `g` does not use any randomness—only the subsequent calls to `g` do—and coherence constraints are upheld by the interpreter by keeping track of which evaluations of `g` exist in the current execution trace. Namely, if the current trace contains evaluations of `g` at the points $x_1, \ldots, x_N$ with return values $y_1, \ldots, y_N$, then the next evaluation of `g` (say, jointly at the points $x_{N+1}, \ldots, x_{N+n}$) will be distributed according to the joint conditional distribution

$$P\left(\texttt{(g}\ x_{N+1}\texttt{)}, \ldots, \texttt{(g}\ x_{N+n}\texttt{)} \;\middle|\; \texttt{(g}\ x_i\texttt{)} = y_i \text{ for } i = 1, \ldots, N\right).$$

In the second view, `g` is a randomly chosen deterministic function, chosen from the space of all deterministic real-valued functions; in this view, the `assume` directive contains *all* the randomness, and subsequent invocations of `g` are deterministic. The first view is procedural and is faithful to the computation that occurs behind the scenes in Venture. The second view is declarative and is faithful to notations like "$g \sim P(g)$" which are often used in mathematical treatments. Because a model program could make arbitrarily many calls to `g`, and the joint distribution on the return values of the calls could have arbitrarily high entropy, it is not computationally possible in finite time to choose the entire function g all at once as in the second view. Thus, it stands to reason that any computationally implementable notion of "nonparametric random functions" must involve incremental random choices in one way or another, and Gaussian processes in Venture are no exception.

2.1 Memoization

Memoization is the practice of storing previously computed values of a function so that future calls with the same inputs can be evaluated by lookup rather than recomputation. Although memoization does not change the semantics of a deterministic program, it does change that of a stochastic program (Goodman et al., 2008). The authors provide an intuitive example: let f be a function that flips a coin and return "head" or "tails". The probability that two calls of f are equivalent is 0.5. However, if the function call is memoized, it is 1. In fact, there is an infinite range of possible caching policies (specifications of when to use a stored value and when to recompute), each potentially having a different semantics. Any particular caching policy can be understood by random world semantics (Poole, 1993; Sato, 1995) over the stochastic program: each possible world corresponds to a mapping from function input sequence to function output sequence (McAllester et al., 2008). In Venture, these possible worlds are first-class objects, and correspond to the *probabilistic execution traces traces* (Mansinghka et al., 2014).

To transfer this idea to probabilistic programming, we now introduce a language construct called a *statistical memoizer*. Suppose we have a function f which can be evaluated but we wish to learn about the behavior of f using as few evaluations as possible. The statistical memoizer, which here we give the name gpmem, was motivated by this purpose. It produces two outputs:

$$\mathtt{f} \xrightarrow{\text{gpmem}} (\mathtt{f}_{\text{probe}}, \mathtt{f}_{\text{emu}}).$$

The function $\mathtt{f}_{\text{probe}}$ calls f and stores the output in a memo table, just as traditional memoization does. The function $\mathtt{f}_{\text{emu}}$ is an online statistical emulator which uses the memo table as its training data. A fully Bayesian emulator, modelling the true function f as a random function $f \sim P(f)$, would satisfy

$$(\mathtt{f}_{\text{emu}}\ \mathtt{x}_1\ \ldots\ \mathtt{x}_k) \sim P\left(f(\mathtt{x}_1), \ldots, f(\mathtt{x}_k) \mid f(\mathtt{x}) = (\mathtt{f}\ \ \mathtt{x}) \text{ for each } \mathtt{x} \text{ in memo table}\right).$$

Different implementations of the statistical memoizer can have different prior distributions $P(f)$; in this paper, we deploy a Gaussian process prior (implemented as gpmem below). Note that we require the ability to sample $\mathtt{f}_{\text{emu}}$ jointly at multiple inputs because the values of $f(\mathtt{x}_1), \ldots, f(\mathtt{x}_k)$ will in general be dependent. To illustrate the linguistic power of gpmem consider a simple model program that uses gpmem procedure abstraction, and a loop:

```
define choose_next_point = proc(em) { gridsearch_argmax( em) }

 // Here stats( em) is the memo table {(x_i, y_i)}.
 // Take the (x,y) pair with the largest y.
define extract_answer = proc(em) { first(max( stats( em, second)))}

 // Hyper-parameter
assume theta =  tag( quote( params), 0, gamma(1,1))
assume (f_probe f_emu) =  gpmem(f, make_squaredexp(1.0, theta))

for t...T:
  f_probe( choose_next_point( f_emu))
extract_answer( f_emu)
```

An equivalent model in typical statistics notation, written in a way that attempts to be as linguistically faithful as possible, is

$$\begin{aligned}
f^{(0)} &\sim P(f) \\
\mathtt{x}^{(t)} &= \arg\max_x f^{(t)}(x) \\
f^{(t+1)} &\sim P\left(f^{(t)} \;\middle|\; f^{(t)}(\mathtt{x}^{(t)}) = (\mathtt{f}\ \mathtt{x}^{(t)})\right).
\end{aligned}$$

The linguistic constructs for abstraction are not present in statistics notation. The equation $\mathsf{x}^{(t)} = \arg\max_x f^{(t)}(x)$ has to be inlined in statistics notation: while something like

$$\mathsf{x}^{(t)} \sim F(P^{(t)})$$

(where $P^{(t)}$ is a probability measure, and F here plays the role of `choose_next_point`) is mathematically coherent, it is not what statisticians would ordinarily write. This lack of abstraction then makes modularity, or the easy digestion of large but finely decomposable models, more difficult in statistics notation.

Adding a single line to the program, such as

```
infer mh( quote( params), one, 50)
```

after line 12 to infer the parameters of the emulator, would require a significant refactoring and elaboration of the statistics notation. One basic reason is that probabilistic programs are written procedurally, whereas statistical notation is declarative; reasoning declaratively about the dynamics of a fundamentally procedural inference algorithm is often unwieldy due to the absence of programming constructs such as loops and mutable state.

We implement `gpmem` by memoizing a target procedure in a wrapper that remembers previously computed values. This comes with interesting implications: 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_{restr} is restricted to only allow evaluation at a specific set of inputs x (Alg. 1). Modelling the data set with a GP then

Algorithm 1 Restricted Function

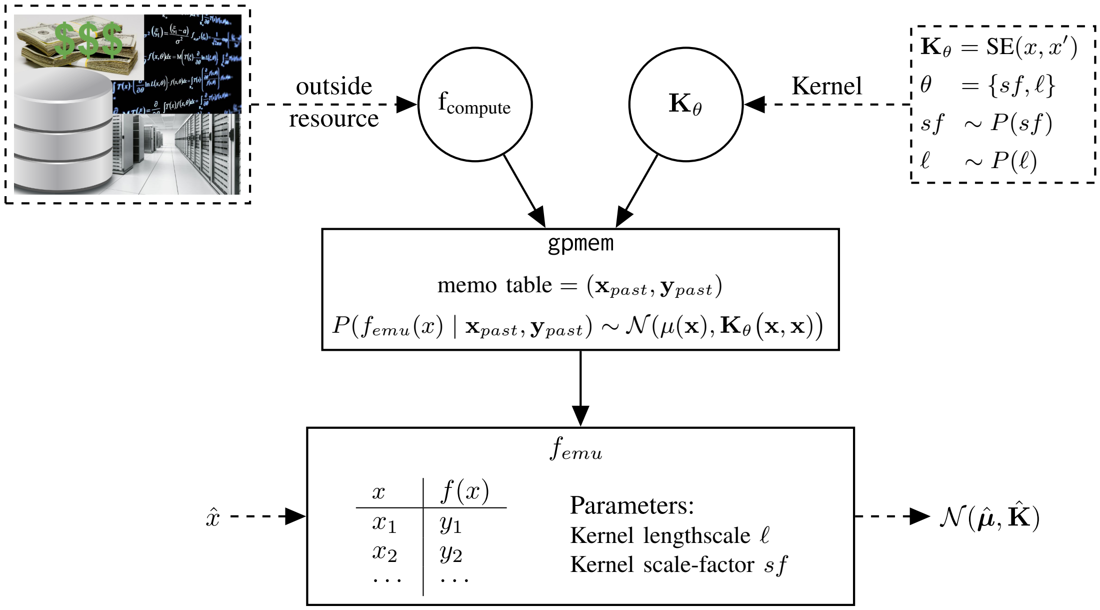
function $f_{\text{RESTR}}(x)$
  if $x \in \mathcal{D}$ **then**
    return $\mathcal{D}[x]$
  else
    raise Exception('Illegal input')
  end if
end function

amounts to trying to learn a smooth function f_{emu} ("emu" stands for "emulator") which extends f to its full domain. Indeed, if f_{restr} is a foreign procedure made available as a black-box to Venture, whose secret underlying pseudo code is in Alg. 1, then the `observe` code can be rewritten using `gpmem` as in Listing 1 (where here the data set `D` has keys `x[1]`,...,`x[n]`):

Listing 1: Observation with `gpmem`

```
assume (f_compute f_emu) =  gpmem( f_restr)
for i=1 to n:
  predict f_compute( x[i])
  infer mh(quote(hyper-parameters), one, 100)
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.




```
define f = proc( x) {
    exp(-0.1*abs(x-2))) *
    10* cos(0.4*x) + 0.2
}
assume (f_compute f_emu) =  gpmem( f, Kθ)
sample f_emu( array( -20, ···, 20))
```

```
predict f_compute( 12.6)

sample f_emu( array( -20, ···, 20))
```

```
predict f_compute( -6.4)

sample f_emu( array( -20, ···, 20))
```

```
observe f_emu( -3.1) = 2.60
observe f_emu( 7.8) = -7.60
observe f_emu( 0.0) =  10.19

sample f_emu( array( -20, ···, 20))
```

```
infer mh(quote(hyper-parameter), one, 50)

sample f_emu( array( -20, ···, 20))
```

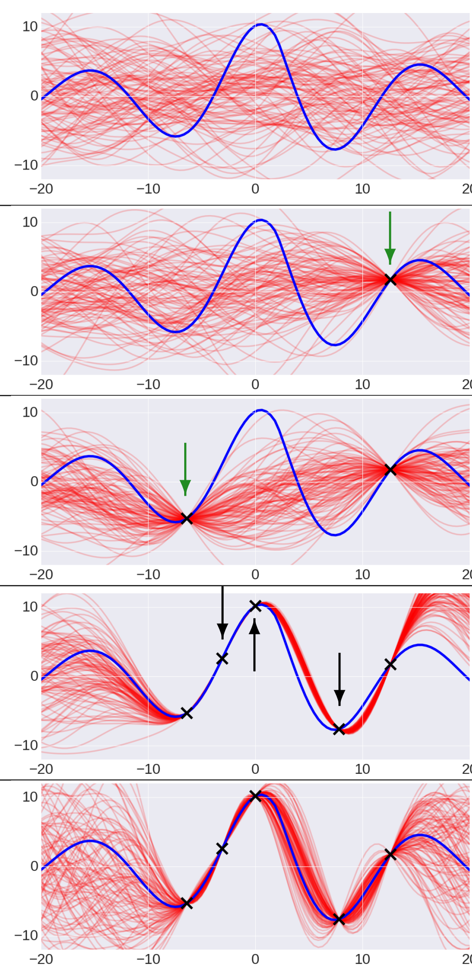
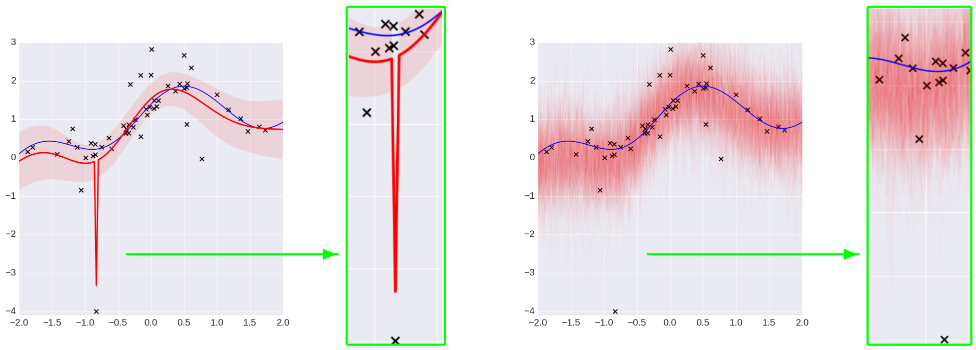


Figure 1: gpmem tutorial. The top shows a schematic of gpmem. $f_{com} =$ f_compute probes an outside resource. This can be expensive (top left). Every probe is memoized and improves the GP-based emulator. Below the schematic we see a movie of the evolution of gpmem's state of believe of the world given certain Venture directives.



(a) (b)

Figure 2: (a) a shows deterministic inferece, that is optimization for an example of Neals synthetic function with an extreme outlier (green).

3 Example Applications

gpmem is an elegant linguistic framework for function learning-related tasks. The technique allows language constructs from programming to help express models which would be cumbersome to express in statistics notation. We will now illustrate this with three example applications.

3.1 Hyperparameter estimation with structured hyper-prior

The probability of the hyper-parameters of a GP as defined above and given covariance function structure $\mathbf{K}$ is:

$$P(\boldsymbol{\theta} \mid \mathbf{D}, \mathbf{K}) = \frac{P(\mathbf{D} \mid \boldsymbol{\theta}, \mathbf{K}) P(\boldsymbol{\theta} \mid \mathbf{K})}{P(\mathbf{D} \mid \mathbf{K})}. \tag{2}$$

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

$$\ell^{(t)} \sim \Gamma(\alpha_1, \beta_1), \ \sigma^{(t)} \sim \Gamma(\alpha_2, \beta_2) \tag{3}$$

and in turn sample the α and β from Γ distributions as well:

$$\alpha_1^{(t)} \sim \Gamma(\alpha_\alpha^1, \beta_\alpha^1), \ \alpha_2^{(t)} \sim \Gamma(\alpha_\alpha^2, \beta_\alpha^2), \cdots \tag{4}$$

One can represent this kind of model using gpmem (Fig. 3). 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:

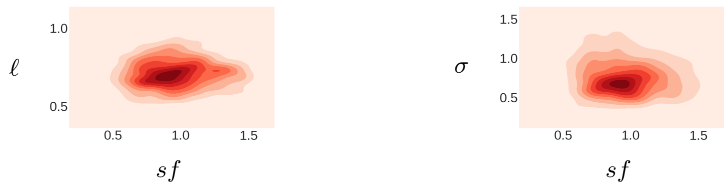
$$f(x) = 0.3 + 0.4x + 0.5\sin(2.7x) + \frac{1.1}{(1+x^2)} + \eta \quad with \ \ \eta \sim \mathcal{N}(0, \sigma) \tag{5}$$

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. 2). Note that Neal devises an additional noise model and performs a large number of Hybrid-Monte Carlo and Gibbs steps.

We illustrate the hyper-parameters by showing a comparison between σ (Fig. 2). We see that gpmem learns the posterior distribution well, the posterior even exhibits a bimodal histogram when sampling σ 100 times reflecting the two modes of data generation, that is normal noise and outliers.

[1] In (Neal, 1997) the sum of an SE plus a constant kernel is used. We keep the WN kernel for illustrative purposes.

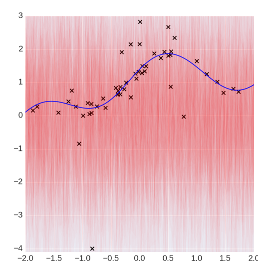
Hyper-Parameters for the Kernel:



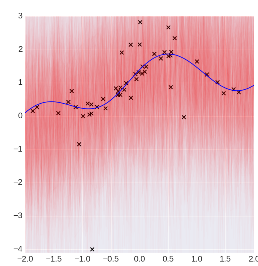

```
// Data and look-up function
define data = array(array(-1.87,0.13),..., array(1.67,0.81))
assume f_look_up = proc(index) {lookup( data, index)}
```

```
assume sf = tag(quote(hyper), 0, gamma(alpha_sf, beta_sf)))
assume l = tag(quote(hyper), 1, gamma(alpha_l, beta_l)))
assume sigma = tag(quote(hyper), 2, uniform_continuous(0, 2))
```

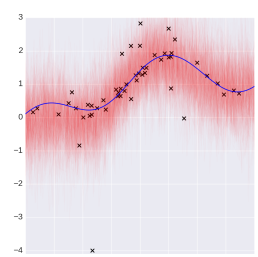
```
// The covariance function
assume se = make_squaredexp(sf, l)
assume wn = make_whitenoise(sigma)
assume composite_covariance = add_funcs(se, wn)

// Create a prober and emulator using gpmem
assume (f_compute, f_emu)
      = gpmem(f_look_up, composite_covariance)

sample f_emu( array( -2, ···, 2))
```



```
// Observe all data points
for n ... N
    observe f_emu(first(lookup(data,n)))
                = second(lookup(data,n))
// Or: probe all data points
for n ... N
    predict f_compute(first(lookup(data,n)))

sample f_emu( array( -2, ···, 2))
```



```
// Metropolis-Hastings
infer repeat( 100, do(
                   mh( quote(hyperhyper), one, 2),
                   mh( quote(hyper),      one, 1)))

sample f_emu( array( -2, ···, 2))
```



```
// Optimization

infer map( quote(hyper), all,0.01, 15)

sample f_emu( array( -2, ···, 2))
```

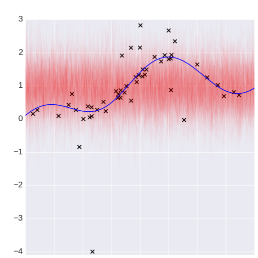


Figure 3: Hyper-parameterization

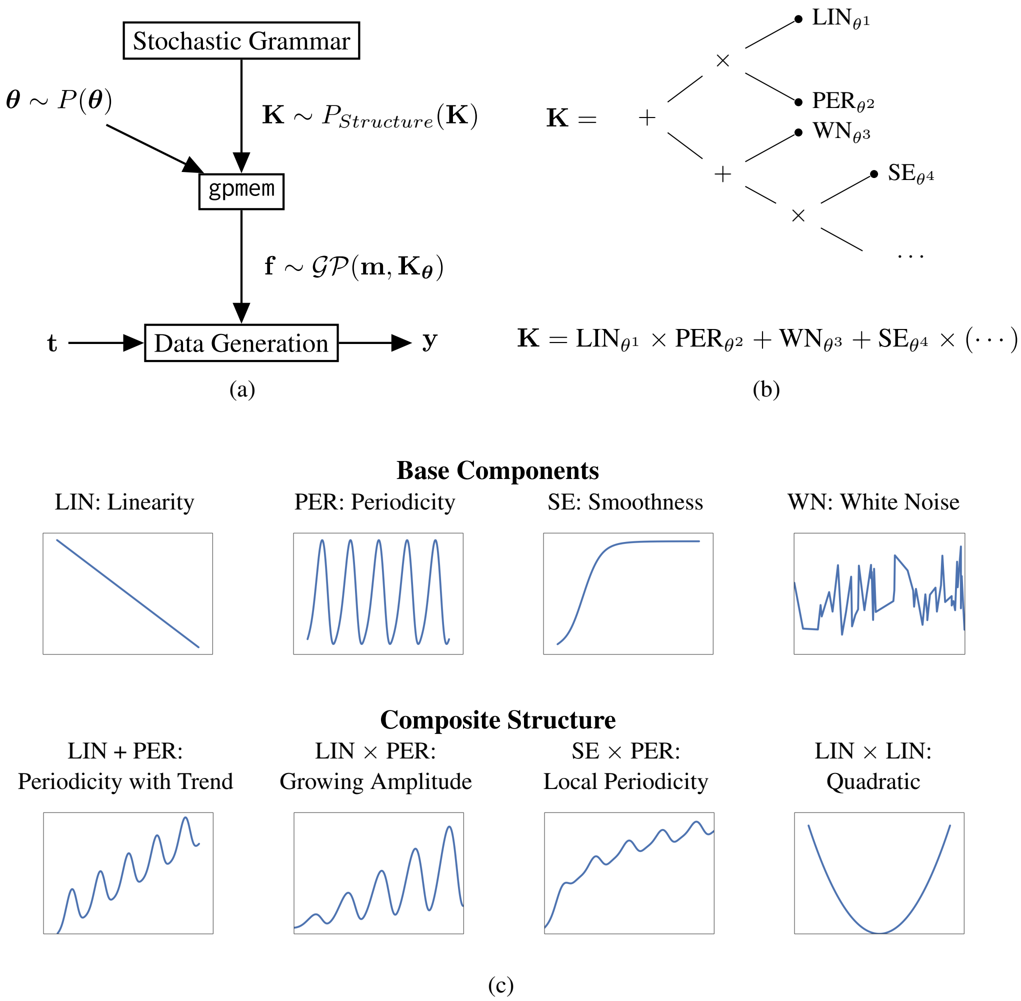


Figure 4: (a) Graphical description of Bayesian GP structure learning. (b) Composite structure. (c) The natural language interpretation of the structure.

3.2 Discovering symbolic models for time series

Inductive learning of symbolic expression for continuous-valued time series data is a hard task which has recently been tackled using a greedy search over the approximate posterior of the possible kernel compostions for GPs (Duvenaud et al., 2013; Lloyd et al., 2014)[2].

With `gpmem` we can provide a fully Bayesian treatment of this, previously unavaible, using a stochastic grammar (see Fig. 4).

We deploy a probabilistic context free grammar for our prior on structures. An input of non-composite kernels (base kernels) is supplied to generate a posterior distributions of composite structure to express local and global aspects of the data.

We approximate the following intractable integrals of the expectation for the prediction:

$$\mathbb{E}[y^* \mid x^*, \mathbf{D}, \mathbf{K}] = \iint f(x^*, \boldsymbol{\theta}, \mathbf{K})\, P(\boldsymbol{\theta} \mid \mathbf{D}, \mathbf{K})\, P(\mathbf{K} | \boldsymbol{\Omega}, s, n)\; \mathbf{d}\boldsymbol{\theta}\mathbf{d}\mathbf{K}. \tag{6}$$

[2]`http://www.automaticstatistician.com/`

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

$$y^* \approx \frac{1}{T} \sum_{t=1}^{T} f(x^* | \boldsymbol{\theta}^{(t)}, \mathbf{K}^{(t)}). \tag{7}$$

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

$$\mathbf{K}^{(t)} \sim P(\mathbf{K} \mid \boldsymbol{\Omega}, s, n) \tag{8}$$

Here, we start with the set of given base kernels and draw a random subset. For this subset of size n, we sample a set of possible operators $\boldsymbol{\Omega}$ combining base kernels. The marginal probability of a composite structure

$$P(\mathbf{K} \mid \boldsymbol{\Omega}, s, n) = P(\boldsymbol{\Omega} \mid s, n) \times P(s \mid n) \times P(n), \tag{9}$$

is characterized by the prior $P(n)$ on the number of base kernels used, the probability of a uniformly chosen subset of the set of n possible covariance functions

$$P(s \mid n) = \frac{n!}{\mid s \mid !}, \tag{10}$$

and the probability of sampling a global or a local structure, which is given by a binomial distribution:

$$P(\boldsymbol{\Omega} \mid s, n) = \binom{n}{r} p_{+\times}^{k} (1 - p_{+\times})^{n-k}. \tag{11}$$

Many equivalent covariance structures can be sampled due to covariance function algebra and equivalent representations with different parameterization (Lloyd et al., 2014). To inspect the posterior of these equivalent structures we convert each kernel expression into a sum of products and subsequently simplify. All base kernels can be found in Appendix A, rules for this simplification can be found in appendix B. The code for learning of kernel structure is as follows:

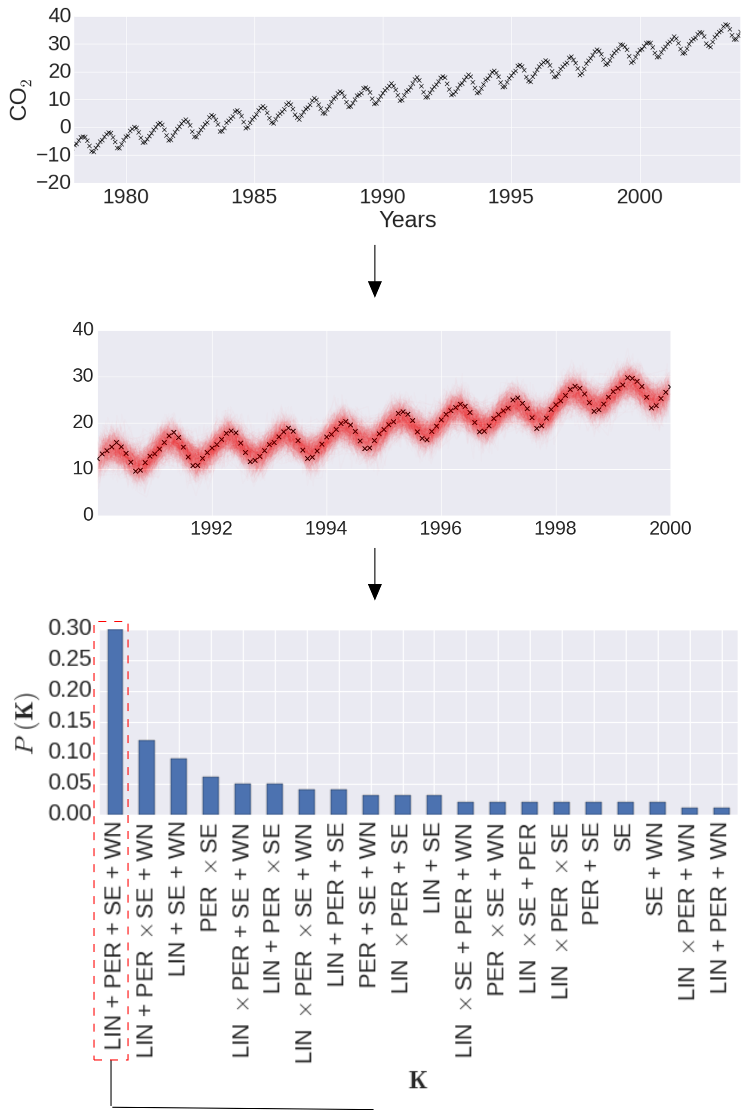
```
// GRAMMAR FOR KERNEL STRUCTURE
assume kernels = list(se, wn, lin, per, rq) // defined as above

// prior on the number of kernels
assume p_number_k = uniform_structure(n)
assume sub_s = tag(quote(grammar), 0,
                               subset(kernels, p_number_k))

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

assume K = tag(quote(grammar), 1, grammar(sub_s))

assume (f_compute f_emu) = gpmem(f_restr, K)

// Probe all data points
for n ... N
    predict f_compute(get_data_xs(n))

// PERFORMING INFERENCE
infer  repeat(2000, do(
                        mh(quote(grammar), one, 1),
                        for kernel ∈ K
                            mh(quote(hyper_kernel), one, 1)))
```

We defined the space of covariance structures in a way that allows us to produce results coherent with work presented in Automatic Statistician. For example, for the airline data set describing monthly totals of international airline passengers (Box et al., 1997, according to Duvenaud et al., 2013). Our most frequent 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_2 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 see that the most probable alternatives for a structural description both recover the data dynamics (Fig. 12 for the airline data set).

Confident about our results, we can now query the data for certain structures being present. We illustrate this using the Mauna Loa data used in previous work on automated kernel discovery (Duvenaud et al., 2013). We assume a relatively simple hypothesis space consisting of only four kernels, a linear, a smoothing, a periodic and a white noise kernel. In this experiment, we resort to the white noise kernel instead RQ (similar to (Lloyd et al., 2014)). We can now run the algorithm, compute a posterior of structures (see Fig. 5). We can also query this posterior distribution for the marginal of certain simple structures to occur. We demonstrate this in Fig. 6

3.3 Bayesian optimization via Thompson sampling

In this section we present a probabilistic meta-program for Bayesian optimization, along with optimization routines implemented as concrete applications of the meta-program. Figure 7 shows a probabilistic meta-program for Bayesian optimization. We use the term "meta-program" because this program defines a generic rule for combining abstract components to perform optimization. The components are themselves subprograms, whose implementations may vary. A traditional example of generic programming is the tree search meta-program of Norvig Norvig (1992), written in LISP, which we present alongside the optimization meta-program for comparison.



$$\boxed{\mathbf{K} = \text{LIN} + \text{PER} + \text{SE} + \text{WN}}$$

$$= 2.7^2(xx') + 5.6^2 \exp\left(\frac{2\sin^2(\pi(x-x')/3.7}{6.4^2}\right) + 0.4^2 \exp(-\frac{(x-x')^2}{2\times 6.3^2}) + 1.9^2\delta_{x,x'}$$

Qualitative Interpretation: The the posterior peaks at a kernel structure with four additive components. Additive components hold globally, that is there are no higher level, qualitative aspects of the data that vary with the input space. The additive components are as follows: (i) a linearly increasing function or trend; (ii) a periodic function; (iii) a smooth function; and (iv) white noise.

Figure 5: Posterior of structure and qualitative, human interpretable reading. We take the raw data (top), compute a posterior distribution on structures (bar plot). We take the peak of this distribution (LIN + PER + SE + WN) and show its human readable interpretation (left of bar plot). Below the bar plot show one sample of this structure with corresponding parameters. On the bottom, we sample from a GP with with this kernel-hyper-parameter combination.

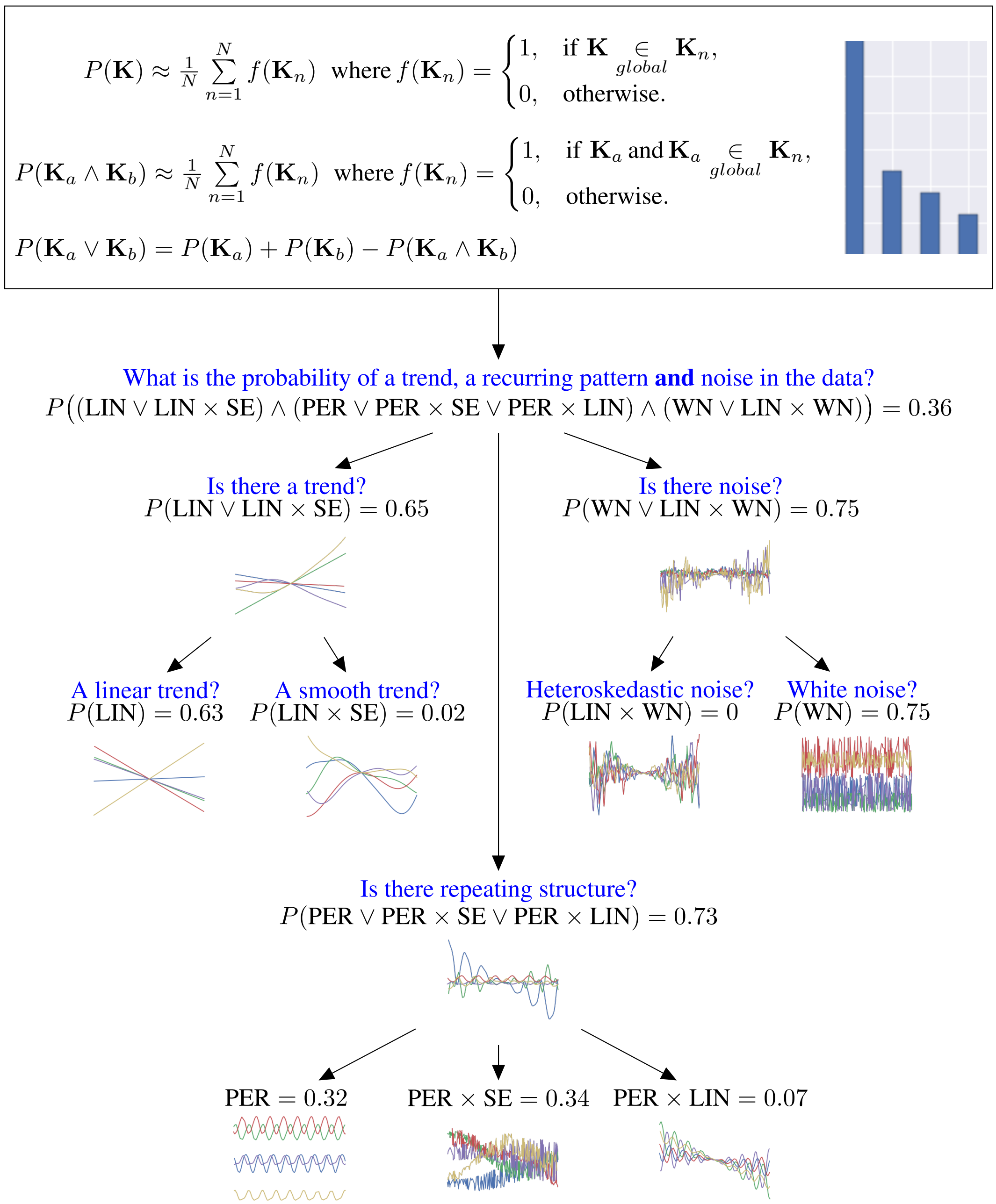


Figure 6: We can query the data if some logical statements are probable to be true, for example, is it true that there is a trend?

```lisp
(defun tree-search (states goal-p successors combiner)
  "Find a state that satisfies goal-p.  Start with states,
  and search according to successors and combiner."
  (cond ((null states) fail)
        ((funcall goal-p (first states)) (first states))
        (t (tree-search
             (funcall combiner
                      (funcall successors (first states))
                      (rest states))
             goal-p successors combiner))))
```

```scheme
(define optimize
  (lambda (probe do_search search_state_box
           post_probe_inference extract_answer finished?)
    (let loop ()
      (if (finished?)
        (extract_answer)
        (begin
          (do_search)
          (if (contents_changed? search_state_box)
            (predict (probe ,(contents search_state_box))))
          (post_probe_inference)
          (loop))))))
```

Figure 7: Top: Norvig's LISP meta-program for tree search. Bottom: A probabilistic meta-program for Bayesian optimization, written in VentureScheme, an abstract, Scheme-like syntax that can be used for Venture.

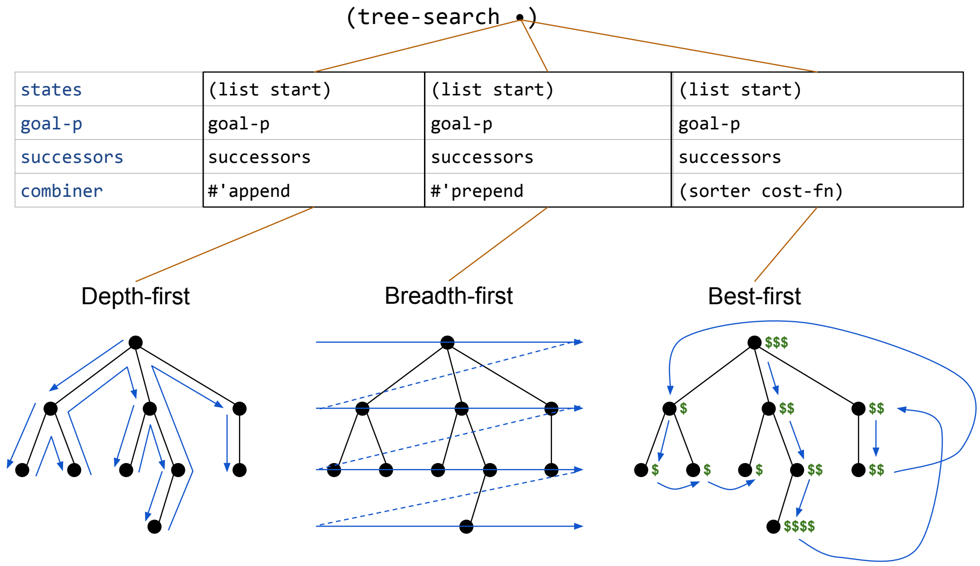


Figure 8: Invocations of Norvig's tree search meta-procedure with different arguments to perform a variety of different tree searches.

Figure 8 shows the flexibility of Norvig's meta-program. The procedure `tree-search` can be turned into a concrete implementation of depth-first, breadth-first or best-first search (among others) by simply supplying the appropriate combiner and set of initial states. Similarly, the meta-procedure `optimize` can make use of a variety of statistical emulators (e.g., GP-based emulators or polynomial regressions), a variety of acquisition heuristics (e.g., randomized grid search or Gaussian drift) and even a variety of rules for choosing an optimum based on the final state of the program (e.g., return the best probe so far, or return the analytically determined optimum of the emulator).

The specifications for the arguments to the meta-procedure `optimize` in Figures 7 are as follows:

- **`probe`:** A procedure for querying the true function `f` (and storing its value in the appropriate table, if caching is desired).
- **`do_search`:** A procedure to search for a new probe point and, if one is found, store it in `search_state_box`.
- **`search_state_box`:** A container for the next value to be probed. In each iteration of the loop, if the contents of `search_state_box` have changed, a new probe is performed.
- **`post_probe_inference`:** Any inference instructions which should be run after each probe, such as inferring hyperparameters.
- **`extract_answer`:** A procedure to produce an approximate optimum, based on the probes and inference that have been done so far.
- **`finished?`:** A procedure to decide whether optimization should be truncated here or should continue.

The meta-program is quite simple: Until `finished?` decides that optimization is finished, we choose new probe points and call `probe` on them. After each probe, we perform post-probe inference. Once optimization is finished, we call `extract_answer` to obtain an approximate optimum.

Thompson Sampling

We introduce Thompson sampling, the basic solution strategy underlying the Bayesian optimization with `gpmem`. Thompson sampling Thompson (1933) is a widely used Bayesian framework for addressing the trade-off between exploration and exploitation in multi-armed (or continuum-armed) bandit problems. We cast the multi-armed bandit problem as a one-state Markov decision process, and describe how Thompson sampling can be used to choose actions for that Markov Decision Processes (MDP).

Here, an agent is to take a sequence of actions $a_1, a_2, \ldots$ from a (possibly infinite) set of possible actions $\mathcal{A}$. After each action, a reward $r \in \mathbb{R}$ is received, according to an unknown conditional distribution $P_{\text{true}}(r \mid a)$. The agent's goal is to maximize the total reward received for all actions in an online manner. In Thompson sampling, the agent accomplishes this by placing a prior distribution $P(\vartheta)$ on the possible "contexts" $\vartheta \in \Theta$. Here a context is a believed model of the conditional distributions $\{P(r \mid a)\}_{a \in \mathcal{A}}$, or at least, a believed statistic of these conditional distributions which is sufficient for deciding an action a. If actions are chosen so as to maximize expected reward, then one such sufficient statistic is the believed conditional mean $V(a \mid \vartheta) = \mathbb{E}[r \mid a; \vartheta]$, which can be viewed as a believed value function. For consistency with what follows, we will assume our context ϑ takes the form $(\theta, \mathbf{a}_{\text{past}}, \mathbf{r}_{\text{past}})$ where $\mathbf{a}_{\text{past}}$ is the vector of past actions, $\mathbf{r}_{\text{past}}$ is the vector of their rewards, and θ (the "semicontext") contains any other information that is included in the context.

In this setup, Thompson sampling has the following steps:

Algorithm 2 Thompson sampling.

Repeat as long as desired:

1. **Sample.** Sample a semicontext $\theta \sim P(\theta)$.
2. **Search (and act).** Choose an action $a \in \mathcal{A}$ which (approximately) maximizes $V(a \mid \vartheta) = \mathbb{E}[r \mid a; \vartheta] = \mathbb{E}[r \mid a;\, \theta, \mathbf{a}_{\text{past}}, \mathbf{r}_{\text{past}}]$.
3. **Update.** Let r_{true} be the reward received for action a. Update the believed distribution on θ, i.e., $P(\theta) \leftarrow P_{\text{new}}(\theta)$ where $P_{\text{new}}(\theta) = P(\theta \mid a \mapsto r_{\text{true}})$.

Note that when $\mathbb{E}[r|a; \vartheta]$ (under the sampled value of θ for some points a) is far from the true value $\mathbb{E}_{P_{\text{true}}}[r \mid a]$, the chosen action a may be far from optimal, but the information gained by probing action a will improve the belief ϑ. This amounts to "exploration." When $\mathbb{E}[r \mid a; \vartheta]$ is close to the true value except at points a for which $\mathbb{E}[r \mid a; \vartheta]$ is low, exploration will be less likely to occur, but the chosen actions a will tend to receive high rewards. This amounts to "exploitation." The trade-off between exploration and exploitation is illustrated in Figure 9. Roughly speaking, exploration will happen until the context ϑ is reasonably sure that the unexplored actions are probably not optimal, at which time the Thompson sampler will exploit by choosing actions in regions it knows to have high value.

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

A Mathematical Specification

Our mathematical specification assert the following properties:

- The regression function has a Gaussian process prior.
- The actions $a_1, a_2, \ldots \in \mathcal{A}$ are chosen by a Metropolis-like search strategy with Gaussian drift proposals.
- The hyperparameters of the Gaussian process are inferred using Metropolis–Hastings sampling after each action.

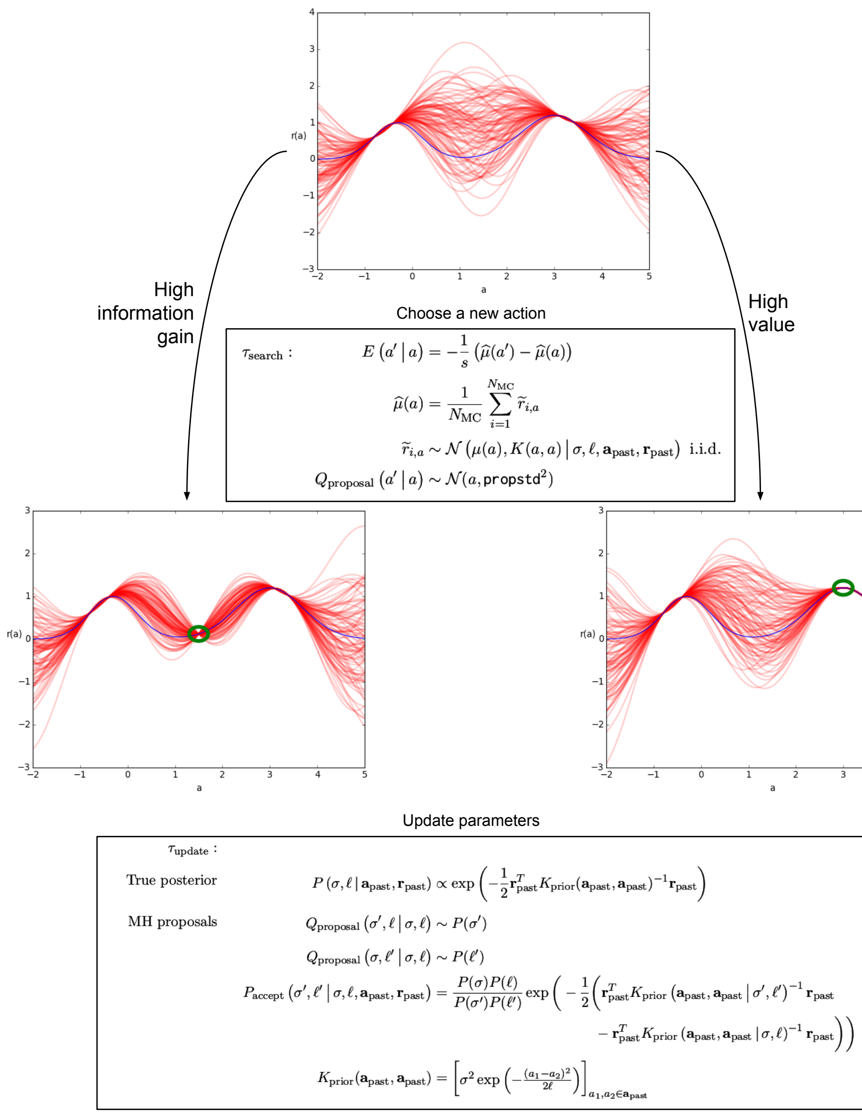


Figure 9: Two possible actions (in green) for an iteration of Thompson sampling. The believed distribution on the value function V is depicted in red. In this example, the true reward function is deterministic, and is drawn in blue. The action on the right receives a high reward, while the action on the left receives a low reward but greatly improves the accuracy of the believed distribution on V. The transition operators τ_{search} and τ_{update} are described in Section 3.3.

In this version of Thompson sampling, the contexts ϑ are Gaussian processes over the action space $\mathcal{A} = [-20, 20] \subseteq \mathbb{R}$. That is,

$$V \sim \mathcal{GP}(\mu, K),$$

where the mean μ is a computable function $\mathcal{A} \to \mathbb{R}$ and the covariance K is a computable (symmetric, positive-semidefinite) function $\mathcal{A} \times \mathcal{A} \to \mathbb{R}$. This represents a Gaussian process $\{R_a\}_{a \in \mathcal{A}}$, where R_a represents the reward for action a. Computationally, we represent a context as a data structure

$$\vartheta = (\theta, \mathbf{a}_{\text{past}}, \mathbf{r}_{\text{past}}) = (\mu_{\text{prior}}, K_{\text{prior}}, \eta, \mathbf{a}_{\text{past}}, \mathbf{r}_{\text{past}}),$$

where μ_{prior} is a procedure to be used as the prior mean function. w.l.o.g. we set $\mu_{\text{prior}} \equiv 0$. K_{prior} is a procedure to be used as the prior covariance function, parameterized by η.

The posterior mean and covariance for such a context ϑ are gotten by the usual conditioning formulas (assuming, for ease of exposition as above, that the prior mean is zero):[3]

$$\begin{aligned}
\mu(\mathbf{a}) &= \mu\left(\mathbf{a} \mid \mathbf{a}_{\text{past}}, \mathbf{r}_{\text{past}}\right) \\
&= K_{\text{prior}}(\mathbf{a}, \mathbf{a}_{\text{past}})\, K_{\text{prior}}(\mathbf{a}_{\text{past}}, \mathbf{a}_{\text{past}})^{-1}\, \mathbf{r}_{\text{past}} \\
K(\mathbf{a}, \mathbf{a}) &= K\left(\mathbf{a}, \mathbf{a} \mid \mathbf{a}_{\text{past}}, \mathbf{r}_{\text{past}}\right) \\
&= K_{\text{prior}}(\mathbf{a}, \mathbf{a}) - K_{\text{prior}}(\mathbf{a}, \mathbf{a}_{\text{past}})\, K_{\text{prior}}(\mathbf{a}_{\text{past}}, \mathbf{a}_{\text{past}})^{-1}\, K_{\text{prior}}(\mathbf{a}_{\text{past}}, \mathbf{a}).
\end{aligned}$$

Note that the context space Θ is not a finite-dimensional parametric family, since the vectors $\mathbf{a}_{\text{past}}$ and $\mathbf{r}_{\text{past}}$ grow as more samples are taken. Θ is, however, representable as a computational procedure together with parameters and past samples, as we do in the representation $\vartheta = (\mu_{\text{prior}}, K_{\text{prior}}, \eta, \mathbf{a}_{\text{past}}, \mathbf{r}_{\text{past}})$.

We combine the Update and Sample steps of Algorithm 2 by running a Metropolis–Hastings (MH) sampler whose stationary distribution is the posterior $P\left(\theta \mid \mathbf{a}_{\text{past}}, \mathbf{r}_{\text{past}}\right)$. The functional forms of μ_{prior} and K_{prior} are fixed in our case, so inference is only done over the parameters $\eta = \{\sigma, \ell\}$; hence we equivalently write $P\left(\sigma, \ell \mid \mathbf{a}_{\text{past}}, \mathbf{r}_{\text{past}}\right)$ for the stationary distribution. We make MH proposals to one variable at a time, using the prior as proposal distribution:

$$Q_{\text{proposal}}\left(\sigma', \ell \mid \sigma, \ell\right) = P(\sigma')$$

and

$$Q_{\text{proposal}}\left(\sigma, \ell' \mid \sigma, \ell\right) = P(\ell').$$

The MH acceptance probability for such a proposal is

$$P_{\text{accept}}\left(\sigma', \ell' \mid \sigma, \ell\right) = \min\left\{1,\ \frac{Q_{\text{proposal}}\left(\sigma, \ell \mid \sigma', \ell'\right)}{Q_{\text{proposal}}\left(\sigma', \ell' \mid \sigma, \ell\right)} \cdot \frac{P\left(\mathbf{a}_{\text{past}}, \mathbf{r}_{\text{past}} \mid \sigma', \ell'\right)}{P\left(\mathbf{a}_{\text{past}}, \mathbf{r}_{\text{past}} \mid \sigma, \ell\right)}\right\}$$

Because the priors on σ and ℓ are uniform in our case, the term involving Q_{proposal} equals 1 and we have simply

$$\begin{aligned}
P_{\text{accept}}\left(\sigma', \ell' \mid \sigma, \ell\right) &= \min\left\{1,\ \frac{P\left(\mathbf{a}_{\text{past}}, \mathbf{r}_{\text{past}} \mid \sigma', \ell'\right)}{P\left(\mathbf{a}_{\text{past}}, \mathbf{r}_{\text{past}} \mid \sigma, \ell\right)}\right\} \\
&= \min\Bigg\{1,\ \exp\Bigg(-\frac{1}{2}\Bigg(\mathbf{r}_{\text{past}}^T K_{\text{prior}}\left(\mathbf{a}_{\text{past}}, \mathbf{a}_{\text{past}} \mid \sigma', \ell'\right)^{-1} \mathbf{r}_{\text{past}} \\
&\qquad - \mathbf{r}_{\text{past}}^T K_{\text{prior}}\left(\mathbf{a}_{\text{past}}, \mathbf{a}_{\text{past}} \mid \sigma, \ell\right)^{-1} \mathbf{r}_{\text{past}}\Bigg)\Bigg)\Bigg\}.
\end{aligned}$$

The proposal and acceptance/rejection process described above define a transition operator τ_{update} which is iterated a specified number of times; the resulting state of the MH Markov chain is taken as the sampled semicontext θ in Step 1 of Algorithm 2.

For Step 2 (Search) of Thompson sampling, we explore the action space using an MH-like transition operator τ_{search}. As in MH, each iteration of τ_{search} produces a proposal which is either accepted or rejected, and the state of this Markov chain after a specified number of steps is the new action a.

[3] Here, for vectors $\mathbf{a} = (a_i)_{i=1}^n$ and $\mathbf{a}' = (a'_i)_{i=1}^{n'}$, $\mu(\mathbf{a})$ denotes the vector $(\mu(a_i))_{i=1}^n$ and $K(\mathbf{a}, \mathbf{a}')$ denotes the matrix $\left[K(a_i, a'_j)\right]_{1 \le i \le n, 1 \le j \le n'}$.

The Markov chain's initial state is the most recent action, and the proposal distribution is Gaussian drift:

$$Q_{\text{proposal}}\left(a' \mid a\right) \sim \mathcal{N}(a,\, \texttt{propstd}^2),$$

where the drift width `propstd` is specified ahead of time. The acceptance probability of such a proposal is

$$P_{\text{accept}}\left(a' \mid a\right) = \min\left\{1,\ \exp\left(-E\left(a' \mid a\right)\right)\right\},$$

where the energy function $E\left(\bullet \mid a\right)$ is given by a Monte Carlo estimate of the difference in value from the current action:

$$E\left(a' \mid a\right) = -\frac{1}{s}\left(\widehat{\mu}(a') - \widehat{\mu}(a)\right)$$

where

$$\widehat{\mu}(a) = \frac{1}{N_{\text{avg}}}\sum_{i=1}^{N_{\text{avg}}} \widetilde{r}_{i,a}$$

and

$$\widetilde{r}_{i,a} \sim \mathcal{N}(\mu(a), K(a,a))$$

and $\{\widetilde{r}_{i,a}\}_{i=1}^{N_{\text{avg}}}$ are i.i.d. for a fixed a. Here the temperature parameter $s \geq 0$ and the population size N_{avg} are specified ahead of time. Proposals of estimated value higher than that of the current action are always accepted, while proposals of estimated value lower than that of the current action are accepted with a probability that decays exponentially with respect to the difference in value. The rate of the decay is determined by the temperature parameter s, where high temperature corresponds to generous acceptance probabilities. For $s = 0$, all proposals of lower value are rejected; for $s = \infty$, all proposals are accepted. For points a at which the posterior mean $\mu(a)$ is low but the posterior variance $K(a,a)$ is high, it is possible (especially when N_{avg} is small) to draw a "wild" value of $\widehat{\mu}(a)$, resulting in a favorable acceptance probability.

Indeed, taking an action a with low estimated value but high uncertainty serves the useful function of improving the accuracy of the estimated value function at points near a (see Figure 9).[4,5] We see a comlete probabilistic program with `gpmem` implementing Bayesian optimization with Thompson Sampling below (Listing 2).

[4] At least, this is true when we use a smoothing prior covariance function such as the squared exponential.

[5] For this reason, we consider the sensitivity of $\widehat{\mu}$ to uncertainty to be a desirable property; indeed, this is why we use $\widehat{\mu}$ rather than the exact posterior mean μ.

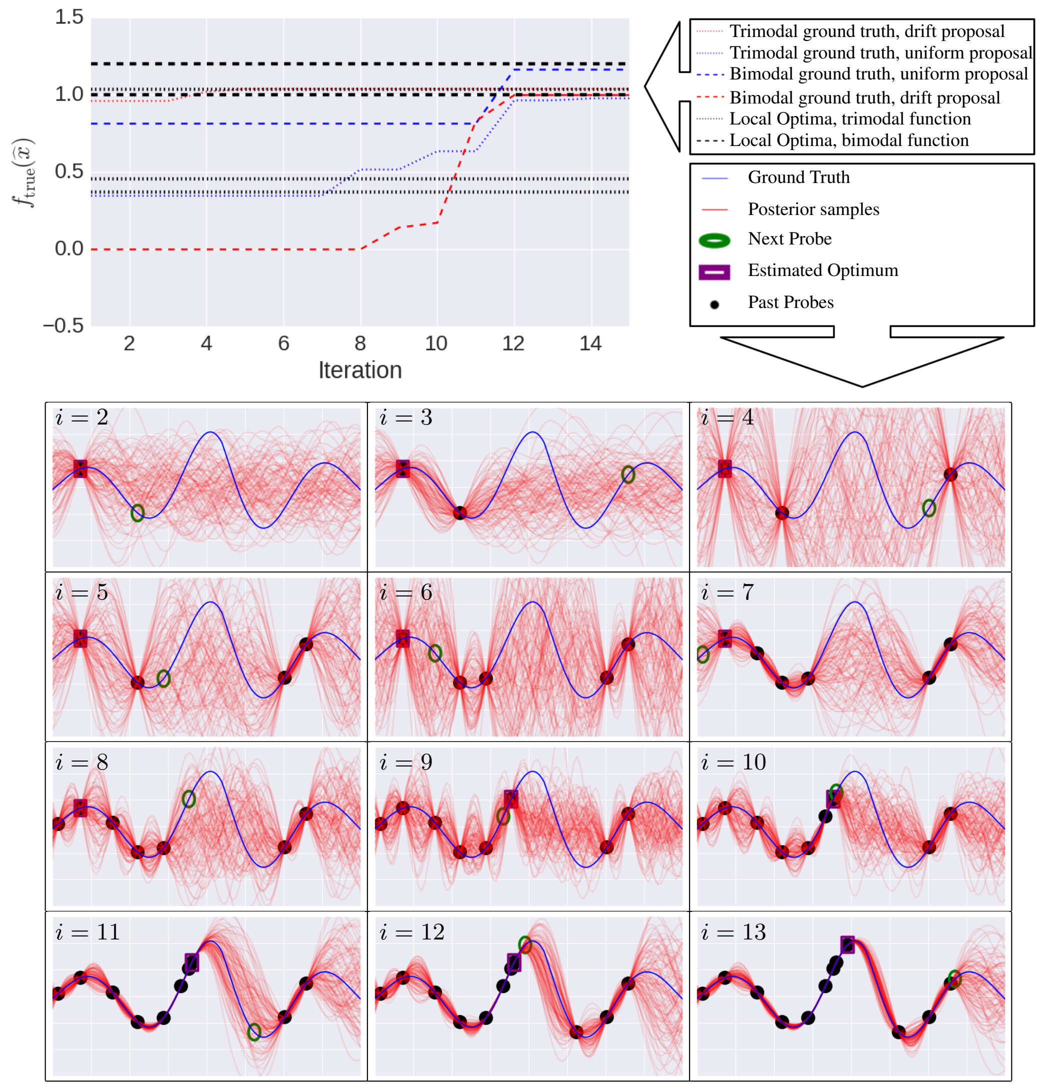


Figure 10: Top: the estimated optimum over time. Blue and Red represent optimization with uniform and Gaussian drift proposals. Black lines indicate the local optima of the true functions. Bottom: a sequence of actions. Depicted are iterations 7-12 with uniform proposals.

Listing 2: Bayesian optimization using gpmem

```
assume sf = tag(quote(hyper), 0, uniform_continuous(0, 10))
assume l = tag(quote(hyper), 1, uniform_continuous(0, 10))
assume se = make_squaredexp(sf, l)
assume blackbox_f = get_bayesopt_blackbox()
assume (f_compute, f_emulate) = gpmem(blackbox_f, se)

// A naive estimate of the argmax of the given function
define mc_argmax = proc(func) {
  candidate_xs = mapv(proc(i) {uniform_continuous(-20, 20)},
                      arange(20));
  candidate_ys = mapv(func, candidate_xs);
  lookup(candidate_xs, argmax_of_array(candidate_ys))
};

// Shortcut to sample the emulator at a single point without packing
// and unpacking arrays
define emulate_pointwise = proc(x) {
    run(sample(lookup(f_emulate(array(unquote(x))), 0)))
};

// Main inference loop
infer repeat(15, do(pass,
    // Probe V at the point mc_argmax(emulate_pointwise)
    predict(f_compute(unquote(mc_argmax(emulate_pointwise)))),
    // Infer hyperparameters
    mh(quote(hyper), one, 50)));
```

4 Discussion

We provided gpmem, an elegant linguistic framework for function learning-related tasks such as Bayesian optimization and GP kernel structure learning. We highlighted how gpmem overcomes shortcomings of the notations currently used in statistics, and how language constructs from programming allow the expression of models which would be cumbersome (prohibitively so, in some cases) to express in statistics notation. We evaluated our contribution on a range of hard problems for state-of-the-art Bayesian nonparametrics.

Appendix

A Covariance Functions

$$
\begin{aligned}
\mathrm{SE} &= \sigma^2 \exp(-\frac{(x-x')^2}{2\ell^2}) && (12)\\
\mathrm{LIN} &= \sigma^2(xx') && (13)\\
\mathrm{C} &= \sigma^2 && (14)\\
\mathrm{WN} &= \sigma^2\delta_{x,x'} && (15)\\
\mathrm{RQ} &= \sigma^2\left(1+\frac{(x-x')^2}{2\alpha\ell^2}\right)^{-\alpha} && (16)\\
\mathrm{PER} &= \sigma^2 \exp\left(\frac{2\sin^2(\pi(x-x')/p}{\ell^2}\right). && (17)
\end{aligned}
$$

B Covariance Simplification

```
SE × SE                    → SE
{SE,PER,C,WN} × WN         → WN
LIN + LIN                  → LIN
{SE,PER,C,WN,LIN} × C      → {SE,PER,C,WN,LIN}
```

Rule 1 is derived as follows:

$$
\begin{aligned}
\sigma_c^2 \exp(-\frac{(x-x')^2}{2\ell_c^2}) &= \sigma_a^2 \exp(-\frac{(x-x')^2}{2\ell_a^2}) \times \sigma_b^2 \exp(-\frac{(x-x')^2}{2\ell_b^2})\\
&= \sigma_c^2 \exp(-\frac{(x-x')^2}{2\ell_a^2}) \times \exp(-\frac{(x-x')^2}{2\ell_b^2})\\
&= \sigma_c^2 \exp\left(-\frac{(x-x')^2}{2\ell_a^2} - \frac{(x-x')^2}{2\ell_b^2}\right)\\
&= \sigma_c^2 \exp\left(-\frac{(x-x')^2}{2\ell_c^2}\right)
\end{aligned}
\tag{18}
$$

For stationary kernels that only depend on the lag vector between x and x' it holds that multiplying such a kernel with a WN kernel we get another WN kernel (Rule 2). Take for example the SE kernel:

$$
\sigma_a^2 \exp\left(-\frac{(x-x')^2}{2\ell_c^2}\right) \times \sigma_b\delta_{x,x'} = \sigma_a\sigma_b\delta_{x,x'} \tag{19}
$$

Rule 3 is derived as follows:

$$
\theta_c(x \times x') = \theta_a(x \times x') + \theta_b(x \times x') \tag{20}
$$

Multiplying any kernel with a constant obviously changes only the scale parameter of a kernel (Rule 4).

C Additional Structure Learning Results

Below we depict additional results for the airline data set using a hypothesis space of LIN, PER, SE and RQ covariance functions as base kernels for the composition. Fig 11 shows the training data and posterior samples drawn from the GP with posterior composite structure.

Fig. 12 shows why it advantageous to be Bayesian here. We see two possible hypotheses for the composite structure of $\mathbf{K}$.

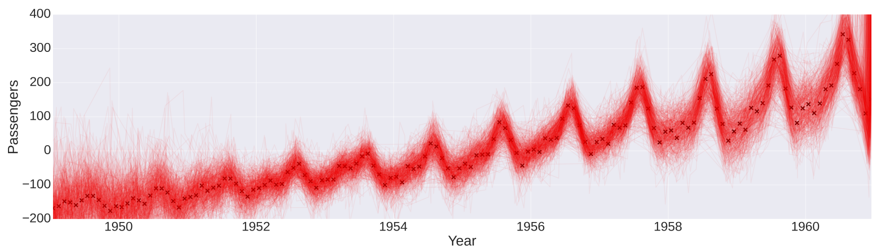


Figure 11: Data (black x) and posterior samples (red) for the airline data set.

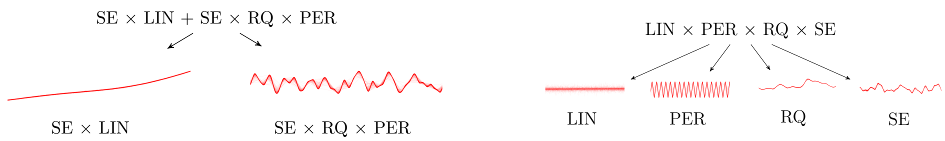


Figure 12: We see two possible hypotheses for the composite structure of $\mathbf{K}$. (a) Most frequent sample drawn from the posterior on structure. We have found two global components. First, a smooth trend (LIN × SE) with a non-linear increasing slope. Second, a periodic component with increasing variation and noise. (b) Second most frequent sample drawn from the posterior on structure. We found one global component. It is comprised of local changes that are periodic and with changing variation.

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