Time Series Structure Discovery via Probabilistic Program Synthesis

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Abstract

There is a widespread need for techniques that can discover structure from time series data. Recently introduced techniques such as Automatic Bayesian Covariance Discovery (ABCD) provide a way to find structure within a single time series by searching through a space of covariance kernels that is generated using a simple grammar. While ABCD can identify a broad class of temporal patterns, it is difficult to extend and can be brittle in practice. This paper shows how to extend ABCD by formulating it in terms of probabilistic program synthesis. The key technical ideas are to (i) represent models using abstract syntax trees for a domain-specific probabilistic language, and (ii) represent the time series model prior, likelihood, and search strategy using probabilistic programs in a sufficiently expressive language. The final probabilistic program is written in under 70 lines of probabilistic code in Venture. The paper demonstrates an application to time series clustering that involves a non-parametric extension to ABCD, experiments for interpolation and extrapolation on real-world econometric data, and improvements in accuracy over both non-parametric and standard regression baselines.

1 Introduction

Time series data are widespread, but discovering structure within and among time series can be difficult. Recent work by Duvenaud et al. [2] and Lloyd et al. [5] showed that it is possible to learn the structure of Gaussian Process covariance kernels and thereby discover interpretable structure in time series data. This paper shows how to reimplement the ABCD approach from Duvenaud et al. [2] using under 70 lines of probabilistic code in Venture [7]. We formulate structure discovery as a form of "probabilistic program synthesis". The key idea is to represent probabilistic models using abstract syntax trees (ASTs) for a domain-specific language, and then use probabilistic programs to specify the AST prior, model likelihood, and search strategy over models given observed data.

Several recent projects have applied probabilistic programming techniques to Gaussian process time series. Schaechtle et al. [10] embed GPs into Venture with fully Bayesian learning over a limited class of covariance structures with a heuristic prior. Tong and Choi [11] describe a technique for learning GP covariance structures using a relational variant of ABCD, and then compile the models into Stan [1]. However, probabilistic programming is only used for prediction, not for structure learning or for hyperparameter inference.

The contributions of this paper are as follows. First, we formulate ABCD as probabilistic program synthesis. Second, our implementation supports combinations of gradient-based search for hyperparameters, and Metropolis-Hastings sampling for structure and hyperparameters. Third, we show competitive performance on extrapolation and interpolation tasks from real-world data against several baselines. Fourth, we show that 10 lines of code are sufficient to extend ABCD into a nonparametric Bayesian clustering technique that identifies time series which share covariance structure.
Synthesis Model (AST Prior + AST Interpreter) \hspace{2cm} Prediction Model (AST Interpreter)

Synthesis Inference Strategy

Observed Dataset \( D = \{ (d_{in}^i, d_{out}^i) \} \)

Probabilistic Programming Engine

\[ \text{Probabilistic Programming Engine} \]

Synthesized AST

Probe Outputs \( \{ d_{out}^j \} \)

Probable Outputs \( \{ d_{in}^j \} \)

\begin{figure}
\centering
\includegraphics[width=\textwidth]{figure_1.png}
\caption{Overview of Bayesian structure learning as probabilistic program synthesis.}
\end{figure}

\begin{table}
\centering
\begin{tabular}{l|l|l}
\hline
synthesized abstract syntax tree of model program & equivalent Venture code of model program & Gaussian process datasets from model program executions \\
\hline
\includegraphics[width=0.3\textwidth]{ast_tree.png} & \includegraphics[width=0.3\textwidth]{venture_code.png} & \includegraphics[width=0.3\textwidth]{gp_datasets.png} \\
\hline
\end{tabular}
\caption{Executing synthesized model programs to produce Gaussian process datasets. \textbf{Left:} A symbolic structure generated by the AST prior. \textbf{Center:} Equivalent source code of the Venture GP model program, produced by the AST interpreter. \textbf{Right:} Executions of the model program probed with inputs in the region \([0, 10]\), which outputs datasets of GP time series.}
\end{table}

\section{Bayesian structure learning as probabilistic program synthesis}

Our objective in probabilistic program synthesis for Bayesian structure learning is to learn a symbolic representation of a probabilistic model program, by observing outputs of the model program given the inputs at which it was evaluated. The basic idea is to define a joint probabilistic model over (i) the symbolic representation of the program in terms of an abstract syntax tree (AST); (ii) the model program synthesized from the AST; and (iii) data \( D = \{ (d_{in}^i, d_{out}^i) : i = 1, \ldots, N \} \) that specifies constraints on observed input-output behavior of \( N \) independent executions of the synthesized model program. This framework, summarized in Figure 1, is implemented using:

1. A pair of probabilistic programs, an AST prior and AST interpreter, which together form the synthesis model. The AST prior \( G \) specifies a generative model over ASTs \( T \) for a class of probabilistic model programs, denoted \( p_G(T) \). The AST interpreter \( I \) takes as input \( T \) and synthesizes an executable model program \( M \) from it. The interpreter’s distribution over model programs is \( p_I(M|T) \).

2. A synthesized probabilistic model program \( M \), whose structure and hyperparameters are determined by its AST, with a distribution \( p_M(d_{out}^{\text{syn}}|d_{in}^{\text{syn}}) \) over output data given input data.

3. A probabilistic inference program named the synthesis strategy. Given \( N \) input-output data pairs \( D \) generated by an unknown model program \( M \) from the class of programs specified by the synthesis model, it searches over the execution trace of \( G \) to find probable symbolic structures (i.e. ASTs) that explain the data.
We now describe the synthesis model (AST prior and AST interpreter), and the class of synthesized

We briefly review the Gaussian process, a nonparametric regression technique that learns a function

The distributions

Applying the framework to Bayesian learning of Gaussian process covariance structures

Recent work by Duvenaud et al. [2] and Lloyd et al. [5] showed it is possible to use Gaussian Processes (GPs) to discover covariance structure in univariate time series. In this section, we extend the basic approach from Duvenaud et al. [2] by using probabilistic program synthesis for Bayesian learning over the symbolic structure of GP covariance kernels. The technique is implemented in under 70 lines of Venture code, shown in Figure 3.

We briefly review the Gaussian process, a nonparametric regression technique that learns a function \( f : X \rightarrow \mathcal{Y} \). The GP prior can express both simple parametric forms (such as polynomial functions) as well as more complex relationships dictated by periodicity, smoothness, and so on. Following the notation of [9], we formalize a Gaussian process \( f \sim \mathcal{GP}(m, k) \) with mean function \( m : X \rightarrow \mathcal{Y} \) and covariance function \( k : X \times X \rightarrow \mathbb{R} \) as follows: \( f \) is a collection of random variables \( \{ f(x) : x \in X \} \), any finite subcollection \( \{ f(x_1), \ldots, f(x_n) \} \) of which are jointly Gaussian with mean vector \( \{ m(x_1), \ldots, m(x_n) \} \) and covariance matrix \( \{ k(x_i, x_j) \}_{1 \leq i, j \leq n} \). The mean \( m \) is typically set to zero as it can be absorbed by the covariance. The functional form of the covariance \( k \) defines essential features of the unknown function \( f \) and so provides the inductive bias which lets the GP (i) fit patterns in data, and (ii) generalize to out-of-sample predictions. Rich GP kernels can be created by composing simple (base) kernels through sum, product, and change-point operators [9, Section 4.2.4].

We now describe the synthesis model (AST prior and AST interpreter), and the class of synthesized model programs for learning GP covariances structures. The AST prior \( \mathcal{G} \) (Codebox 3a) specifies a prior over binary trees. Each leaf \( n \) of \( \mathcal{T} \) is a pair \( (k_n, h_n) \) comprised of a base kernel and its hyper-parameters. The base kernels are: white noise (WN), constant (C), linear (LIN), squared exponential (SE), and periodic (PER). Each base kernels has a set of hyperparameters; for instance, PER has a lengthscale and period, and LIN has an x-intercept. Each internal node \( n \) represents a composition operator \( o_n \), which are: sum (+), product (×), and changepoint (CP, whose hyperparameters are the \( x \)-location of the change, and decay rate). The structure of \( \mathcal{T} \) is encoded by the index \( n \) of each internal node (whose left child is 2n and right child is 2n + 1) and the operators and base kernels at each node. Let \( N = |\mathcal{T}| \) denote the number of nodes. We write \( \mathcal{T} = \bigcup_{n=1}^{N} \{ x_n \} \) as a collection of \( N \) random variables, where \( x_n = (b_n, o_n, k_n, h_n) \) is a bundle of random variables for node \( n \): \( b_n = 1 \) if the tree branches at \( n \) (and 0 if \( n \) is a leaf); \( o_n \) is the operator (or \( \varnothing \) if \( b_n = 0 \)); \( k_n \) is the base kernel (or \( \varnothing \) if \( b_n = 1 \)); and \( h_n \) is the hyperparameter vector (or \( \varnothing \) if \( n \) has no hyperparameters, e.g., if \( b_n = 1 \) and \( o_n = \varnothing \)). Letting \( \pi(n) \) denote the list of all nodes in the path from \( n \) up to the root, the tree prior is:

\[
p_{\mathcal{G}}(T) = \prod_{n=1}^{N} p_g(x_n | x_{\pi(n)});
\]

\[
= \prod_{n=1}^{N} \begin{cases} 
(1 - p_{\text{branch}}) p_{\text{kernel}}(k_n) p_{\text{hyper}}(h_n | \text{kernel} = k_n) & \text{if } b_n = 0, \\
p_{\text{branch}} p_{\text{operator}}(o_n) p_{\text{hyper}}(h_n | \text{operator} = o_n) & \text{if } b_n = 1, \\
0 & \text{if } x_n | x_{\pi(n)} \text{ is inconsistent.}
\end{cases}
\]

The distributions \( p_{\text{branch}}, p_{\text{kernel}}, \) and \( p_{\text{hyper}} \) are all fixed constants in \( \mathcal{G} \). An example covariance kernel AST generated by Eq (2) is shown the first column of Figure 2. As for the AST interpreter \( \mathcal{I} \) (Codebox 3b), it parses \( \mathcal{T} \) and deterministically outputs a GP model program with mean 0 and covariance function encoded by \( \mathcal{T} \), plus baseline noise. Outcomes of the synthesis step are shown in the second column of Figure 2. The synthesized GP model program \( \mathcal{M} \) takes as input \( k \) probe points \( d^{\text{in}} \in \mathbb{R}^k \), and produces as output a (noisy) joint sample \( d^{\text{out}} \in \mathbb{R}^k \) of the GP at the probe points:

\[
\log P_{\mathcal{M}}(d^{\text{out}} | d^{\text{in}}) = \log N(e^{\text{out}} | 0, \mathbf{K}^{\text{cov}} + \sigma^2 I) \quad \text{(with } \mathbf{K}^{\text{cov}} = \text{cov(a}_n d^{\text{in}}, d^{\text{out}})_{1 \leq a, b \leq k})
\]

\[
= -\frac{1}{2} d^{\text{out}} (\mathbf{K}^{\text{cov}} + \sigma^2 I)^{-1} d^{\text{out}} - \frac{1}{2} \log |\mathbf{K}^{\text{cov}} + \sigma^2 I| - \frac{k}{2} \log 2\pi.
\]
(a) Synthesis model: AST prior $G$

```plaintext
assume tree_root = () -> {1};

assume get_hyper_prior ~ mem((node_index) -> {
    // Gradient-safe exponential prior.
    -log_logistic(log_odds_uniform() #hypers:node_index)
});

assume choose_primitive = (node) -> {
    base_kernel ~ categorical(simplex(.2, .2, .2, .2, .2),
    ["WN", "C", "LIN", "SE", "PER"]) #structure:pair("base_kernel", node);
    cond(
        (base_kernel == "WN") ("WN", get_hyper_prior(pair("WN", node))));
        (base_kernel == "C") ("C", get_hyper_prior(pair("C", node))));
        (base_kernel == "LIN") ("LIN", get_hyper_prior(pair("LIN", node))));
        (base_kernel == "SE") ("SE", .01 + get_hyper_prior(pair("SE", node))));
        (base_kernel == "PER") ("PER",
            .01 + get_hyper_prior(pair("PER_1", node)),
            .01 + get_hyper_prior(pair("PER_t", node))));
    )
});

assume choose_operator = mem((node) -> {
    operator_symbol ~ categorical(simplex(0.45, 0.45, 0.1),
        ["+", "/", "CP"]) #structure:pair("operator", node);
    if (operator_symbol == "CP") {
        [operator_symbol, get_hyper_prior(pair("CP", node))]
    } else {
        choose_primitive(node)
    }
});

assume generate_random_program = mem((node) -> {
    if (flip(.3) #structure:pair("branch", node)) {
        operator ~ choose_operator(node);
        [operator, generate_random_program(2 * node), generate_random_program(2 * node + 1)]
    } else {
        generate_random_program(node)
    }
});

assume produce_covariance = (source) -> {
    cond(
        (source[0] == "WN") (gp_cov_scale(source[1], gp_cov_bump)),
        (source[0] == "C") (gp_cov_const(source[1])),
        (source[0] == "LIN") (gp_cov_linear(source[1])),
        (source[0] == "SE") (gp_cov_se(source[1]**2)),
        (source[0] == "PER") (gp_cov_periodic(source[1]**2, source[2])),
        (source[0] == "+") (gp_cov_sum(produce_covariance(source[1]), produce_covariance(source[2]))),
        (source[0] == "/") (gp_cov_product(produce_covariance(source[1]), produce_covariance(source[2]))),
        (source[0][0] == "CP") (gp_cov_cp(source[0][1], .1, produce_covariance(source[1]), produce_covariance(source[2]))));
});

assume produce_executable = (source) -> {
    baseline_noise = gp_cov_scale(.1, gp_cov_bump);
    covariance_kernel = gp_cov_sum(produce_covariance(source), baseline_noise);
    make_gp(gp_mean_const(0.), covariance_kernel)
};
```

(b) Synthesis model: AST interpreter $I$

```plaintext
assume source ~ generate_random_program(tree_root());
assume gp_executable = produce_executable(source);
define xs = get_data_xs("./data.csv");
define ys = get_data_ys("./data.csv");
observe gp_executable(xs) = ys;
```

(c) Data observation program

```plaintext
(d) Synthesis inference strategy: MH + Gradients

for_each(arange(T), (_) -> {
    infer gradient(
        minimal_subproblem(/?hypers, steps=100);
    infer resimulate(
        minimal_subproblem(one(/?structure), steps=100)))
});
```

Figure 3: Structure discovery in time series via probabilistic program synthesis. Panels (a)–(d) present interacting programs in Venture which correspond to the components in Figure 1.
4 Bayesian structure learning and hyperparameter inference in the covariance kernel AST

Our implementation of program synthesis for GP covariances described in the previous section simplifies Eq (1) in that \( I \) deterministically interpreters a GP model given the AST, so that \( P_I(M | T) = \delta [M = \text{interpret}(I ; T)] \). The key inference problem becomes search over the space of GP kernel compositions in \( T \), and hyperparameters \( h_n \in T \) of base kernels. This section describes the synthesis strategy for posterior inference over the AST.

Our strategy for inference on structure is to simulate a Markov chain whose target distribution is \( p_G(T | D) \). The following Metropolis-Hastings algorithm is implemented by the Venture inference program \( \text{infer resimulate(minimal_subproblem(?structure))} \) (invoked in Codelbox 3d). Suppose the current AST is \( T \). Design a proposal distribution \( Q(T \rightarrow T') \) using a three-step process. First, identify a node \( x_n \in T \), and let \( T_n \) denote the subtree of \( T \) rooted at \( n \). Second, “detach” \( x_n \) and all its descendants from \( T \), which gives an intermediate tree \( T_{\text{detach}} := T \setminus T_n \). Third, “resimulate”, starting from \( T_{\text{detach}} \), the random choice \( x_n' \) using a resimulational distribution \( q(x_n' | T_{\text{detach}}) \equiv p_G \) equal to the prior Eq (2). If \( b_n' = 0 \) (i.e., a branch node), recursively resimulate its children until all downstream random choices are leaf nodes. This operation results in a new subtree \( T' \), and we set \( T' = T_{\text{detach}} \cup T_n \) to be the proposal. To compute the reversal \( Q(T' \rightarrow T) \), we make the following key observation: when resimulating node \( x_n' \) starting from \( T' \), the intermediate trees \( T_{\text{detach}} = T_n \) are identical for \( Q(T \rightarrow T') \) and \( Q(T' \rightarrow T) \). Using this insight, the MH ratio is therefore:

\[
\alpha(T \rightarrow T') = \frac{p_G(T', D)Q(T \rightarrow T')}{p_G(T, D)Q(T' \rightarrow T)} = \frac{\prod_{n=1}^{N} p_G(x_n' | x_{\sigma(n)}') p_G(D | T')Q(T' \rightarrow T)}{\prod_{n=1}^{N} p_G(x_n | x_{\sigma(n)}) p_G(D | T)Q(T \rightarrow T')}
\]

\[
= \frac{\prod_{n \in T_{\text{detach}}} p_G(x_n | x_{\sigma(n)}) \left( \prod_{n \in T_n} q(x_n' | x_{\sigma(n)}) p_G(D | T') \right) \prod_{n \in T_n} p_G(x_n | x_{\sigma(n)})}{\prod_{n \in T_{\text{detach}}} p_G(x_n | x_{\sigma(n)}) \left( \prod_{n \in T_n} p_G(x_n' | x_{\sigma(n)}) p_G(D | T) \right) \prod_{n \in T_n} p_G(x_n | x_{\sigma(n)})} = \frac{p_G(D | T')}{p_G(D | T)}.
\]

This likelihood-ratio can be computed without revisiting the entire trace [7]. Algorithm 1 summarizes the key elements of the MH resimulation algorithm described above.

As for hyperparameter inference, our synthesis strategy uses either MH (for each hyperparameter separately) or gradient ascent (for all hyperparameters jointly). The gradient optimizer uses reverse-mode auto-differentiation [3], propagating gradients down the root of \( T \) to the leaves, and partial derivatives of hyperparameters from leaves back up to the root. Algorithms 2 and 3 describe hyperparameter inference in the AST using MH and gradient-based inference, respectively. All three algorithms are implemented as general purpose inference machinery in Venture.

Algorithm 1 Resimulation MH for the covariance AST.
Inference program: \( \text{infer resimulate(minimal_subproblem(?structure)=pair("branch", n)))} \)

Require: Index \( n \) of node in the AST whose subtree structure \( T_n \) to transition.
Ensure: MH transition \( T_n \rightarrow T'_n \), targeting \( p_G(T_n | T'_n, D) \).
1: \( T_{\text{detach}} \leftarrow T \setminus T_n \) \( \triangleright \) Detach the subtree rooted at \( n \).
2: \( T'_n \leftarrow p_G(\mathbf{\cdot} | T_{\text{detach}}) \) \( \triangleright \) Resimulate the subtree rooted at \( n \) from the prior.
3: \( T' \leftarrow T_{\text{detach}} \cup T'_n \) \( \triangleright \) Construct the proposal tree.
4: \( \alpha \leftarrow p_G(D | T') / p_G(D | T) \) \( \triangleright \) Compute the acceptance ratio.
5: if Uniform(0, 1) \leq \alpha then \( \triangleright \) Accept the proposal with probability \( \alpha \).
6: \( T'_n \leftarrow T'_n \)

Algorithm 2 MH transition on hyperparameters of covariance base kernels and operators.
Inference program: \( \text{infer resimulate(minimal_subproblem(?hypers=\{\}), steps=T)} \)

Require: Index \( n \) of node in AST whose hypers to transition; number \( T \) of MH steps.
Ensure: MH transition targeting \( p_G(h_n | D, T \setminus \{ h_n \}) \).
1: for \( t = 1, \ldots, T \) do
2: \( h_n' \leftarrow q(\mathbf{\cdot} | T, D) \) \( \triangleright \) Propose a new value of \( h_n' \).
3: \( q_{\text{revers}} = p(\mathbf{\cdot} | T \setminus \{ h_n \}, h_n'; D) q(h_n | T \cup h_n') \setminus \{ h_n \}, D) \) \( \triangleright \) Compute density of reversal proposal.
4: \( q_{\text{forward}} = p(\mathbf{\cdot} | T, D) q(h_n' | T, D) \) \( \triangleright \) Compute density of forward proposal.
5: \( \alpha \leftarrow q_{\text{revers}} / q_{\text{forward}} \) \( \triangleright \) Compute the acceptance ratio.
6: if Uniform(0, 1) \leq \alpha then \( \triangleright \) Accept the proposal with probability \( \alpha \).
7: \( T \leftarrow (T \cup h_n') \setminus \{ h_n \} \)
We next applied the technique to regression problems on real-world time series. Figure 7a shows

holds.

Algorithm 3 Reverse auto-differentiation jointly optimizing hyperparameters of all kernels.
Inference program: infer gradient(minimal_subproblem(/hypers), steps=T, step_size=g)

Require: Number $T$ of gradient steps; gradient step size $\gamma$.
Ensure: Gradient ascent on all hypers $h = (h_n : n \in T)$ optimizing un-normalized posterior $p(D, h, T \setminus \{h\})$.
1: $\triangleright$ Posterior factors as $p(D, h, T \setminus \{h\}) = \mathcal{L}(h)p(h|T \setminus \{h\})p(T \setminus \{h\})$, where $\mathcal{L}(h) = p(D|h, T \setminus \{h\})$.
2: for $t = 1, \ldots, T$ do
3: $(C^1, \ldots, C^T) \leftarrow$ Compute-Covariance-Matrices($T$) $\triangleright$ Recompute covariance matrices at all subtrees.
4: $dC^t \leftarrow \nabla \log p(D|C^t)$ $\triangleright$ Compute gradient of $\log \mathcal{L}$ w.r.t $C^t$.
5: Backpropagate-Gradient-Subtree($T, 1$) $\triangleright$ Compute gradients of $\log \mathcal{L}$ w.r.t $C^t$, $h_n$ at all subtrees.
6: $dh \leftarrow dh + \nabla \log p(h|T \setminus \{h\})$ $\triangleright$ Add gradient of the prior on $h$.
7: $h \leftarrow h + \gamma dh$ $\triangleright$ Jointly update all hyperparameters.
8: procedure Backpropagate-Gradient-Subtree($T$, node index $n$)
9: if $h_n$ is 1 then $\triangleright$ A leaf node.
10: if $\alpha_n$ is ‘+’ then $\triangleright$ Child gradient is the parent gradient.
11: $dC^t_n \leftarrow dC^p_n$ $\triangleright$ Update left child.
12: $dC^t_{2n-1} \leftarrow dC^p_{2n-1}$ $\triangleright$ Update right child.
13: else ($\alpha_n$ is ‘*’) $\triangleright$ Child gradient is element-wise product of parent gradient and sibling covariance.
14: $dC^t_n \leftarrow dC^p_n \odot C^t_{2n}$ $\triangleright$ Update left child.
15: $dC^t_{2n} \leftarrow dC^p_n \odot C^t_{2n}$ $\triangleright$ Update right child.
16: Backpropagate-Gradient-Subtree($T, 2n$) $\triangleright$ Backpropagate down left subtree.
17: Backpropagate-Gradient-Subtree($T, 2n + 1$) $\triangleright$ Backpropagate down right subtree.
18: else ($h_n$ is 0) $\triangleright$ A leaf node.
19: $dh_n \leftarrow \text{vec}(dC^t_n) : f_{h_n}(K_o(D^n, D^n | h_n))$ $\triangleright$ Gradient is product of covariance with kernel’s Jacobian.

5 Applications to synthetic and real-world datasets

In this section, we apply the probabilistic program synthesis framework for learning GP covariance
structures to a collection of synthetic and real-world examples.

The first experiment compares the outcomes of hyperparameter inference using two different inference
programs: MH sampling (Algorithm 2) and gradient optimization (Algorithm 3), given data from
a periodic GP with period 3 and lengthscale 1.4. By encapsulating inference algorithms as top-
level inference programs, it is possible to easily compare both their performance in searching the
hyperparameter space, and their predictive outcomes. Refer to the figure caption for further details.

To explore the advantage of Bayesian learning versus greedy search over structures, we ran inference
on 50 data points from a GP with a LIN + PER composite covariance kernel. The posterior distribution
over structures is shown in Figure 5. The ground truth structure is the second most probable, while
the MAP estimate is incorrectly identified as LIN + WN. GP predictives from model averaging over
the posterior structure distribution provide a better fit than using the MAP structure.

To assess the flexibility and extensibility of time series discovery as probabilistic program synthesis,
we extended the observation program from Codebox 3c to specify a non-parametric mixture of several
GP curves, as shown in Figure 6a. We simulated four datasets, (two linear, and two periodic), and
then ran joint MH inference over their structures, hyperparameters, and cluster identities. Clusterings
based on 64 posterior samples correctly recover the ground-truth partitioning, shown in red and green
in Figure 6b. It is worthwhile to note that this significant change to the probabilistic model is achieved
by modifying less than 10 lines of the original code, suggesting it is possible to extend the basic
synthesis template from Figure 3 to a variety of time series analysis tasks.

We next applied the technique to regression problems on real-world time series. Figure 7a shows
extrapolation performance on a dataset of airline passenger volume between 1949 and 1960. The GP
detects the linear trend with periodic variation, leading to very accurate predictions. Figure 7b shows
interpolation on a dataset of solar radiation between the years 1660 and 2010. The GP successfully
models the qualitative change at around 1760, which correctly results in different interpolation
characteristics at both ends. In contrast, Bayesian linear regression is forced to treat such structural
effects as unmodeled noise.
Figure 4: Comparing Metropolis-Hastings sampling and gradient ascent as synthesis strategies for learning GP hyperparameters. The data are drawn from a periodic kernel with length scale 1.4 and period 3. **Left:** The surface of the unnormalized posterior after observing 200 data points. The gradient ascent steps converge to a local mode at period 6 (a multiple of the true period); the MH sampler explores both posterior modes at periods of 3 and 6. **Right:** By averaging over modes, posterior predictive curves from the MH inference program (top) illustrate smoother behavior than predictive curves from gradient inference (bottom), which center on a single mode. The mean squared prediction errors on held-out data (red crosses) are 0.18 and 0.20 for MH and gradients, respectively.

Figure 5: Structure recovery from synthetic data. **Left:** Histogram of the posterior distribution over AST structures, given data from a LIN + PER Gaussian process. The MAP structure (posterior mode) is LIN + WN. **Right:** Posterior GP curves sampled from the LIN + WN (blue) and LIN + PER (gray) structures; LIN + PER, which is not the MAP, achieves better predictions on the held-out data (red crosses). Model averaging (green) smooths predictions over all structures.

```plaintext
assume crp = make_crp(0.5);
assume get_cluster_id = mem((ts_index) -> {crp()});
assume get_source = (ts_index) -> {
    cluster_id ~ get_cluster_id(integer(ts_index));
    generate_random_program(
        get_tree_root(), cluster_id)
};
assume obs_function = (ts_index, data) -> {
    source = get_source(ts_index);
    produce_executable(source)(data)
};
```

(a) Observation program for clustering GP curves. 

Figure 6: Clustering data according to structural characteristics. **Left:** A small modification to the model program from Codebox 3a suffices to extend it for clustering time series by their covariance structures. **Right:** Detected clustering among four synthetic time series of 100 points each.
Figure 7: Comparing GP regression via probabilistic program synthesis and Bayesian linear regression for extrapolating and interpolating on held-out data (red crosses) in real-world time series. The GP learns combinations of periodic and change-point structures, improving predictive performance.

Figure 8: Held-out predictive performance of GP regression via probabilistic program synthesis versus non-parametric regression and standard machine learning baselines on 4 real-world datasets. Each point for the GP methods is the RMSE of a posterior sample, standardized to lowest overall error = 1. The ABCD baseline learns hyperparameters (in Venture) for structures reported by [5].

Figure 9: Lines of code comparison between probabilistic program synthesis in Venture, and ABCD.

Finally, we compared the predictive performance against six baselines on four datasets from Lloyd et al. [5], shown in Figure 8. The GP based on probabilistic program synthesis achieved very competitive prediction error on all tasks. Figure 9 illustrates that implementing probabilistic program synthesis in Venture, an expressive probabilistic programming system with reusable inference machinery, leads to large reductions in code length and complexity.

6 Discussion

We have described and implemented a framework for time series structure discovery using probabilistic program synthesis. We also have assessed efficacy of the approach on synthetic and real-world experiments, and demonstrated improvements in model discovery, extensibility, and predictive accuracy. It seems promising to apply probabilistic program synthesis to several other settings, such as fully-Bayesian search in compositional generative grammars for other model classes [4], or Bayes net structure learning with structured priors [6]. We hope the formalisms in this paper encourage broader use of probabilistic programming techniques to learn symbolic structures in other applied domains.
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