Running head: COMPOSITIONAL INDUCTIVE BIASES

Compositional Inductive Biases in Function Learning

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### COMPOSITIONAL INDUCTIVE BIASES

2

#### Abstract

How do people recognize and learn about complex functional structure? Taking inspiration from other areas of cognitive science, we propose that this is achieved by harnessing compositionality: complex structure is decomposed into simpler building blocks. We formalize this idea within the framework of Bayesian regression using a grammar over Gaussian process kernels, and compare this approach with other structure learning approaches. Participants consistently chose compositional (over non-compositional) extrapolations and interpolations of functions. Experiments designed to elicit priors over functional patterns revealed an inductive bias for compositional structure. Compositional functions were perceived as subjectively more predictable than non-compositional functions, and exhibited other signatures of predictability, such as enhanced memorability and reduced numerosity. Taken together, these results support the view that the human intuitive theory of functions is inherently compositional.

*Keywords:* Function learning; Pattern recognition; Compositionality; Structure search; Gaussian process

## COMPOSITIONAL INDUCTIVE BIASES

3

# Compositional Inductive Biases in Function Learning

# Introduction

Recognizing functional patterns is a ubiquitous problem in everyday cognition, underlying the perception of time, space and number. How much food should you cook to satisfy every guest at a party? How far do you have to turn the faucet handle to get the right temperature? Should you invest in a particular stock that seems to be going up? Since the space of such mappings is theoretically infinite, inductive biases are necessary to constrain the plausible inferences (Griffiths, Chater, Kemp, Perfors, & Tenenbaum, 2010; Mitchell, 1980). But what is the nature of these inductive biases over functions?

The major theoretical accounts of function learning, which we review below, offer two radically different answers to this question. Rule-based accounts posit a fixed set of parametric forms (or rules) that serve as a "vocabulary" for functions; these accounts imply strong inductive biases for the rules in the functional vocabulary. By contrast, similarity-based accounts posit a nonparametric representation of functions, implying relatively weak inductive biases.

A major challenge for humans is how to accommodate the virtually infinite diversity of functions in the real world. Rule-based models can only represent linear combinations of a fixed set of parametric functions. Similarity-based models can in principle represent an infinite variety of functions, but their typically weak inductive biases do not support strong inferences from small amounts of data—an important characteristic of human learning (Lake, Ullman, Tenenbaum, & Gershman, 2016).

A ubiquitous strategy in many areas of cognition, from language (Chomsky, 1965) to concept learning (Goodman, Tenenbaum, Feldman, & Griffiths, 2008; Kemp, 2012; Piantadosi, Tenenbaum, & Goodman, 2016) and visual perception (Biederman, 1987; Lake, Salakhutdinov, & Tenenbaum, 2015), is to divide and conquer: construct complex representations out of simpler building blocks using a set of compositional rules. Compositional systems support strong inferences from small amounts of data by imposing structural constraints, without sacrificing the capacity for representing an infinite variety of forms. The primary claim in this paper is that human function learning is structurally

## COMPOSITIONAL INDUCTIVE BIASES

4

constrained by compositional inductive biases.

To formalize this idea, we need a theoretical framework for function learning that can represent and reason about compositional function spaces. Lucas, Griffiths, Williams, and Kalish (2015) recently presented a normative theory of function learning using the formalism of Gaussian processes (GPs). As we will describe more formally, GPs are distributions over functions that can encode properties such as smoothness, linearity, periodicity, symmetry, and many other inductive biases found by past research on human function learning (Brehmer, 1974b; DeLosh, Busemeyer, & McDaniel, 1997). Lucas et al. (2015) showed how Bayesian inference with GP priors can be expressed in both parametric (rule-based) and nonparametric (similarity-based) forms. GPs can therefore serve as a computational-level theory of function learning that bridges different mechanistic implementations.

We build on the GP theory to study, both theoretically and experimentally, the compositional nature of inductive biases in human function learning. We first define a compositional grammar for intuitive functions based on work by Duvenaud, Lloyd, Grosse, Tenenbaum, and Ghahramani (2013). This grammar allows us to construct a GP prior that obeys compositionally structured constraints. We then test the predictive power of this model in several function learning experiments, comparing the compositional prior to a flexible non-compositional prior (the spectral mixture representation proposed by Wilson & Adams, 2013, which we will describe later). Both models use Bayesian inference to reason about functions, but differ in their inductive biases. Finally, we investigate how compositional functions influence memory, change detection, and the perception of numerosity and predictability.

### Prior research on human function learning

The general problem of inferring how one variable depends functionally on another is important for many aspects of cognition. Traditionally ,it has been studied in paradigms assessing how people learn about input-output mappings or how they make sense of spatiotemporal patterns. Additionally, the way in which we learn about and recognize functional patterns is also crucial in the modern world as we look at data – either as scientists

## COMPOSITIONAL INDUCTIVE BIASES

5

or non-scientist decision makers – in trying to understand what function the data reveal. We are interested in all of these aspects of function learning, but will focus first on the latter because it can potentially reveal how people recognize and perform inference about structure very quickly. However, we believe that a strength of the compositional account of functional inductive biases that we put forward here is that it can account for empirical effects across a diverse set of paradigms.

Donald Broadbent was among the first psychologists to investigate how people learn and control functions between inputs and outputs (Broadbent, 1958). In his experiments, participants controlled functions within an industrial setting called the "sugar factory," in which they learned the relationship between work force and sugar production. Broadbent showed that participants had difficulty controlling some functions, such as exponential or power functions, but were good at learning others, for example linear functions (Berry & Broadbent, 1984).

Since Broadbent's pioneering work, further studies have established several empirical regularities (see McDaniel & Busemeyer, 2005, for a review). For example, studies using interpolation judgments—predictions of function outputs for inputs inside the convex hull of training inputs—have found that linear, increasing functions are easier to learn than non-linear, non-monotonic or decreasing functions (Brehmer, 1974a; Brehmer, Alm, & Warg, 1985; Byun, 1995). Presentation order also matters: it is easier to learn functions if the input is ordered by increasing output (DeLosh et al., 1997).

Important constraints on theories of function learning have come from studies of extrapolation judgments—predictions of function outputs for inputs outside the convex hull of training inputs (DeLosh et al., 1997; McDaniel & Busemeyer, 2005). People tend to make linear extrapolations with a positive slope and an intercept of zero (Kalish, Lewandowsky, & Kruschke, 2004; Kwantes & Neal, 2006). This linear bias holds true even when the underlying function is nonlinear; for example, when trained on a quadratic function, average predictions fall between the true function and straight lines fitted to the closest training points (DeLosh et al., 1997).

Two families of theories have been developed to explain these and other regularities.

## COMPOSITIONAL INDUCTIVE BIASES

6

Rule-based theories (Carroll, 1963; Koh & Meyer, 1991) propose that people learn explicit parametric functions, for example linear, polynomial or power-law functions, or some combination of simpler functions. While rule-based theories have had some success in predicting function learning performance, they have trouble accounting for the aforementioned "order-of-difficulty effects" in interpolation tasks (McDaniel & Busemeyer, 2005), fail to fully predict extrapolation performance (DeLosh et al., 1997), especially for non-linear functions, and are unable to learn a partitioning of the input space (the knowledge partitioning effect; Kalish et al., 2004).

Similarity-based theories (e.g., Busemeyer, Byun, Delosh, & McDaniel, 1997; DeLosh et al., 1997) propose that people learn functions by associating inputs and outputs: if input x is paired with output y, then inputs similar to x should produce outputs that are similar to y. Busemeyer et al. (1997) formalized this intuition using a connectionist model (Associative-Learning Model; ALM) in which inputs activate an array of hidden units representing a range of possible input values; each hidden unit is activated in proportion to its similarity to the current input. Learned associations between the hidden units and the response units map the similarity-based activation pattern to output predictions. ALM successfully captures aspects of interpolation performance, but fails to explain extrapolation and knowledge partitioning phenomena.

In order to overcome some of these problems, hybrid versions of the two approaches have been put forward (McDaniel & Busemeyer, 2005). Hybrid models normally contain an associative learning process that acts on explicitly-represented rules. One such hybrid is EXAM (Extrapolation-Association Model; Busemeyer et al., 1997). EXAM assumes similarity-based interpolation, but extrapolates using a simple linear rule. The model effectively captures the human bias towards linearity, and predicts human extrapolations for a variety of functions, but without accounting for non-linear extrapolation (Bott & Heit, 2004). POLE (population of Linear Experts; Kalish et al., 2004), which approximates functions using piece-wise linear representations, can capture knowledge partitioning and order-of-difficulty effects (McDaniel, Dimperio, Griego, & Busemeyer, 2009). However, it is unclear if a combination of linear functions is able to explain human function learning in more complex,

## COMPOSITIONAL INDUCTIVE BIASES

7

naturalistic contexts, especially given that humans are capable of learning non-linear functions as well (see Bott & Heit, 2004).

Another area of explaining how people make sense of functional structure could be called "intuitive science" or forecasting. Here, participants are normally confronted with multiple data points at once and then have to predict future or left out points.

Various reviews have established factors that influence participants predictions of visually presented data (see Bolger & Harvey, 1998; Goodwin & Wright, 1993, for example). Broadly speaking, these factors fall within 4 categories. First, people seem to damp trends when they make forecasts from noisy data. This means that their forecasts lie below upward trend lines but above downward ones. Therefore, it appears that forecasters tend to underestimate the steepness of functions (Andreassen & Kraus, 1990; Keren, 1983). Trend damping is greater for downward than for upward trended data, especially when the data representation format is visual rather than in a table (Harvey & Bolger, 1996). Second, forecasts tend to overestimate functions lacking a trend (Eggleton, 1982). Third, people seem to deliberately attach random noise to their forecasts, and add more noise to forecasts from noisier data series. This means that their forecasts appear to represent the way the series will appear once the outcome has occurred (Harvey, Ewart, & West, 1997). Fourth, forecasts for independent series should lie on the series mean, but instead they have been found to lie between the mean and the last revealed data point (Eggleton, 1982), similar to findings in more traditional function learning paradigms.

#### Gaussian process regression as a normative theory of function learning

The theories of function learning summarized in the previous section are process models, specifying mechanistic hypotheses about representations and learning rules. However, mechanistic hypotheses do not directly give insight into inductive biases, since different mechanisms may or may not produce the same bias. Thus, if our goal is to understand human inductive biases, we require a computational-level analysis of function learning that is agnostic to mechanism. The GP theory of function learning developed by Lucas et al. (2015) fills this gap.

## COMPOSITIONAL INDUCTIVE BIASES

8

Formally, a GP is a collection of random variables, any finite subset of which are jointly Gaussian-distributed (see Rasmussen & Williams, 2006, for an introduction). A GP can be expressed as a distribution over functions. Let  $f : \mathcal{X} \to \mathbb{R}$  denote a function over input space  $\mathcal{X}$  that maps to real-valued scalar outputs.<sup>1</sup> The function can be modeled as a random draw from a GP:

$$f \sim \mathcal{GP}(m,k),\tag{1}$$

where m is a mean function specifying the expected output of the function given input  $\mathbf{x}$ , and k is a kernel (or covariance) function specifying the covariance between outputs.

$$m(\mathbf{x}) = \mathbb{E}[f(\mathbf{x})] \tag{2}$$

$$k(\mathbf{x}, \mathbf{x}') = \mathbb{E}\left[ (f(\mathbf{x}) - m(\mathbf{x}))(f(\mathbf{x}') - m(\mathbf{x}')) \right].$$
(3)

Intuitively, the mean function encodes an inductive bias about the expected shape of the function, and the kernel encodes an inductive bias about the expected smoothness. To simplify exposition, we follow standard convention in assuming a prior mean of **0**.

Conditional on observed data  $\mathcal{D} = {\mathbf{x}_n, y_n}_{n=1}^N$ , where  $y_n \sim \mathcal{N}(f(\mathbf{x}_n), \sigma^2)$  is a noise-corrupted draw from the latent function, the posterior predictive distribution for a new input  $\mathbf{x}_*$  is Gaussian with mean and variance given by:

$$\mathbb{E}[f(\mathbf{x}_*)|\mathcal{D}] = \mathbf{k}_*^\top (\mathbf{K} + \sigma^2 \mathbf{I})^{-1} \mathbf{y}$$
(4)

$$\mathbb{V}[f(\mathbf{x}_*)|\mathcal{D}] = k(\mathbf{x}_*, \mathbf{x}_*) - \mathbf{k}_*^\top (\mathbf{K} + \sigma^2 \mathbf{I})^{-1} \mathbf{k}_*,$$
(5)

where  $\mathbf{y} = [y_1, \dots, y_N]^\top$ , **K** is the  $N \times N$  matrix of covariances evaluated at each pair of observed inputs, and  $\mathbf{k}_* = [k(\mathbf{x}_1, \mathbf{x}_*), \dots, k(\mathbf{x}_N, \mathbf{x}_*)]$  is the covariance between each observed input and the new input  $\mathbf{x}_*$ . See Appendix A for further technical details.

As pointed out by Griffiths, Lucas, Williams, and Kalish (2009) (see also Lucas et al. 2015), the predictive distribution can be viewed as an exemplar (similarity-based) model of function learning (DeLosh et al., 1997; McDaniel & Busemeyer, 2005), since it can be written

<sup>&</sup>lt;sup>1</sup>In general  $\mathcal{X}$  can be multidimensional and discrete, but in this paper we focus on functions with onedimensional, continuous inputs since these have received the most attention in the function learning literature.

## COMPOSITIONAL INDUCTIVE BIASES

9

as a linear combination of the covariance between past and current inputs:

$$f(\mathbf{x}_*) = \sum_{n=1}^{N} \alpha_n k(\mathbf{x}_n, \mathbf{x}_*),$$
(6)

where  $\alpha = (\mathbf{K} + \sigma^2 \mathbf{I})^{-1} \mathbf{y}$ . Equivalently, by Mercer's theorem any positive definite kernel can be expressed as an outer product of feature vectors:

$$k(\mathbf{x}, \mathbf{x}') = \sum_{d=1}^{\infty} \lambda_d \phi_d(\mathbf{x}) \phi_d(\mathbf{x}'), \tag{7}$$

where  $\{\phi_d(\mathbf{x})\}\$  are the eigenfunctions of the kernel and  $\{\lambda_d\}\$  are the eigenvalues. The posterior predictive mean is a linear combination of the features, which from a psychological perspective can be thought of as encoding "rules" mapping inputs to outputs (Carroll, 1963; Koh & Meyer, 1991). Thus, a GP can be expressed as both a similarity-based model and as a rule-based model, thereby unifying the two dominant families of function learning theories in cognitive science (Lucas et al., 2015).

#### Understanding human inductive biases with Gaussian processes

The GP theory provides insight into human inductive biases for functions, by making explicit the prior over functions. Intuitively, a GP favors functions that are "smooth" in a certain sense defined by the kernel function.<sup>2</sup> The critical question then is what kind of smoothness do humans prefer.

Experiments have begun to study this question. One experimental technique, known as *iterated learning*, estimates priors by simulating a Markov chain across multiple people—essentially a "game of telephone". Under certain assumptions, the Markov chain is guaranteed to converge to a stationary distribution, such that asymptotically it will generate samples from the prior (Griffiths & Kalish, 2007). In a function learning version of this task, participants see a set of points, which they then have to remember and re-draw. The resulting points are presented to another participant, who is asked to repeat the same procedure. Iterating this procedure multiple times will reveal participants' priors over functions. Kalish, Griffiths, and Lewandowsky (2007) showed that participants consistently converged to linear

<sup>&</sup>lt;sup>2</sup>A mathematically precise characterization of smoothness induced by a given kernel function is given by the theory of reproducing kernel Hilbert spaces (Schölkopf & Smola, 2002).

## COMPOSITIONAL INDUCTIVE BIASES

10

functions with a positive slope, even when the starting points came from a linear function with a negative slope, quadratic functions, or when they were generated at random.

Lucas et al. (2015) explained the iterated learning results by postulating a GP with a mixture of experts kernel that is mostly dominated by a positively linear kernel but can also generate smooth non-linear extrapolations by utilizing a non-linear radial basis function kernel. Additionally, their proposed kernel contained negatively linear and quadratic components. Samples from the GP parameterized in this way tend to be positively linear lines. This parametrization was able to explain a number of findings from the human function learning literature, such as the partitioning of the learning space, the linear-polynomial mixture-like patterns of extrapolations, and the difficulty of learning some functions (e.g., exponential patterns) relative to others (e.g., linear patterns).

Going further, Wilson, Dann, Lucas, and Xing (2015) attempted to infer the "human kernel" by having participants generate extrapolations for different functions sampled from a radial basis kernel and fitting a non-parametric kernel (the spectral mixture defined by Wilson & Adams, 2013, which we will describe in detail below) to their extrapolations. They found that participants expected long-distance correlations between points. These correlations could be viewed as arising from a mixture between linear and radial basis components<sup>3</sup>. In a second experiment, they showed that participants could effectively learn functions sampled from a mixture of a product of linear and spectral kernels.

These studies suggest that participants' represent complex functions as compositions of simpler ones. In the next section, we will motivate compositionality as a core principle of cognition, and then proceed to formalizing a fully compositional theory of function learning.

## Beyond smoothness: compositionality as a core principle of function learning

Humans can adapt to a wide variety of structural forms (Gershman & Niv, 2010; Kemp & Tenenbaum, 2009); the space of such forms is essentially unbounded, raising the question of how an infinite variety of forms can be represented. One approach (arguably the only tractable approach) is to define a compositional system that can build complex structures

<sup>&</sup>lt;sup>3</sup>A mixture of linear and radial basis function extrapolations can lead to longer-distance dependencies between points than a radial basis function alone.

## COMPOSITIONAL INDUCTIVE BIASES

11

through the composition of simpler elements. For example, in functional programming languages, functional primitives can be combined to create more complex functions which can then be re-combined to create even more complex functions (Peyton Jones, 1987). Via re-combinations, compositionality leads to a large increase of productivity—an infinite number of representations can be constructed from a finite set of primitives (Fodor, 1975; Fodor & Pylyshyn, 1988).

One source of evidence for compositionality in cognition comes from studies of rule-based concept learning. In these studies, the rules can be expressed as functions of logical primitives (e.g. Bruner, Goodnow, & George, 1956; Shepard, Hovland, & Jenkins, 1961). By studying participants' mistakes and the relative learning difficulty of different concepts, researchers tried to unravel the primitives of symbolic thought and how these primitives are combined. This work has led to a rich set of theoretical ideas and empirical constraints on compositionality in concept learning (Goodman et al., 2008; Lake et al., 2015; Nosofsky, Palmeri, & McKinley, 1994; Piantadosi et al., 2016).

Kemp (2012) provided an exhaustive characterization of compositionality in logical domains, showing how a "conceptual universe" can be formed by a rule inference scheme based on minimal description length that explains logical reasoning data across a wide set of domains. Recently, Piantadosi et al. (2016) showed how different sets of structural primitives, embedded in an approximate Bayesian inference framework, can predict distinct learning curves in rule-based concept learning experiments. Based on these and other studies, Lake et al. (2016) argued that compositionality is a necessary requirement for designing algorithms "that learn and think like people."

Given the widespread theoretical and empirical support for compositionality in cognitive science, it is natural to ask whether humans make use of compositionality in representing and learning about functions. With a few exceptions (Gershman, Malmaud, & Tenenbaum, 2016; Gershman, Tenenbaum, & Jäkel, 2016), prior work on function learning with GPs has assumed a fixed, non-compositional kernel<sup>4</sup>. Thus, our goal is to formalize a compositional approach to function learning and compare it to alternative non-compositional

<sup>&</sup>lt;sup>4</sup>This is also true for approaches utilizing a mixture of expert kernel, which is fixed *a priori*.

## COMPOSITIONAL INDUCTIVE BIASES

12

approaches. We accomplish this by positing two candidate kernel parametrizations that express conceptually different (compositional vs. non-compositional) inductive biases. We will then present a series of experimental tests that pit these kernels against each other.

## Structure learning with Gaussian processes

Broadly speaking, there are two approaches to parametrizing the kernel space: a fixed functional form with continuous parameters, or a combinatorial space of functional forms. These approaches are not mutually exclusive; indeed, the success of the combinatorial approach depends on optimizing the continuous parameters for each form. Nonetheless, this distinction is useful because it allows us to separate different forms of functional complexity. A function might have internal structure such that when this structure is revealed, the apparent functional complexity is significantly reduced. For example, a function composed of many piece-wise linear segments might have a long description length under a typical continuous parametrization (e.g., the radial basis kernel described below), because it violates the smoothness assumptions of the prior. However, conditional on the change-points between segments, the function can be decomposed into independent parts each of which is well-described by a simple continuous parametrization (see Lee & Yuille, 2006, for a discussion of how this strategy is used by the brain for early vision). If internally structured functions are "natural kinds", then the combinatorial approach may be a good model of human intuitive function representation.

In the rest of this section, we describe three kernel parametrizations. The first two are continuous, differing in their expressiveness. The third one is combinatorial, allowing it to capture complex patterns by composing simpler kernels. For all kernels, we take the standard approach of choosing the parameter values that optimize the log marginal likelihood (see Appendix for details).

## **Radial basis kernel**

The radial basis kernel is a commonly used kernel in machine learning applications, embodying the assumption that the covariance between function values decays exponentially

## COMPOSITIONAL INDUCTIVE BIASES

13

with input distance:

$$k(\boldsymbol{x}, \boldsymbol{x}') = \theta^2 \exp\left(-\frac{|\boldsymbol{x} - \boldsymbol{x}'|^2}{2l^2}\right),$$
(8)

where  $\theta$  is a scaling parameter and l is a length-scale parameter determining the speed of the decay over the distance between inputs. This kernel assumes that the same smoothness properties apply globally for all inputs. It provides a standard baseline to compare with more expressive kernels.

# Spectral mixture kernel

The second approach is based on the fact that any stationary kernel<sup>5</sup> can be expressed as an integral using Bochner's theorem. Letting  $\tau = x - x' \in \mathbb{R}^P$ , then

$$k(\boldsymbol{\tau}) = \int_{\mathbb{R}^P} e^{2\pi i \boldsymbol{S}^\top \boldsymbol{\tau}} \psi(\mathbf{d}\boldsymbol{s}).$$
(9)

If  $\psi$  has a density S(s), then S is the spectral density of k; S and k are thus Fourier duals (Rasmussen & Williams, 2006, see Appendix). This means that a spectral density over the kernel space fully defines the kernel and that furthermore every stationary kernel can be expressed as a spectral density. Wilson and Adams (2013) showed that the spectral density can be approximated by a mixture of Q Gaussians, such that

$$k(\boldsymbol{\tau}) = \sum_{q=1}^{Q} w_q \prod_{p=1}^{P} \exp\left(-2\pi^2 \tau_p^2 v_q^p\right) \cos\left(2\pi \tau_p \mu_q^{(p)}\right),$$
(10)

where the *q*th component has mean vector  $\mu_q = (\mu_q^{(1)}, \ldots, \mu_q^{(P)})$  and a covariance matrix  $\mathbf{M}_q = \operatorname{diag}(v_q^{(1)}, \ldots, v_q^{(P)})$ . The result is a flexible and expressive parametrization of the kernel, in which complex kernels are approximated by mixtures of simpler ones. Further technical details can be found in Appendix B.

This approach is appealing when simpler kernels (e.g., the radial basis function) fail to capture functional structure. Its main drawback is that because structure is captured implicitly via the spectral density, the building blocks are psychologically less intuitive: humans appear to have preferences for linear (Kalish et al., 2007) and periodic (Bott & Heit, 2004) functions, which are not straightforwardly encoded in the spectral mixture (though of course the mixture

<sup>&</sup>lt;sup>5</sup>A stationary kernel is a function of  $\mathbf{x} - \mathbf{x}'$ . Thus, it is invariant to translation of the inputs.

#### COMPOSITIONAL INDUCTIVE BIASES

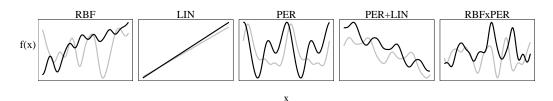
14

can approximate these functions). Since the spectral kernel has been successfully applied to reverse engineering human kernels (Wilson et al., 2015), it is a useful reference of comparison to more structured compositional approaches.

## **Compositional kernel**

As positive semi-definite kernels are closed under addition and multiplication, we can create richly structured and interpretable kernels from well-understood base components. For example, by summing kernels, we can model the data as a sum of independent functions. Imagine a function that is linearly increasing over time but also shows some seasonal periodicity; then a combination of a linear and a periodic kernel added together might be a good description of that function.

Figure 1 shows an example of how different kernels (radial basis, linear, periodic) can be combined. Our approach, following Duvenaud et al. (2013), is to define a simple grammar over kernels that generates new kernels through summation or multiplication of simpler kernels. Table 1 summarizes the kernels used in our grammar. Given a set of input-output pairs, the task facing the learner is to identify both the function and an underlying parse tree. As with the other kernel parametrizations, the parse tree is chosen to maximize the marginal likelihood.



*Figure 1*. Examples of base and compositional kernels. The base kernels are radial basis (**RBF**), linear (**LIN**), and periodic (**PER**); the composition operators are addition and multiplication. Adding a periodic and a linear kernel creates functions with trends and seasonality. Multiplying a periodic kernel with a radial basis kernel results in more localized periods than a standard periodic kernel would be able to capture.

Many other compositional grammars are possible. For example, we could have included a more diverse set of kernels, and other composition operators (e.g., convolution, scaling) that

## COMPOSITIONAL INDUCTIVE BIASES

15

### Table 1

Base kernels in the compositional grammar.

Name	Definition
Linear	$k(oldsymbol{x},oldsymbol{x'})=(oldsymbol{x}- heta_1)(oldsymbol{x'}- heta_1)$
Radial basis	$k(oldsymbol{x},oldsymbol{x}')= heta_2^2\exp\left(-rac{(oldsymbol{x}-oldsymbol{x}')^2}{2 heta_3^2} ight)$
Periodic	$k(oldsymbol{x},oldsymbol{x}') =  heta_4^2 \exp\left(-rac{2\sin^2(\pi oldsymbol{x}-oldsymbol{x}'  heta_5)}{ heta_6^2} ight)$

generate valid kernels. However, we believe that our simple grammar is a useful starting point, since the components are intuitive and likely to be psychologically plausible. For tractability, we fix the maximum number of combined kernels to be 3 and do not allow for repetition of kernels in order to restrict the complexity of the inference. The complete set of resulting kernels is shown in Table 2.

### **Experiment 1a: Pattern completions of compositional functions**

Our first experiment examined whether participants prefer compositional over non-compositional predictions of functions if the ground truth is indeed compositional. Although this mainly tells us whether people make predictions in accordance with the underlying structure (i.e., it is not informative about inductive biases *per se*), Experiment 1b will examine the case where the ground truth is non-compositional.

We used a "pattern completion" paradigm, motivated by prior research on pattern perception as a window into cognitive representations (e.g., Buffart, Leeuwenberg, & Restle, 1981; Kanizsa, 1979). Participants chose among 3 different completions of a partial one-dimensional function.<sup>6</sup> The candidate completions were generated by the different structure learning approaches described above. Our hypothesis was that if participants have structured, compositional representations of functions, then they should prefer pattern completions generated from the compositional kernel.

<sup>&</sup>lt;sup>6</sup>This is essentially a form of extrapolation judgment, but unlike typical extrapolation paradigms that test inputoutput pairs one at a time, pattern completion asks participants to consider a set of input-output pairs.

## COMPOSITIONAL INDUCTIVE BIASES

16

### Table 2

Kernel combinations in the compositional grammar and their interpretations.

Combination	Interpretation		
Linear	Linear function		
Radial basis	Locally smooth function		
Periodic	Repeated pattern		
Linear + Periodic	Linear trend plus repeated pattern		
Linear + RBF	Linear trend plus local deviations		
RBF + Periodic	Repeated pattern plus local deviations		
Linear $\times$ Periodic	Repeated pattern with increasing amplitude		
Linear $\times$ RBF	Local deviations with increasing amplitude		
$RBF \times Periodic$	Slowly changing repeated pattern		
Linear + RBF + Periodic	Linear trend plus local deviations plus repeated pattern		
$Linear + Periodic \times RBF$	Linear trend plus slowly changing repeated pattern		
$\text{Periodic} + \text{Linear} \times \text{RBF}$	Repeated pattern plus local deviations with increasing amplitude		
Linear $\times$ RBF $\times$ Periodic Slowly changing repeated pattern with increasing amplitude of the state of the s			

# Methods

**Participants.** 52 participants (29 women) with an average age of 36.15 (SD = 9.11) were recruited via Amazon Mechanical Turk and received \$1 for their participation.

**Design.** We sampled 20 different functions from a Gaussian process parametrized by various compositional kernels within an input space of  $x = [0, 0.1, 0.2, \dots, 10]$ . Afterwards, the functional outputs for  $x_{\text{learn}} = [0, 0.1, 0.2, \dots, 7]$  were used as a training set to which all three approaches were fitted and then used to generate predictions for the test set  $x_{\text{test}} = [7.1, 7.2, \dots, 10]$ . The hyper-parameters of the radial basis kernel as well as the number of components and the hyper-parameters of the spectral mixture kernel were fitted by optimizing the marginal likelihood given the training set. The best prediction of the compositional kernel approach was found by choosing the composition from the grammar that produced the best marginal likelihood (following Duvenaud et al., 2013, see Appendix). All of

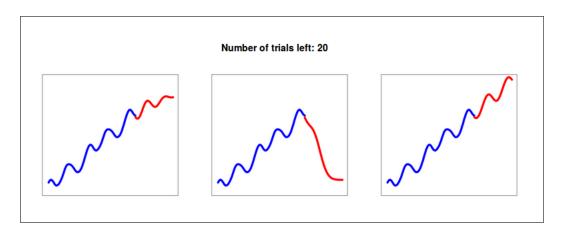
## COMPOSITIONAL INDUCTIVE BIASES

17

the models were only fitted to the training set (the observed input-output pairs) and used to complete the patterns (predict the functions) for the test inputs.

The different mean predictions were then used to generate 3 plots (one for every kernel approach) that showed the given input as a blue curve and the new predictions (the extrapolation pattern) as a red curve. The procedure was repeated for 20 different compositions, each corresponding to a separate trial.

**Procedure.** Participants were asked to select one of 3 extrapolations (pattern completions) they thought best completed a given function (Figure 2). The position at which a kernel's predictions appeared was randomized on every trial.

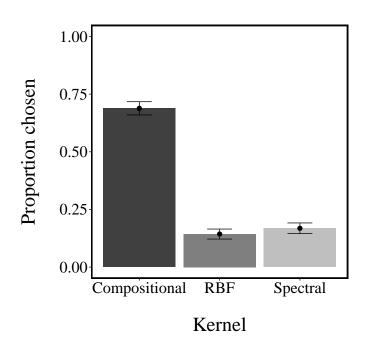


*Figure 2*. Screen shot of Experiment 1a. Pattern completions (shown in red) were generated by a spectral mixture (left), a radial basis (middle), and a compositional kernel (right).

### **Results and discussion**

Participants chose the compositional completions on 69% of the trials, the spectral mixture completions on 17%, and the radial basis completions on 14% (Figure 3). Overall, the compositional completions were chosen significantly more often than the other two completions ( $\chi^2 = 591.2$ , p < 0.01). The results thus supported our hypothesis that participants will prefer compositional pattern completions when the ground truth is compositional.

COMPOSITIONAL INDUCTIVE BIASES



*Figure 3*. Experiment 1a results: proportion of pattern completion choices for three kernels. Error bars represent the standard error of the mean.

## **Experiment 1b: Pattern completions of non-compositional functions**

While the results of Experiment 1a suggest a preference for compositionally structured functions, they do not indicate whether humans have an inductive bias for such functions, since the results are perfectly compatible with the possibility that participants adapted to the ground truth structure without a compositional inductive bias. In Experiment 1b, we subject our theory to a stronger test, measuring pattern completion preferences when the ground truth is non-compositional (specifically, functions drawn from a GP with the spectral mixture kernel). If participants prefer compositional completions in this experiment, we can be more confident that the preference for such functions arises from an inductive bias.

#### Methods

**Particpants.** 65 participants (mean age=30, SD = 9.84, 31 male) were recruited from Amazon's Mechanical Turk web service and received \$0.5 for their participation.

**Design.** The design was identical to the one used in Experiment 1a, apart from the fact that in this experiment the underlying functions were sampled from a GP with the spectral

19

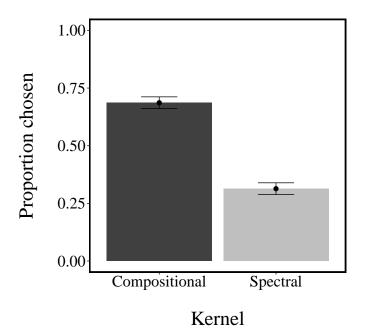
## COMPOSITIONAL INDUCTIVE BIASES

mixture kernel parametrized with a randomly assigned number of components (sampled uniformly between 2 and 5). We also only generated completions for the compositional and the spectral kernel in this experiment. We did not generate completions for the radial basis kernel because in some cases these completions corresponded closely to predictions of the compositional kernel. This correspondence arose due to the fact that there was not much compositional structure for the compositional kernel to capture in samples from the spectral mixture kernel.

**Procedure.** The procedure was as described in Experiment 1a, with the one difference that participants made choices between two (rather than three) completions.

## **Results and discussion**

As in Experiment 1a, participants chose compositional completions more frequently than non-compositional (spectral mixture) completions (68% vs. 32%,  $\chi^2 = 172.8$ , p < 0.01; Figure 4). This finding is consistent with the claim that human inductive biases for functions are compositional—and sufficiently strong to induce preference for compositional completions even when the ground truth is non-compositional.



*Figure 4*. Experiment 1b results: proportions of pattern completion choices. Error bars represent the standard error of the mean.

## COMPOSITIONAL INDUCTIVE BIASES

20

### Markov chain Monte Carlo with people

In our next set of experiments, we sought to elicit samples from the posterior predictive distribution over functions in order to gain finer-grained insight into the subjective representation of functions. We accomplished this using a technique called *Markov chain Monte Carlo with People* (MCMCP; Sanborn, Griffiths, & Shiffrin, 2010). This technique asks participants to accept or reject proposed hypotheses, effectively simulating a Markov chain whose stationary distribution is the prior over hypotheses. In our experiments, we condition on a training set and ask participants to choose between completions (as in Experiments 1a and 1b); thus the stationary distribution is the posterior predictive distribution over pattern completions.

If the proposal distribution is symmetric (the probability of proposing a new state  $x^*$  from the current state x is the same as the probability of proposing x from  $x^*$ ), then one psychologically plausible acceptance function is Barker's acceptance function:

$$A(x^*, x) = \frac{\pi(x^*)}{\pi(x^*) + \pi(x)},$$
(11)

where  $\pi(x) \propto P(x)$ . Letting  $\mathcal{D}$  indicate the training set, this leads to the following expression for the acceptance function in our experiments:

$$A(x^*, x) = \frac{p(x^*|\mathcal{D})}{p(x^*|\mathcal{D}) + p(x|\mathcal{D})}$$
(12)

which corresponds to Luce's choice rule, the most common model for discrete choice distributions in psychology. Thus, under fairly standard assumptions about the choice process, we can elicit samples from the desired distribution.

#### **Experiment 2a: Compositional ground truth**

In the first MCMCP experiment, we sampled the underlying functions from compositional kernels in order to see if the posterior over compositional completions converges to patterns that match the underlying kernel.

### COMPOSITIONAL INDUCTIVE BIASES

21

### Methods

**Design.** We generated completions from all possible kernel combinations (up to a maximum of 3 combined kernels), optimizing each kernel's hyper-parameters on the training set and then generating the completions for the extrapolation set. On each trial, participants chose between their most recently accepted extrapolation and a new proposal.

Eight different functions were sampled from various compositional kernels, the input space was split into training and test sets, and then all kernel combinations were used to generate completions for the test set. Proposals were sampled uniformly from this set. We mainly focused on combinations containing linear and periodic components, as these provide more interesting structure than the smoothness induced by samples from the radial basis kernel.

**Participants.** 51 participants (27 male) with an average age of 32.55 (SD = 8.21) were recruited via Amazon's Mechanical Turk web service and paid \$1.

**Procedure.** There were 8 blocks of 30 trials, where each block corresponded to a single extrapolation set. The order of the blocks was randomized for each participant.

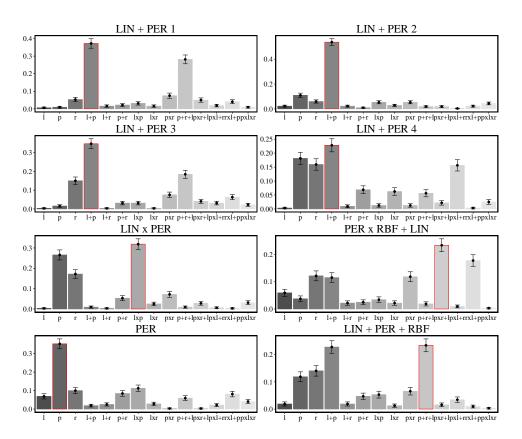
### **Results and discussion**

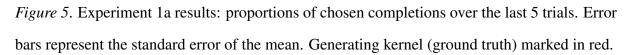
We calculated the average proportion of accepted kernels over the last 5 trials, as shown in Figure 5. The first 25 trials were excluded to avoid trials on which participants might not have converged yet to their subjective posterior extrapolations, a process commonly called "burn-in".

In all cases, participants' subjective probability distribution over completions placed the greatest mass on the data-generating kernel (marked in red). Furthermore, we observed a strong rank correlation between the true posterior probability over completions and participants' subjective distribution ( $\rho = 0.91$ , p < 0.01). Thus, participants approximately converged to the true posterior when the functions were generated from compositional kernels.

22

## COMPOSITIONAL INDUCTIVE BIASES





### **Experiment 2b: Real-world functions**

The second MCMCP experiment assessed what structures people converged to when faced with real-world data, where the ground truth is unknown. We hypothesized that real-world data is often intrinsically compositional (see Duvenaud et al., 2013), and hence human inductive biases may be adapted to such functions.

**Participants.** 51 participants with an average age of 32.55 (SD = 12.14) were recruited via Amazon Mechanical Turk and received \$1 for their participation.

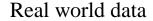
**Procedure.** We used four real-world time series (Figure 6): airline passenger data, volcano CO2 emission data, the number of gym memberships over 5 years, and the number of times people googled the band "Wham!" over the last 8 years. Some of these functions have been extensively analyzed in the time series modeling literature and all of them showed interesting patterns a priori. Participants were not told any information about the data sets

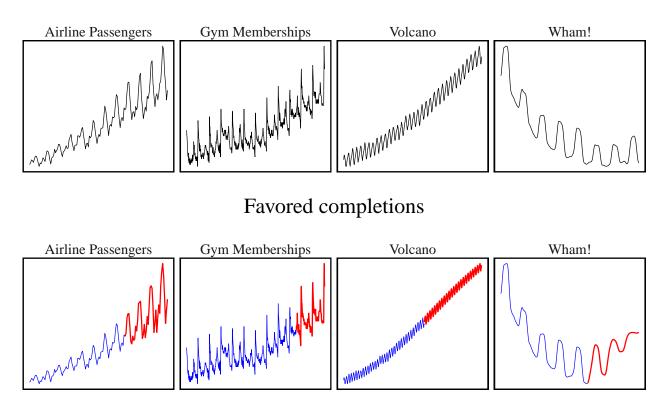
## COMPOSITIONAL INDUCTIVE BIASES

23

(including input and output descriptions); they were simply shown the unlabeled input-output pairs in the experiment.

The input space was split into training (75% of the data) and test sets (25% of the data), and then all kernel combinations were fitted to the training set and used to generate completions for the test set. Proposals were sampled uniformly from this set. As periodicity in the real world is rarely ever purely periodic, we adapted the periodic component of the grammar by multiplying a periodic kernel with a radial basis kernel, thereby locally smoothing the periodic part of the function.<sup>7</sup> Apart from the different training sets, the procedure was identical to Experiment 2a.





*Figure 6*. (Top) Real-world data sets used in Experiment 2b. Descriptions and origin of the data were unknown to participants. (Bottom) Participants were shown the region in blue; most frequently selected completions are shown in red.

<sup>&</sup>lt;sup>7</sup>See the following page for an example: http://learning.eng.cam.ac.uk/carl/mauna.

24

#### COMPOSITIONAL INDUCTIVE BIASES

**Results and discussion.** Results (again taken from the last 5 trials) are shown in Figure 7, demonstrating that participants converged to intuitively plausible patterns. In particular, for both the volcano and the airline passenger data, participants converged to compositions resembling those found in previous analyses Duvenaud et al. (2013). The most frequently chosen completions for each data set are shown in Figure 7. The rank correlation between the subjective distributions and the posterior over completions was significantly positive ( $\rho = 0.83$ , p < 0.01), supporting the hypothesis that the compositional pattern completions capture human inferences about functions.

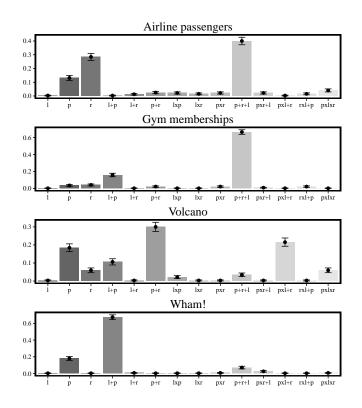


Figure 7. Experiment 2b results: proportions of chosen predictions over last 5 trials.

#### **Experiment 3: Manual pattern completion**

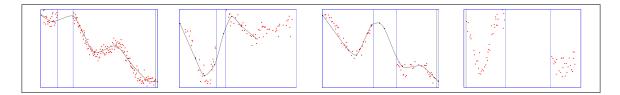
In our previous experiments, we asked participants to make choices between a discrete set of pattern completions. In our next experiment, we measured pattern completion in a less constrained task, by having participants draw the pattern completions manually (see Cox, Kachergis, & Shiffrin, 2012, for related work).

### COMPOSITIONAL INDUCTIVE BIASES

25

# Methods

**Design.** On each round of the experiment, functions were sampled from the compositional grammar, the number of points to be presented on each trial was sampled uniformly between 100 and 200, and the noise variance was sampled uniformly between 0 and 25. Finally, the size of an unobserved region of the function (for completion) was sampled to be of a size between 5 and 50. Participants were asked to manually draw the function best describing the observed data and to complete this function within the observed and unobserved regions. A screen shot of the experiment is shown in Figure 8.



*Figure 8*. Screen shots of manual pattern completions (Experiment 3). The unobserved region (for completion) is delimited by vertical lines.

**Participants.** 36 participants with a mean age of 30.5 (SD = 7.15) were recruited from Amazon Mechanical Turk and received \$2 for their participation.

**Procedure.** Participants were asked to draw lines in a cloud of dots that they thought best described the given data. To facilitate this process, participants placed black dots into the cloud, which were then automatically connected by a black line based on a cubic Bezier smoothing curve (see Forrest, 1972). They were asked to place the first dot on the left boundary and the final dot on the right boundary of the graph. In between, participants were allowed to place as many dots as they liked (from left to right) and could remove previously placed dots. There were 50 trials in total. The dots were sampled from a function that was in turn sampled from a kernel chosen at random out of all possible combinations in our compositional grammar.

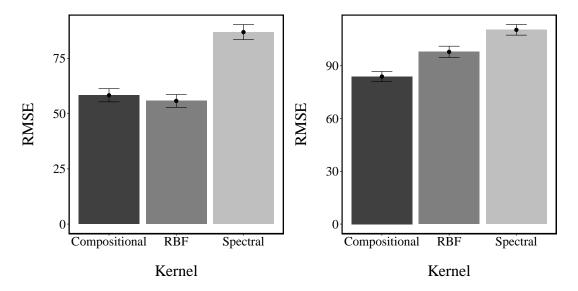
#### **Results and discussion**

We assessed the average root mean squared distance between participants' predictions (the line they drew) and the mean predictions of each kernel given the data points participants

26

## COMPOSITIONAL INDUCTIVE BIASES

had seen, for both interpolation and extrapolation areas. Again, we optimized the parameters for the radial basis kernel and the number of components as well as the parameters for the spectral mixture kernel by optimizing the log marginal likelihood. Predictions of the compositional kernel were also generated by choosing the composition that produced the best marginal log-likelihood given the presented dots. Results are shown in Figures 9.



*Figure 9*. Experiment 3 results: average root mean squared error for interpolation (left) and extrapolation (right) drawings. Error bars show standard error of the mean.

The mean distance between the model predictions and participants' drawings was significantly higher for the spectral mixture kernel than for the compositional kernel in both interpolation (86.96 vs. 58.33, t(1291.1) = -6.3, p < 0.001) and extrapolation areas (110.45 vs 83.91, t(1475.7) = 6.39, p < 0.001). The radial basis kernel produced similar distances as the compositional kernel in interpolation (55.8), but predicted participants' drawings significantly worse in extrapolation areas (97.9, t(1459.9) = 3.26, p < .01). As extrapolation is normally seen as the best criterion to judge between different models of function learning (DeLosh et al., 1997), the difference in extrapolation judgments provides further evidence for the compositional kernel model.

## **Generating comparison functions**

One potential concern with the previous experiments is that compositional and non-compositional functions may differ in terms of low-level perceptual characteristics, and

## COMPOSITIONAL INDUCTIVE BIASES

these differences (rather than the hypothesized high-level structural differences) are driving the behavioral effects. To address this concern, we need a set of non-compositional functions whose low-level perceptual characteristics are matched with a set of compositional functions.

We generated 500 functions from both compositional and non-compositional kernels. The compositional functions were sampled randomly from our compositional grammar by first randomly sampling a kernel composition and then sampling a function from that kernel, whereas the non-compositional functions were sampled from the spectral mixture kernel, where the number of components was varied between 2 and 6 uniformly. We then calculated the standardized spectral entropy (or "forecastability") for each function, following Goerg (2013):

$$\Omega(f) = 1 - \frac{H(f)}{\ln(2\pi)} \tag{13}$$

27

where  $H(\cdot)$  is the Shannon entropy of the function's normalized spectral density  $S_f$  (see Appendix C for details),

Forecastability can be seen as a measure of how well future output values of a function can be predicted. It takes values between 0% and 100%, representing the proportional reduction in entropy a given function achieves relative to white noise. Although forecastability technically assumes stationary functions, it has also been shown to produce reliable measures for non-stationary functions in practice (Hyndman, Wang, & Laptev, 2015). Of the 500 non-compositional functions that we generated, we selected those that had a forecastability of higher than 20%, but set the maximum predictability for the compositional kernel functions to be less than 40 and the minimum predictability for the spectral mixture kernel functions to be higher than 40%. This means that theoretically the functions generated from the spectral mixture kernel are more forecastable on average (i.e., contain lower entropy in their spectral density) than the functions sampled from the compositional kernel. Because of this forecastability advantage for non-compositional functions, behavior consistent with the compositional kernel predictions would provide especially strong evidence for our framework.

We verified that all of the functions were matched in terms of low level visual properties, as measured by a similarity measure based on the discrete wavelet Haar transform (Montero, Vilar, et al., 2014, see Appendix C). The basic idea of this similarity measure is to

28

## COMPOSITIONAL INDUCTIVE BIASES

replace the original series by its wavelet approximation coefficients at an appropriate scale, and then to measure similarity between the wavelet coefficients. Specifically, we ranked each function based on its wavelet similarity to other functions and selected the top functions (20 compositional and 20 spectral) from this set. These functions, which are used in the experiments reported below, are shown in Figures 10 and 11. We will subsequently refer to these functions as the "matched set."

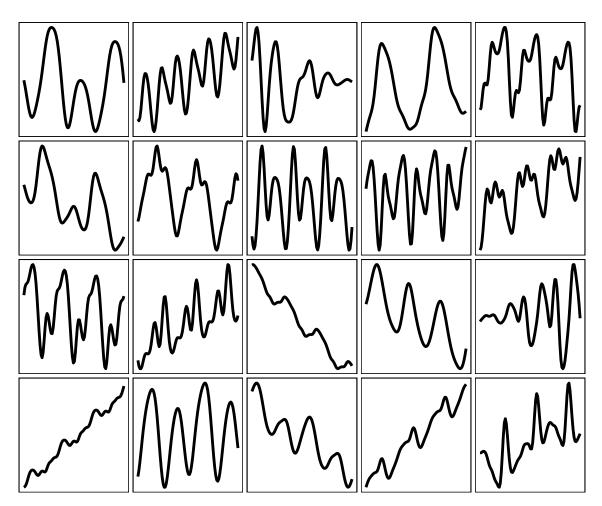


Figure 10. Sampled compositional functions.

# **Experiment 4: Assessing predictability**

If human inductive biases for functions are inherently compositional, then compositional functions should be perceived as more *predictable*.<sup>8</sup> In our previous work

<sup>&</sup>lt;sup>8</sup>Predictability is closely related to forecastability, insofar as both measures can be characterized in terms of the eigenspectrum (Sollich, 2001). Here we focus on predictability since it has a more intuitive interpretation.

29

#### COMPOSITIONAL INDUCTIVE BIASES

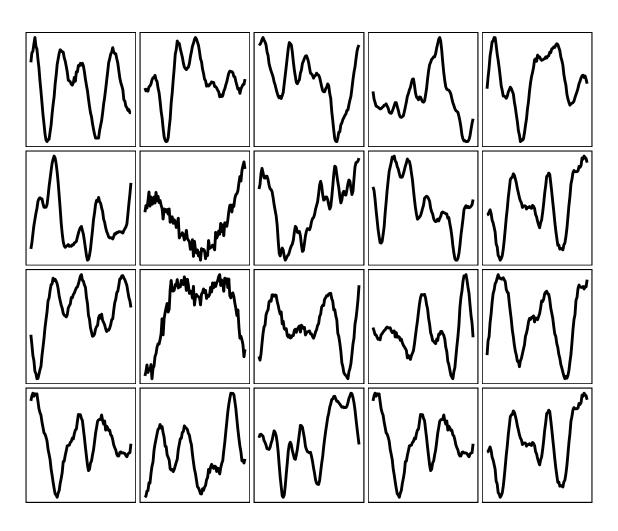


Figure 11. Sampled spectral mixture functions.

(Schulz, Tenenbaum, Reshef, Speekenbrink, & Gershman, 2015), we operationalized predictability in terms of generalization error. Intuitively, more predictable functions should lead to lower generalization error on new inputs. This analysis identified several key factors determining the predictability of a function; specifically, predictability increases with sample size and smoothness, and decreases with noise.

Here we posit compositionality as another key factor. If inductive biases for functions are compositional, then we expect such functions to be perceived as more predictable. We assess this by collecting both absolute and relative measures of subjective predictability.

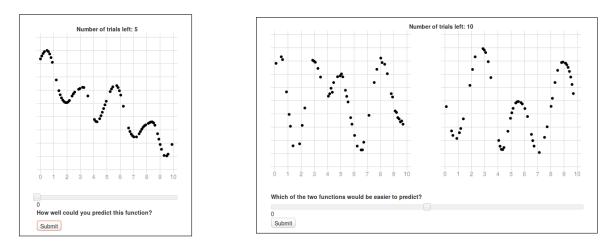
### Methods

**Participants.** 50 participants (mean age=32, SD=7.2; 32 males) were recruited via Amazon Mechanical Turk and received \$0.5 for their participation.

30

#### COMPOSITIONAL INDUCTIVE BIASES

**Procedure.** On each trial, one of the "matched" functions defined above was randomly subsampled with a sample size  $n_j$  was drawn uniformly from  $\{50, 60, \ldots, 100\}$ . Participants were asked to judge how well they thought they could predict a newly sampled input point for the function on a scale ranging from 0 (not at all) to 100 (very well). After judging the subjective predictability for all 40 of the matched functions in a randomized order, participants then had to make pairwise comparisons between compositional and non-compositional functions from -100 (function presented on the left is definitely easier to predict) to 100 (function presented on the right is definitely easier to predict). As with the absolute predictability judgments, the sample size  $n_j$  was varied randomly, with the constraint that both functions had the same sample size. Screen shots of the two tasks are shown in Figure 12.



*Figure 12*. Screen shots of the two predictability judgment tasks (Experiment 4). (Left) Absolute predictability judgments. (Right) Relative predictability judgments.

#### **Results and discussion**

As shown in Figure 13, we found that compositional functions were perceived as more predictable (mean predictability judgment=55.92) than non-compositional functions (mean predictability judgment=37.88, t(998) = 14.96, p < 0.001). Moreover, the predictability judgments for compositional judgments were more strongly correlated with sample size (r = 0.28, p < 0.001) compared to predictability judgments for non-compositional functions (r = 0.18, p < 0.001).

To analyze these results further, we fit a regression model of subjective predictability

### COMPOSITIONAL INDUCTIVE BIASES

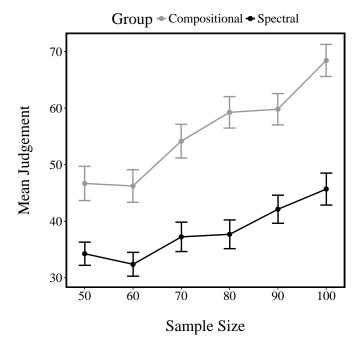


Figure 13. Mean predictability judgments. Error bars represent the standard error of the mean.

with two predictors: samples size and a dummy variable indicating whether or not a presented function was compositional. The results of this analysis, summarized in Table 3, demonstrate main effects of both compositionality and sample size.

The relative predictability judgments tell a similar story (Figure 14). As with the absolute judgments, compositional functions were perceived to be more predictable relative to non-compositional functions (t(499) = 13.502, p < 0.001), and this difference increased with sample size (r = 0.14, p < 0.001).

To understand how subjective probability judgments match theoretical predictability, we approximated the generalization error using the average squared error for a randomly sampled new input point. We computed this approximation for every sample that a participant saw under different kernel choices: linear, RBF, spectral mixture, or a compositional kernel. To generate predictions from each kernel, we chose the hyper-parameters (including the composition for the compositional kernel) that maximized the log marginal likelihood. Figure 15 shows the average correlation between the each kernel's generalization error and participants' predictability judgments, averaged over all trials and participants.

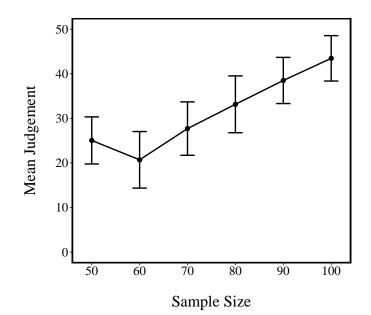
The spectral mixture kernel (t-test against a correlation of 0: t(49) = -2.351, p < 0.05),

## COMPOSITIONAL INDUCTIVE BIASES

#### Table 3

Regression model of predictability judgments. Overall model fit:  $R^2 = 0.17$ .

	Estimate	Std. Error	t-value	<b>Pr(&gt; t )</b>
Intercept	13.06	3.50	3.72	0.0002
Compositional	17.44	1.53	11.39	0.0000
Sample size	0.34	0.04	7.42	0.0000



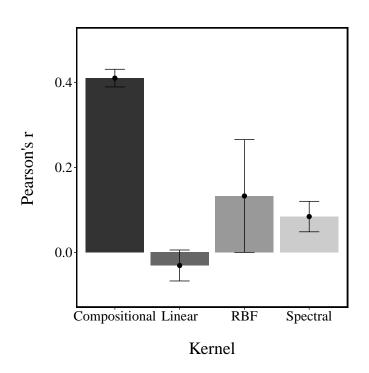
## **Direct Comparison**

*Figure 14*. Relative predictability judgments. Positive values indicate that the compositional function was judged to be more predictable than the non-compositional function. Error bars represent the standard error of the mean.

the compositional kernel (t(49) = -19.73, p < 0.001) as well as the RBF kernel (t(49) = -4.3, p < 0.01) all described participants' judgments better than chance. The linear (t(49) = 0.846, p > 0.1) kernel did not predict participants' judgments better than chance. Crucially, the compositional kernel predicted judgments significantly better than the spectral mixture kernel (t(98) = -7.86, p < 0.001).

In summary, compositional functions were perceived as more predictable, even though they were generated to be theoretically less "forecastable" than the non-compositional functions sampled from the spectral mixture kernel. The generalization error produced by the

COMPOSITIONAL INDUCTIVE BIASES



*Figure 15*. Model fit for predicting participants' predictability judgments by using the models' average generalization error. As smaller generalizations error should theoretically lead to higher predictability judgments. Therefore, negative correlations imply good model fit. Error bars represent the standard error of the mean.

compositional structure learning approach matched participants' predictability judgments more closely than any of the alternative models.

## **Experiment 5: Traditional function learning paradigm**

The experiments presented so far have mostly focused on visual pattern completions, either by choosing completions in forced choice or MCMCP tasks or by manual pattern completions. However, psychological experiments on function learning have traditionally focused on a different task, in which participants produce output predictions given inputs presented one at a time. For example, Carroll (1963) asked participants to predict the height of one bar given another bar's height. After each prediction, participants received feedback about how close their prediction was to the actual output.

We sought to compare compositional and non-compositional functions using the traditional function learning paradigm. Additionally, we used this as an opportunity to assess which account of function learning best captures participants' trial-by-trial learning.

### COMPOSITIONAL INDUCTIVE BIASES

34

#### Methods

**Participants.** 46 participants (mean age=31, SD=11; 30 males) were recruited via Amazon Mechanical Turk and received \$0.5 for their participation.

**Procedure.** Participants were asked to predict an output indicated by the height of a red bar given the current input indicated by the height of a blue bar (Figure 16). On each trial, they saw the current input (a blue bar) and had to indicate their predictions by adjusting the height of an orange bar using a slider. After submitting their prediction, the actual output appeared marked as a red bar directly next to the orange bar. Additionally, participants also saw the actual numbers of the current input, their prediction and –after they submitted their predictions– the output, as well as the difference between their prediction and the actual output. It was explicitly stated to participants that the input is related to the output by an underlying function and that they had to learn that function in order to produce the smallest possible difference between their predictions and the outputs.

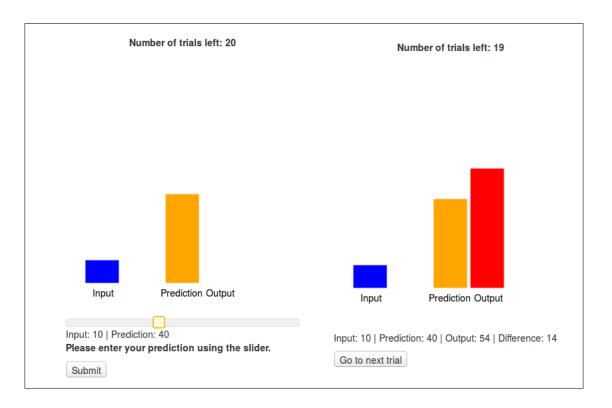
Participants learned 4 different functions over 4 blocks. Each block consisted of 20 trials (input-output pairs). The input was randomly sampled to be within 0 and 100, and the output was also transformed to range between 0 and 100. Out of the 4 different functions participants had to learn, 2 were sampled from the set of matched compositional functions and 2 were sampled from the set of matched non-compositional functions.

# **Results and discussion**

On average, participants' predictions were more accurate for the compositional functions than for the non-compositional functions (t(269) = 2.5, p < 0.05), as shown in Figure 17. Performing a linear regression with the absolute difference between participants' predictions and the actual outputs as the dependent variable and a factor variable encoding whether or not the underlying function was compositional as well as the trial number (how many predictions participants had made before) resulted in the model summarized in Table 4.

Participants clearly improved over the course of each block, as evidenced by the main effect of trial. Even though compositional functions are on average predicted more easily  $(\beta = -1.56)$ , this effect turned out to be rather small, perhaps because both compositional and

### COMPOSITIONAL INDUCTIVE BIASES



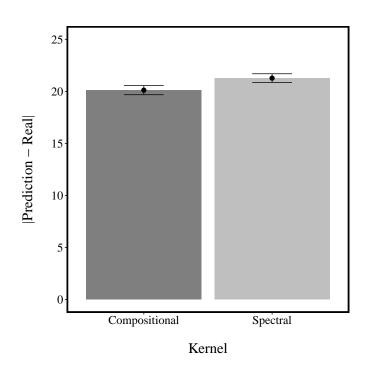
*Figure 16*. Screen shots of the input-output learning experiment. The height of the blue bar indicates the input. The height of the orange output marks the prediction and can be adjusted by using the slider. After the prediction was submitted, the actual output, marked by the height of the red bar, appeared and participants were told the absolute difference between their prediction and the actual outcome.

non-compositional functions are non-linear, which are notoriously hard to learn in the traditional function learning paradigm (Byun, 1995) and also because they were created to be quite similar when we designed the matched set.

To further disentangle the different models, we created the trial-by-trial predictions for the linear, compositional, spectral mixture and RBF kernels, and assessed how well each model's predictions for the n + 1 trial after having seen n outputs matched participants' predictions. As shown in Figure 18, the compositional kernel described participants' predictions best (r = 0.54, p < 0.01) followed by the linear kernel (r = 0.21, p < 0.01). The correlation for both the RBF kernel (r = 0.03) and the spectral mixture kernel did not differ significantly from zero (r = 0.04). Thus, the compositional kernel appears to provide a substantially better account of trial-by-trial learning in the traditional function learning

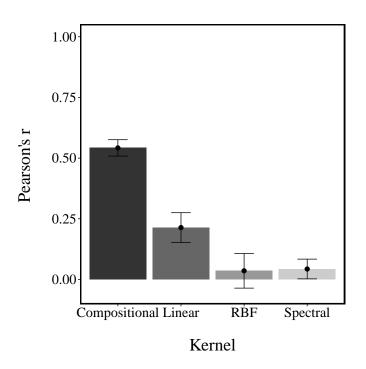
35

### COMPOSITIONAL INDUCTIVE BIASES



*Figure 17*. Mean difference between predictions and outcomes for compositional and spectral kernel in Experiment 5. Error bars represent the standard error of the mean.

paradigm.



*Figure 18.* Model fit (Pearson correlation coefficient) for predicting participants' next predictions given the current input over all trials. Error bars represent the standard error of the mean.

## COMPOSITIONAL INDUCTIVE BIASES

Trial

37

### Table 4

	Estimate	Std. Error	t value	Pr(> t )
Intercept	23.01	0.72	32.02	0.0000
Compositional	-1.56	0.62	-2.52	0.0118

-0.30

*Regression model of the traditional function learning paradigm. Overall model fit:*  $R^2 = 0.14$ .

## **Experiment 6: Assessing numerosity**

0.0535

-5.65

0.0000

In our next series of experiments, we explore the broader implications of compositional function representation for 3 domains of cognition: numerosity perception, change detection, and short-term memory. We begin with a standard numerosity judgment task, in which participants estimate the number of dots appearing briefly on a screen. Zhao and Yu (2016) showed that, in the absence of explicit grouping cues, structured configurations of dots led to lower estimates compared to random configurations. This effect of structure on perceived numerosity appears to arise from the fact that dots belonging to structured configurations are more likely to be perceptually grouped together; these groups then become the units which are enumerated. In a related study, Zhao, Ngo, McKendrick, and Turk-Browne (2011) showed that the accuracy of numerosity judgments improves when statistical regularities are removed, indicating a direct relationship between statistical learning and numerosity perception.

If compositional functions are perceived as more "structured" than non-compositional functions (as suggested indirectly by our predictability experiment), then a natural hypothesis is that dot configurations generated from compositional functions will be perceived as less numerous. We tested this prediction using a standard numerosity judgment task.

## Methods

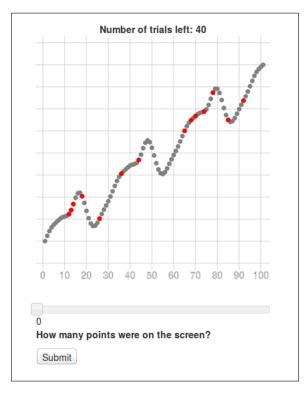
**Participants.** 91 participants (mean age=37.84, SD=7.87, 48 female) were recruited via Amazon Mechanical Turk and received \$0.5 for their participation.

**Procedure.** Each participant completed a total of 40 trials. On each trial, participants were presented with a function drawn from the set of matched functions, discretely sampled

38

#### COMPOSITIONAL INDUCTIVE BIASES

into 100 equidistant gray dots on the screen. This configuration was displayed for one second, after which the dots vanished. Out of the 100 dots, n = [5, 6, 7, ..., 15] randomly selected dots were marked as red. Participants were asked to estimate the number of red dots (between 0 and 20) after all the dots had vanished. A screen shot of the experiment is shown in Figure 19.



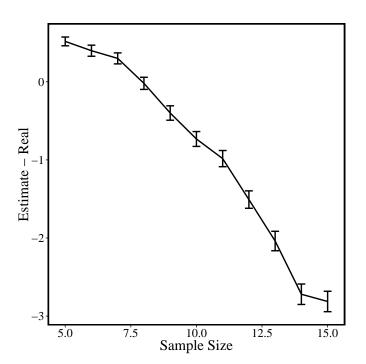
*Figure 19.* Screen shot of the numerosity experiment. Dots stayed on the screen for 1000ms and then vanished before the slider could be used.

#### **Results and discussion**

Figure 20 shows the effect of the number of dots on participants' numerosity judgments, averaged over both compositional and non-compositional functions, demonstrating that increasing the number of red dots led to greater underestimation of the actual number, consistent with the idea that perceived numerosity diminishes as structure becomes more discernible.

We hypothesized that participants would underestimate the red dots if they were superimposed on more structured functions (functions sampled from a compositional kernel) as compared to relatively unstructured functions (sampled from the spectral mixture kernel). Figure 21 shows the direct comparison of numerosity estimates for compositional and

COMPOSITIONAL INDUCTIVE BIASES



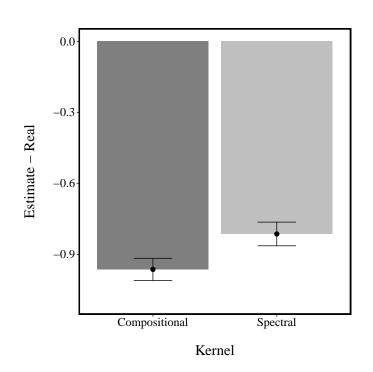
*Figure 20*. Mean difference between presented and estimated number of red dots over number of shown dots. Error bars represent the standard error of the mean. As more red dots are presented, participants tend to under-estimate the actual number more.

non-compositional patterns. Overall, participants underestimated the number of dots more for compositional than for non-compositional patterns (-0.74 vs. -0.53, t(38) = -2.2, p < 0.05), consistent with our hypothesis.

We performed a regression analysis to account for both the number of dots and the function type. The results (presented in Table 5) showed that with an increasing number of red dots, participants showed a stronger tendency to underestimate numerosity ( $\beta = -0.39$ ). Additionally, we found a main effect of function type ( $\beta = -0.17$ ). There was no interaction effect between the number of red dots and function type ( $\beta = -0.02$ ).

Taking together, our results indicate that perceived numerosity is reduced to a greater extent by compositional functions compared to non-compositional functions, a finding that agrees with the results of Zhao and Yu (2016): structural regularity distorts the units of perception, making them appear less numerous. Even though the non-compositional functions we used were in fact structured (as measured by forecastability), they produced a weaker effect on numerosity relative to compositional functions, arguably because their structure is

COMPOSITIONAL INDUCTIVE BIASES



*Figure 21*. Comparative judgments. Lower values mean that participants underestimated the number of red dots. Error bars represent the standard error of the mean.

less "intuitive" (i.e., they lack the inductive bias needed to easily perceive this structure).

#### **Experiment 7: Change detection with functions**

We next examined whether compositional structure influences change detection performance (Pashler, 1988; Rouder, Morey, Morey, & Cowan, 2011). In a typical change detection paradigm, participants judge whether two stimuli presented rapidly in sequence are the same or different. It has been suggested that structured representations facilitate change detection by allowing a summary representation of the stimulus to be stored in short-term memory (Brady & Tenenbaum, 2013). When the stimulus consists of multiple items, those items that are not assimilated into the summary representation are encoded as "outliers". However, because memory is capacity-limited, only a small number of outliers can be encoded. Thus, the summary representation frees up encoding resources for specific items. The more structure in the display that can be encoded, the more resources will be available for encoding specific items.

The critical question concerns the nature of this structure—what are the inductive biases that constrain short-term memory representations? Brady and Tenenbaum (2013) used

## COMPOSITIONAL INDUCTIVE BIASES

## Table 5

	Estimate	Std. Error	t-value	<b>Pr(&gt; t )</b>
Intercept	3.23	0.12	27.631	<2e-16
Number of dots	-0.39	0.01	-35.845	<2e-16
Compositional	-0.17	0.07	-2.43	0.015
Compositional × Number of dots	-0.02	0.02	-0.76	0.446

Parameter estimates from numerosity judgments regression analysis.

Markov random fields to encode information about object features; several other structural assumptions have been explored in the literature (Lew & Vul, 2015; Mathy & Feldman, 2012; Orhan & Jacobs, 2013). Here we explore the possibility that the representation of functions in short-term memory is compositional, leading to the prediction that change detection will be more accurate with compositional functions compared to with non-compositional functions.

# **Participants**

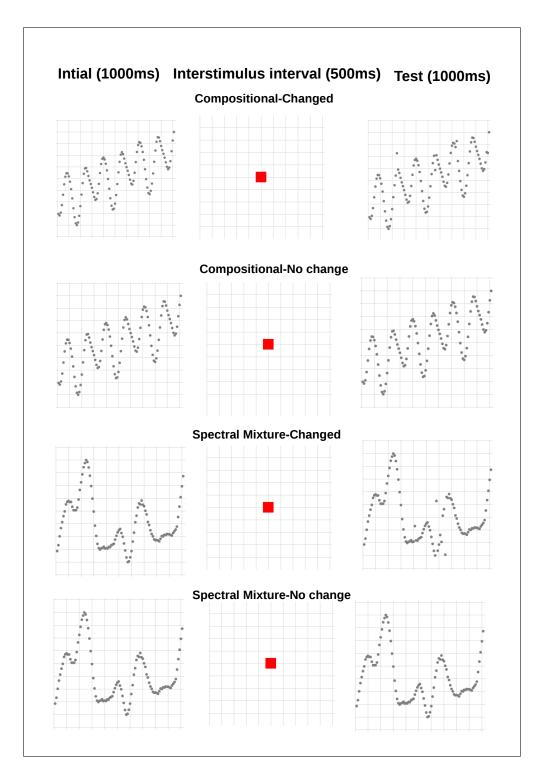
80 participants (mean age=30, SD=8.2, 42 males) were recruited from Amazon Mechanical Turk and received \$0.5 for their participation.

# Procedure

Participants judged whether or not two consecutively displayed patterns were the same or different (Figure 22). As in the numerosity experiment, we used functions from the matched set (20 compositional, 20 non-compositional) and displayed them on the screen as 100 horizontally equidistant gray dots. On each trial, participants saw the original structure for 1000ms, followed by an interstimulus interval (500ms) and then a test probe (1000ms). Unbeknownst to participants, the probe had a 50% chance of being same or different. Change probes were constructed by randomly selecting  $N \in \{2, 3, \dots, 5\}$  dots and permuting them (under the constraint that no point ends up at the same position as before).

# COMPOSITIONAL INDUCTIVE BIASES

42



*Figure 22.* Schematic of change detection task. Initial stimulus was presented for 1000ms, drawn either from the compositional or from the non-compositional (spectral mixture) set. After an interstimulus interval (500ms), a test probe was presented and participants had to make a same/different judgment.

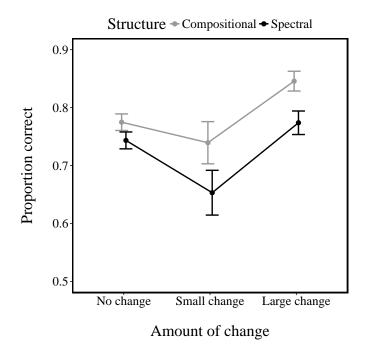
## COMPOSITIONAL INDUCTIVE BIASES

43

# **Results and discussion**

Participants responded correctly on 82% of no-change trials for the compositional functions and on 81% of the no-change trials for the non-compositional functions. Thus, there was no significant difference in correct rejection rate for the two types of functions  $(\chi^2 = 0.21, p > 0.05)$ . However, 77% of the changed compositional functions were correctly identified as having changed, whereas that proportion was only 67% for the changed non-compositional functions. Therefore, change is more easily detected for compositional functions  $(\chi^2 = 12.13, p < 0.001)$ .

We created an indicator variable that was set to 1 if a participant responded correctly, and 0 otherwise. Figure 23 shows the mean proportions of correct responses for compositional and non-compositional trials across different levels of change: "no change", "small change" (between 1 and 2 dots permuted) and "large change" (between 3 and 5 dots permuted). This analysis demonstrated that change detection performance was superior for compositional across levels of change.



*Figure 23*. Proportion of correctly detected changes. Participants were more likely to detect changes in compositional functions. Error bars represent the standard error of the mean.

In order to quantitatively capture these results, we developed a Bayesian theory of

## COMPOSITIONAL INDUCTIVE BIASES

functional change detection. Let  $\mathcal{D}_1$  and  $\mathcal{D}_2$  denote the first and second stimuli (input-output pairs), respectively, and let  $f_1$  and  $f_2$  denote the corresponding functions. The task facing participants is to determine the posterior probability that the two functions are different:

$$P(f_1 \neq f_2 | \mathcal{D}_1, \mathcal{D}_2) = \frac{P(\mathcal{D}_1, \mathcal{D}_2 | f_1 \neq f_2)}{P(\mathcal{D}_1, \mathcal{D}_2 | f_1 \neq f_2) + P(\mathcal{D}_1, \mathcal{D}_2 | f_1 = f_2)},$$
(14)

44

where for simplicity we have assumed that the prior probability of change is 0.5. The change  $(f_1 \neq f_2)$  likelihood is given by:

$$P(\mathcal{D}_1, \mathcal{D}_2 | f_1 \neq f_2) = \int_{f_1} P(\mathcal{D}_1 | f_1) P(f_1) df_1 \int_{f_2} P(\mathcal{D}_2 | f_2) P(f_2) df_2,$$
(15)

and the no-change  $(f_1 = f_2)$  likelihood is given by:

$$P(\mathcal{D}_1, \mathcal{D}_2|f_1 = f_2) = \int_f P(\mathcal{D}_1|f) P(\mathcal{D}_2|f) P(f) df.$$
(16)

We used this probabilistic model to make trial-by-trial predictions of performance on the change detection task. As in our other analyses, we chose hyper-parameters that optimized the marginal likelihood for a given kernel. For the spectral kernel, we treated the number of mixture components as a free hyper-parameter (ranging from 1 to 6).

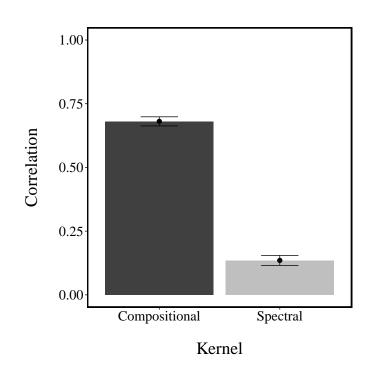
To allow for noise in the decision process, we modeled the binary responses using a logistic function of the model predictions, with separate predictors for compositional and non-compositional predictions. The results of this logistic regression are summarized in Table 6. The compositional model was a significant predictor of human change detection performance ( $\beta = 0.0122$ , p < 0.001), whereas the spectral mixture model was only marginally predictive (p = 0.05).

Table 6

Result of cha	inge d	etection l	logistic	regression.
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	Estimate	Std. Error	z value	Pr(> z )
Intercept	1.3018	0.0918	14.19	0.0000
Compositional prediction	0.0122	0.0006	19.61	0.0000
Spectral mixture prediction	0.0012	0.0006	1.95	0.0517

COMPOSITIONAL INDUCTIVE BIASES



*Figure 24*. Mean point biserial correlation between model predictions and participants' responses in the change detection task. Error bars represent the standard error of the mean.

To show this result in a different way, we computed the point biserial correlation between the model predictions and human responses (Figure 24). The average correlation for the compositional model was significantly higher than the average correlation for the spectral mixture model (r = 0.68 vs. r = 0.15, t(132) = 20.5, p < 0.001).

In summary, we found that changes are more easily detected in compositional functions compared to non-compositional functions, consistent with the idea that compositional functions are more efficiently encoded into a summary representation. Moreover, a GP theory of change detection with a compositional kernel allowed us to quantitatively predict human change detection performance.

# **Experiment 8: Compositional chunking in short-term memory**

The results of Experiment 7 suggested that change detection is facilitated by compositional summary representations. A closely related idea is that structural regularities increase memory capacity because they are "compressible" (Brady, Konkle, & Alvarez, 2011; Mathy & Feldman, 2012). For example, if multiple items can be chunked together, then a greater number of items can be stored in memory (Miller, 1956). Chunking has been posited

## COMPOSITIONAL INDUCTIVE BIASES

46

as the basis of exceptional expert memory (Chase & Simon, 1973; Gobet & Simon, 1998) and story comprehension (Thorndyke, 1977).

In our next experiment, we pursue this idea further, asking whether compositional functions are more compressible (and hence more memorable) than non-compositional functions. We used a standard short-term memory task (the Sternberg paradigm; Sternberg et al., 1966), in which participants are shown a rapid sequence of items (functions in this case) followed by an old/new judgment of a probe item. This task additionally allowed us to measure the interplay between compositionality and set size.

# Methods

**Participants.** 133 participants (mean age=31.05, SD=8.19, 71 male) were recruited via Amazon Mechanical Turk and received \$0.5 for their participation.

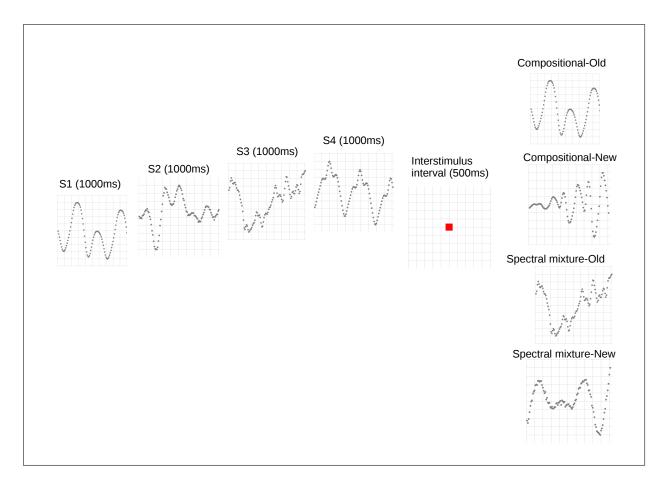
**Procedure.** Participants were shown between 2 and 6 functions sampled randomly from the matched set. Each function appeared on the screen for 1000ms. A 500ms intertrial interval succeeded the final item, followed by a probe item. Participants were asked to judge as quickly as possible whether the probe item was old (i.e., appeared in the preceding set) or new. There were 15 trials in total (3 trials for each set size). The probe was randomly selected to be either compositional or non-compositional, and probes were old on half of the trials. A schematic of the experiment is shown in Figure 25.

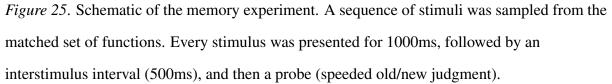
# **Results and discussion**

We excluded 23 participants who failed to respond correctly for more than half of the trials, and removed all trials that took longer than 5 seconds or less than 500ms.

Participants responded correctly on 77.8% of the compositional probes and on 66.7% of the non-compositional probes—a significant difference in accuracy ( $\chi^2 = 14.252, p < 0.001$ ). This result can be decomposed further into a 75% hit rate for compositional probes, compared to a 67% hit rate for the non-compositional probes (a significant difference between hit rates:  $\chi^2 = 5.19, p < 0.05$ ). Finally, there was also a significant difference between the correct rejection rate (78% for compositional probes vs. 65% for non-compositional probes;  $\chi^2 = 8.87, p < 0.01$ ).

## COMPOSITIONAL INDUCTIVE BIASES





To disentangle compositionality and set size, we ran a logistic regression to predict the probability of a correct response from compositionality (i.e., compositional vs. non-compositional probe) and set size factors. As shown in Table 7, the probability of responding correctly decreases with set size ( $\beta = -0.22$ ), and compositional probes are more likely to be correctly identified ( $\beta = -0.37$ ). We also found a significant interaction, whereby the compositional advantage decreases with set size ( $\beta = -0.18$ ; Figure 26). This might be due to an increased guessing rate that could potentially obscure the compositional advantage.

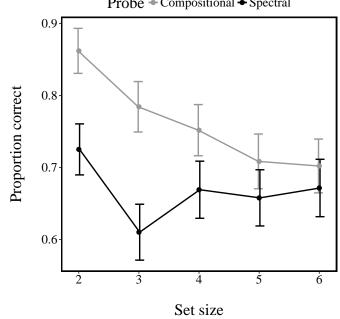
We next developed a Bayesian model of performance in the task, adapting the same basic framework that we applied to the change detection task. A participant is exposed to a study list (sequence of independent input-output datasets), denoted by  $\mathcal{D}_{1:N}$ , generated by underlying functions  $f_{1:N}$ . The task is to compute the posterior probability that a new dataset

# COMPOSITIONAL INDUCTIVE BIASES

# Table 7

Results of logistic regression analysis of the memory experiment.

	Estimate	Std. Error	z-value	<b>Pr</b> (>  <b>z</b>  )
Intercept	2.04	0.29	7	<2.57e-12
Set size	-0.22	0.06	-3.33	< 0.001
Compositional	1.24	0.37	3.33	< 0.001
Set size $\times$ Compositional	- 0.18	0.08	2.2	0.02



Probe - Compositional - Spectral

Figure 26. Proportion of correctly identified probes as a function of set size. Error bars represent the standard error of the mean.

(the test probe), denoted by  $\mathcal{D}'$ , was generated by one of the functions in the study list:

$$P(f' \in f_{1:N}|Y) = \sum_{n=1}^{N} P(f' = f_n | \mathcal{D}_n, \mathcal{D}')$$
(17)

$$\propto \sum_{n=1}^{N} P(f'=f_n) P \mathcal{D}_n, \mathcal{D}' | f'=f_n).$$
(18)

Following the structure of the experiment, we will assume that the probability of an "old" trial,  $\sum_{n=1}^{N} P(f' = f_n)$ , is 0.5. The marginal likelihood is given by:

$$P(\mathcal{D}_n, \mathcal{D}'|f' = f_n) = \int_f P\mathcal{D}_n |f_n = f) P(\mathcal{D}'|f' = f) P(f) df.$$
(19)

## COMPOSITIONAL INDUCTIVE BIASES

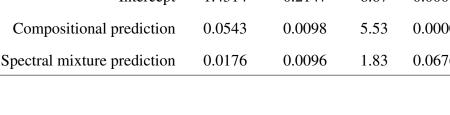
Our general optimization procedure is the same as described in the change detection model.

We entered the model predictions for both the compositional and spectral mixture models into a logistic regression to predict participant's old/new responses. Results of the logistic regression analysis are summarized in Table 8. Only the compositional model was a significant predictor of responses ( $\beta = 0.054$ , p < 0.001), whereas the spectral mixture model was not a significant predictor ( $\beta = 0.01, p = 0.07$ ).

# Table 8

	Estimate	Std. Error	z value	Pr(> z )
Intercept	1.4314	0.2147	6.67	0.0000
Compositional prediction	0.0543	0.0098	5.53	0.0000
Spectral mixture prediction	0.0176	0.0096	1.83	0.0676

Results of logistic regression analysis of the memory experiment.



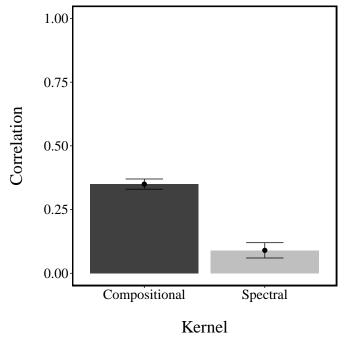


Figure 27. Mean point biserial correlation for the compositional and the spectral mixture models. Error bars represent the standard error of the mean.

Finally, we calculated the correlation between each model's predictions and participants' responses. As shown in Figure 27, the compositional model produced a superior correlation

50

compared to the non-compositional model (r = 0.35 vs. r = 0.09; t(262) = 9.97, p < 0.001).

We conclude that compositional functions are more easily remembered than non-compositional functions in a version of the Sternberg task. Participants' old/new judgments were well-captured by a Bayesian model of short-term memory that used a compositional kernel.

#### **General discussion**

In this paper, we pursued the hypothesis that human inductive biases for functional pattern recognition are compositionally structured—that is, humans prefer to represent complex functions as compositions of simpler building blocks. We formalized this idea using a compositional kernel within a Gaussian Process regression framework, and assessed human inductive biases across a diverse range of experiments. The first set (Experiments 1, 2, 3 and 5) attempted to directly measure inductive biases using extrapolation and interpolation judgments, finding that participants preferred compositional over non-compositional pattern completions. The second set of experiments examined the broader implications of compositionality, finding that compositional functions are perceived as more predictable (Experiment 4) and memorable (Experiment 8) compared to non-compositional functions. Furthermore, discrete displays of items are perceived as less numerous (a signature of statistical regularities; Experiment 6), and changes in such displays are more easily detected (Experiment 7). Taken together, our experimental findings provide strong support for the compositional hypothesis.

## **Related work**

The work presented here is connected to several lines of previous work. Most relevant are the seminal work of Griffiths et al. (2009) and Lucas et al. (2015) on Gaussian processes for function learning in general, and Wilson et al. (2015) more recent attempts to reverse-engineer the human kernel using a non-parametric kernel in particular. We see our work as complementary to this research. If we want to find out how people perceive and reason about functional structure then we need both a bottom-up theory to describe how

# COMPOSITIONAL INDUCTIVE BIASES

51

people make sense of structure as well as a top-down method to indicate what the final structure might look like when represented as a kernel.

Our approach here also ties together neatly with past attempts to model compositional structure in other cognitive domains. Of course, language (e.g., Chomsky, 1965) and object perception (e.g., Biederman, 1987) have long traditions of emphasizing compositionality. More recently, these ideas have been extended to other domains. For example, Gershman, Tenenbaum, and Jäkel (2016) showed how hierarchical motion perception could be understood as a kind of vector analysis, using compositional GPs to model the combination of motion flow fields. This approach has also been applied to decision making; Gershman, Malmaud, and Tenenbaum (2016) used GPs to model utility functions over tree-structured objects (e.g., meals in a restaurant). In both motion perception and decision making, simpler non-compositional models failed to explain human performance.

## Limitations and future directions

While our experiments established the importance of compositional representations for functional pattern recognition, we do not believe that we have fully characterized the base functions and composition architecture. We restricted our framework to a small number of components primarily for practical purposes. Thus, an important direction for future work will be to systematically investigate the boundaries of function composition. Fortunately, the GP formalism can accommodate a wide variety of compositional structures (Duvenaud et al., 2013), so we expect that this task can be accomplished without deviating too far from the analytical framework laid out in this paper.

There are many other potential implications of compositional inductive biases for functions. For example, these inductive biases could shape active learning (i.e., tasks in which participants can choose the next data point). We believe that active learning model comparisons constitute an interesting framework to pit the structured and unstructured approaches against each other (Parpart, Schulz, Speekenbrink, & Love, 2015).

Related issues arise in reinforcement learning tasks, where agents must balance exploration and exploitation. Such tasks have already been modeled using GPs (Schulz,

# COMPOSITIONAL INDUCTIVE BIASES

52

Konstantinidis, & Speekenbrink, 2016), suggesting their amenability to analysis with compositional kernels. This approach could also be applied to designing nonparametric value function approximators, which have been proposed as cognitively and neurally plausible solutions to reinforcement learning problems (Gershman & Daw, 2015). New experiments will be required to discern whether reinforcement learning exploits compositional inductive biases.

Finally, the development of compositional inductive biases for functions is another important and open question. Very little is known in general about the development of function learning. The studies described in this paper could potentially be run in children, which would provide insight into the origin of compositional inductive biases.

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# COMPOSITIONAL INDUCTIVE BIASES

59

## Appendix A

## **Gaussian Process Inference**

In the case that there is only one test point  $x_*$ , the posterior mean  $f_*$  can be calculated as:

$$f_* = k_*^\top (K + \sigma_n^2 I)^{-1} y, \tag{20}$$

where  $k_* = k(x_*, X)$  and K = k(X, X). The posterior variance of the prediction is given by:

$$\mathbb{V}[f_*] = k(x_*, x_*) - k_*^\top (K + \sigma_n^2 I)^{-1} k_*.$$
(21)

The marginal likelihood is given by integrating over the latent function f:

$$p(y|x) = \int p(y|f, X)p(f|X)df.$$
(22)

The log marginal likelihood for a GP with hyper-parameters  $\theta$  is given by:

$$\log p(y|X,\theta) := -\frac{1}{2}y^{\top}(K + \sigma_n^2 I)^{-1}y - \frac{1}{2}\log|K + \sigma_n^2 I| - \frac{n}{2}\log 2\pi.$$
 (23)

where the dependence of K on  $\theta$  is left implicit. The hyper-parameters are chosen to maximize the log-marginal likelihood, using gradient-based optimization.

# COMPOSITIONAL INDUCTIVE BIASES

### Appendix B

# Spectral mixture kernel

# **Bochner's theorem**

A stationary kernel is a function of  $\tau = x - x'$ . A complex-valued function k on  $\mathbb{R}^P$  is the covariance function of a weakly stationary mean-square continuous complex-valued random process on  $\mathbb{R}^P$  if and only if it can be represented as:

$$k(\tau) = \int_{\mathbb{R}^P} e^{2\pi i s^{\top} \tau} \psi(ds)$$
(24)

where  $\psi$  is a positive finite measure. The density S(s) of  $\psi$  is called the spectral density of k; k and S are Fourier duals:

$$k(\tau) = \int S(s)e^{2\pi i s^{\top} \tau} ds$$
(25)

$$S(s) = \int k(\tau) e^{-2\pi i s^{\top} \tau} d\tau$$
(26)

Therefore, every kernel can also be represented by a distribution over the spectral density space.

# Mixture of Gaussians spectral kernel

Our treatment of the spectral kernel follows Wilson et al. (2015), and we refer the reader to that paper for more details. The spectral density modeled with a single Gaussian can be expressed as:

$$\phi(s,\mu,\sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\{-\frac{1}{2\sigma^2}(s-\mu)^2\}$$
(27)

$$S(s) = \frac{1}{2} [\phi(s) - \phi(-s)]$$
(28)

The resulting kernel is given by:

$$k(\tau) = \exp\{-2\pi^{2}\tau^{2}\sigma^{2}\}\cos(2\pi\tau\mu)$$
(29)

Extending this result to a mixture of Q Gaussians results in:

$$k(\tau) = \sum_{q=1}^{Q} w_q \prod_{p=1}^{P} \exp\{-2\pi^2 \tau_p^2 v_q^{(p)}\} \cos(2\pi \tau_p \mu_q^{(p)})$$
(30)

60

61

where the *q*th component has the mean  $\mu_q = (\mu_q^{(1)}, \dots, \mu_q^{(p)})$  and covariance matrix  $M_q = \text{diag}(v_q^{(1)}, \dots, v_q^{(p)})$ , where the inverse mean represents the component periods and the

inverse standard deviation the length scales.

## COMPOSITIONAL INDUCTIVE BIASES

62

## Appendix C

# Details on generation of comparison functions

## Forecastibility

The Shannon entropy of a function f can be measured by the uncertainty of its spectrum  $S_f$ :

$$H(f) = -\int_{-\pi}^{\pi} S_f(\lambda) \ln S_f(\lambda) d\lambda$$
(31)

For any stationary function,

$$H(f) \le H(\text{white noise})$$
  
=  $-\int_{-\pi}^{\pi} \frac{1}{2\pi} \ln \frac{1}{2\pi} d\lambda$   
=  $\ln 2\pi$ , (32)

with equality if and only if f is white noise, the least forecastable signal with a uniform spectrum. The forecastibility measure  $\Omega(f)$  is then defined as

$$\Omega(f) = 1 - \frac{H(f)}{\ln(2\pi)}.$$
(33)

We follow Goerg (2013) and estimate  $\Omega(f)$  by first estimating the spectrum  $S_f$ , normalizing it so that it integrates to 1, and then plugging it back into Eq. 31. We use the periodogram as an unbiased estimator of  $S_f$  (see Goerg, 2013, for details).

# Wavelet transform similarity measure

A discrete wavelet Haar Transform performs a scale-wise decomposition of the time series in such a way that most of the energy of the time series can be represented by a few coefficients. The main idea is to replace the original series by its wavelet approximation coefficients a in an appropriate scale, and then to measure the dissimilarity between the wavelet approximations. A detailed description of wavelet methods for time series analysis can be found in Percival and Walden (2006). We used the R-package TSclust (Montero et al., 2014) to find the appropriate scale of the transform. We then measured the dissimilarity between two series  $x_1$  and  $x_2$  by the Euclidean distance at the selected scale:

$$d(x_1, x_2) = ||\mathbf{a}_1 - \mathbf{a}_2||$$