A Formal Theory of Compositionality

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Abstract

Compositionality is believed to be fundamental to intelligence. In humans, it underlies the structure of thought, language, and higher-level reasoning. In AI, compositional representations can enable a powerful form of out-of-distribution generalization, in which a model systematically adapts to novel combinations of known concepts. However, while we have strong intuitions about what compositionality is, there currently exists no formal definition for it that is measurable and mathematical. Here, we propose such a definition, which we call *representational compositionality*, that accounts for and extends our intuitions about compositionality. The definition is conceptually simple, quantitative, grounded in algorithmic information theory, and applicable to any representation; for instance, it assigns a single scalar quantifying the compositionality of a representation in some intermediate layer of a trained neural network. Intuitively, representational compositionality states that a compositional representation satisfies three properties. First, it must be expressive. Second, it must be possible to redescribe the representation as a function of discrete symbolic sequences, analogous to sentences in natural language. Third, the function that relates these symbolic sequences to the representation—analogous to semantics in natural language—must be simple. Through experiments on both synthetic and real world data, we validate our definition of compositionality and show how it unifies disparate intuitions from across the literature in both AI and cognitive science. We also show that representational compositionality, while theoretically intractable, can be readily estimated using standard deep learning tools. Our definition has the potential to inspire the design of novel, theoretically-driven models that better capture the mechanisms of higher-level human thought, just as formal definitions in other areas of science have traditionally enabled technological breakthroughs.

Keywords compositionality, complexity, deep learning, representation, generalization

1 Introduction

Compositionality is thought to be one of the hallmarks of human cognition. In the domain of language, it lets us produce and understand utterances that we have never heard before, giving us "infinite use of finite means" (Chomsky, 1956). Beyond this, one of the most influential ideas in cognitive science is the *Language of Thought* hypothesis (Fodor, 1975; Quilty-Dunn et al., 2023), which conjectures that *all* thought involved in higher-level human cognition is compositional. Indeed, recent evidence from neuroscience supports the Language of Thought hypothesis and suggests that it is core to human intelligence (Dehaene et al., 2022).

Compositionality has been equally influential in AI, right from its very genesis when approaches relied on symbolic models with structured, rule-based semantics. While "Good Old-Fashioned AI" has largely given way to deep learning, the idea that compositionality is central to intelligence has remained, motivating efforts in neurosymbolic AI (Garcez and Lamb, 2023; Marcus, 2003; Sheth et al., 2023), probabilistic program inference (Ellis et al., 2023; Lake et al., 2017), modular deep neural networks Andreas et al. (2016); Bengio (2017); Goyal and Bengio (2022); Goyal et al. (2021, 2020); Pfeiffer et al. (2023); Schug et al. (2024), disentangled representation learning (Ahuja et al., 2022; Brehmer et al., 2022; Higgins et al., 2017; Lachapelle et al., 2022; Lippe et al., 2022; Sawada, 2018), object-centric learning (Locatello et al., 2020; Singh et al., 2023; Wu et al., 2024), and chain-of-thought reasoning (Hu et al., 2024; Kojima et al., 2022; Wei et al., 2022), to name only a few. One of the primary appeals of compositionality is that it enables a powerful form of out-of-distribution generalization, aptly named *compositional generalization* (Lake and Baroni,

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2018). If a model is compositional with respect to a set of features in its training data, it need not observe all possible combinations of those features in order to generalize to novel ones (Bahdanau et al., 2019; Mittal et al., 2021; Schug et al., 2024; Wiedemer et al., 2024, 2023). For instance, if a vision model's representations are compositional with respect to foreground objects and background scenes, then it should be able to meaningfully represent an image of "a cow on a beach" at inference time after having only observed cows and beaches separately at training time.

Despite its importance, compositionality remains an elusive concept: there is currently no formal, quantitative definition of compositionality that could be used to measure it. It is often described in the following way (Szabó, 2022):

Definition 1 (*Compositionality – colloquial*)

The meaning of a complex expression is determined by its structure and the meanings of its constituents.

In the context of neural representations in brains or deep neural networks (DNNs), we can take these "meanings" to be high-dimensional vectors of activations. While satisfying on some level, this definition lacks formal rigour and breaks down upon inspection.

First, the definition presupposes the existence of a symbolic "complex expression" associated to each meaning. In some cases, this makes sense; for instance, we can consider human languages and the neural representations they elicit. But where do these expressions and their constituent parts come from when considering neural representations themselves such as in the Language of Thought hypothesis, where thoughts are encoded in distributed patterns of neural activity?

Second, it is unclear what the expression's "structure" should be. The definition is motivated from human language, where sentences have syntactic parses and individual words have types (e.g., noun, verb, etc.), but these properties are not intrinsic to the sentences themselves, which are simply strings.

Third, the definition says that meaning is "determined by" the structure and meanings of the constituents through a semantics function, but it does not put any kind of restriction on these semantics for the meanings to qualify as compositional: any function qualifies. For instance, functions that *arbitrarily* map constituents to their meanings (as in the case of idioms like "he kicked the bucket") are functions nonetheless and thus satisfy Definition 1, but it is commonly agreed that they are not compositional (Mabruroh, 2015; Swinney and Cutler, 1979; Weinreich, 1969).

Finally, the colloquial definition of compositionality suggests that it is a binary property of representations, when it should arguably be a matter of degree. For instance, while linguists often model the syntax and semantics of language using hierarchical decompositions that are considered compositional (Chomsky, 1956), human language regularly deviates from this idealization. In particular, language has some degree of context-sensitivity, where the meanings of words depend on those of others in the sentence. Thus, human language does not satisfy the colloquial binary definition of compositionality, even though it is considered largely compositional.

The colloquial definition of compositionality is thus flawed if we wish to formalize and measure it quantitatively, moving beyond mere intuitions that are fundamentally limited in their explanatory reach. In this paper, we introduce such a definition, which we call *representational compositionality*. The definition is grounded in algorithmic information theory, and says that compositional representations are both expressive and easily describable as a simple function of symbolic parts. We argue that this definition not only addresses Definition 1's flaws, but also accounts for and generalizes our many intuitions about compositionality. Finally, we provide empirical experiments that clarify implications of the definition and validate its agreement with intuition. Since representational compositionality is rigorous and quantitative, it has the potential to inspire new principled methods in AI for learning compositional representations.

2 Compressing a representation

The definition that we will propose rests on the idea that compositional representations can be redescribed as a simple function of constituent parts. While there may be many ways to redescribe any given representation, a natural and principled way is through the lens of *optimal compression* and Kolmogorov complexity. We provide a brief introduction to Kolmogorov complexity below, but direct unfamiliar readers to Appendix A.

Kolmogorov complexity Kolmogorov complexity (Kolmogorov, 1965; Li et al., 2008) is a notion of information quantity. Intuitively, the Kolmogorov complexity of an object x, denoted $K(x)$, is the length of the shortest program (in some programming language) that outputs x. A related notion is the conditional Kolmogorov complexity of x given another object y, denoted $K(x|y)$, which is the length of the shortest program that takes y as input and outputs x. Kolmogorov complexity has many intuitive properties as a measure of information quantity. The smaller and the more "structure" an object has (regularity, patterns, rules, etc.), the more easily it can be described in a short program and the lower its complexity. Kolmogorov complexity therefore is deeply rooted in the idea of *compression*.

In the context of ML, an interesting quantity is the Kolmogorov complexity of a dataset $X = (x_1, ..., x_n)$ where each sample is drawn *iid* from a distribution $p(x)$. It turns out that if the dataset is sufficiently large, the optimal method for compressing it is to first specify $p(x)$ and then encode the data using it, giving us $K(X) = K(X|p) + K(p)$ (Fortnow, 2000). For the first term $K(X|p)$, each sample can be optimally encoded using only $-\log_2 p(x_i)$ bits (Witten et al., 1987), as in the case of Shannon information (Shannon, 2001). The second term $K(p)$ refers to the complexity of the data distribution (i.e., the length of the shortest program that outputs the function $p : \mathcal{X} \to \mathbb{R}^+$).

Compressing Z as a function of parts Let us denote a representation by a matrix $Z \in \mathbb{R}^{N \times D}$, where each row z_n is obtained by sampling *iid* from some data distribution and model $p(x)p(z|x)$. For instance, $p(x)$ could be a distribution over natural images, $z_n \sim p(z|x)$ could be the (often deterministic) output of some intermediate layer in a trained image classifier, and the resulting representation $Z \in \mathbb{R}^{N \times D}$ would be a matrix of these layer activations.

We will argue that a natural way to think about compositional representations is: representations Z that can be significantly compressed as a function of constituent parts. In other words, the shortest program that outputs the representation, with length $K(Z)$, has a very particular form: it first describes Z using short parts-based constituents, and then maps these parts to the high-dimensional representation. This program form is shown in Figure 1 and described in detail below. Crucially, the components of this program will be used in Section 3 to construct our formal definition of compositionality, in which representations that are *more* compressible as a function of constituent parts are *more* compositional. Before combining them into a definition of compositionality, we now describe the components of this program in the following steps.

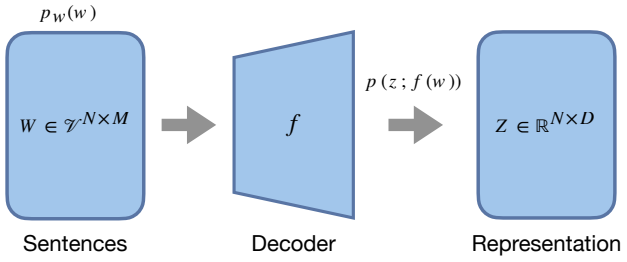
a.

```
def construct_z():
    # 1. Describe Z using a compressed code W
    def p_w(w):  # K(p_w) = length of this function
        ... # returns a probability
    w_compressed = [...]  # K(W | p_w) = ∑ − log p_w(w_n)
    w = decode_algo(w_compressed, p_w)  # K = small constant

    # 2. Decode Z from W
    def f(w):  # K(f) = length of this function
        ... # returns mean and std of a normal distribution
    def p_normal(mu, std):  # K = small constant
        ... # returns a probability
    z_mu, z_std = f(w)  # K = small constant
    z_correction = [...]  # K(Z | W, f) = ∑ − log 𝒩(z_n; z_n^μ, z_n^σ)
    z = decode_algo(z_correction, p_normal, z_mu, z_std)  # K = small constant

    return z
```

b.



c.

$$K(Z) \approx \min_{p_w, W, f} K(p_w) + K(W \mid p_w) + K(f) + K(Z \mid W, f)$$

Figure 1: Hypothesized form of the shortest program that outputs a compositional representation Z. a. Pseudocode showing the skeleton of the program. The program describes the representation using sentences W (sequences of discrete tokens) that are compressed using a prior $p_w(w)$, and then maps these sentences to high-dimensional vectors in representation space using a function $f(w)$ that outputs the sufficient statistics of a Normal distribution. Reconstruction errors are corrected using bit sequences who's length depends on the magnitudes of the errors. `decode_algo()` is a short function that decodes an object compressed using arithmetic coding (Witten et al., 1987). **b.** A visual depiction of the program. **c.** The total Kolmogorov complexity of the representation is estimated by the length of the shortest program that has this form.

Step 1: describe a representation using short parts-based constituents First, we assume that every sample of a the representation z_n of data point x_n can be compressed using a sequence of constituent parts, which in practice are discrete tokens. By analogy to natural language, we will call these discrete token sequences "sentences". Mathematically, we denote these sentences by $W \in \mathcal{V}^{N \times M}$, where $\mathcal{V}$ is a finite set of discrete symbols corresponding to a vocabulary and M is the maximum sentence length. Each row in W is a sentence that describes a high-dimensional vector in the corresponding row of Z. Importantly, these are not sentences in any human language, such as English; they are sequences of discrete tokens that best compress the representation, and can be thought of as an intrinsic representation-specific language. For instance, if the representation describes visual scenes, the sentences might abstractly describe the different objects that the scene is composed of along with the relations between those objects.

For the program to encode these sentences in their most compressed form, it should also define a distribution over the sentences $p_w(w)$. The reason for this is that optimal coding schemes (e.g., arithmetic coding Witten et al., 1987) allow us to encode an object using only $-\log p(x)$ bits so long as p is known (see Equation (7)).

So far, the part of the program in Figure 1 that describes a representation using discrete sentences contributes a total Kolmogorov complexity of:

$$K(p_w) + K(W|p_w) = K(p_w) - \sum_{n=1}^{N} \log p_w(w_n).$$

Step 2: decode representations from their sentences Given sentences W describing representation Z, the program must reconstruct Z. This means that the program must define a function $f : \mathcal{V}^M \to \mathbb{R}^D$—which we call the *semantics* in analogy to natural language—that maps discrete tokens sequences to their high-dimensional vector representations.

Usually, $f(w_n)$ will not perfectly reconstruct any of the z_n's, since w_n is discrete and z_n is continuous. Since Kolmogorov complexity is about *lossless* compression, these errors need to be corrected. The number of bits needed for this correction depends on the magnitudes of the errors in the following way. Instead of outputting a vector in $\mathbb{R}^D$ representing z_n directly, let f output the sufficient statistics of some distribution in $\mathbb{R}^D$. At this point, we can evaluate the probability of the true z_n's under this distribution, $p(z_n; f(w_n))$, and the number of bits needed to specify z_n is equal to $-\log p(z_n; f(w_n))$. For simplicity, we take p to be a Normal distribution who's mean and standard deviation are given by $f(w_n)$, in which case the number of correction bits needed depends on the error of $f(w_n)$: the further the predicted mean is from the true z_n and the higher the uncertainty of the prediction, the lower the probability $p(z_n; f(w_n))$ and the higher the correction bit-length $-\log p(z_n; f(w_n))$.

In sum, the part of the program in Figure 1 that decodes representations from their sentences contributes a total Kolmogorov complexity of:

$$K(f) + K(Z|W, f) = K(f) - \sum_{n=1}^{N} \log p(z_n; f(w_n)).$$

As a small technical note, because Z lives in a continuous space and p is a probability density function, it would take an infinite number of bits to encode the correction term. Thus, in practice, Z must be discretized to some finite precision (e.g., floating-point) and a discrete approximation of the Normal distribution with corresponding probability mass function must be used (e.g., the Skellam distribution).

Summary and further intuition The steps above describe a program that takes no arguments as input and outputs Z, the skeleton of which is shown in Figure 1. We take representations to be compositional if they are highly compressible as a function of constituent parts (justified in Section 3), in which case the shortest possible program that outputs the representation has this form. Under this framework, the total Kolmogorov complexity of the representation decomposes as:

$$\begin{aligned} K(Z) &= \min_{p_w, W, f} K(p_w) + K(W|p_w) + K(f) + K(Z|W, f) \\ &= \min_{p_w, W, f} K(p_w) - \sum_{n=1}^{N} \log p_w(w_n) + K(f) - \sum_{n=1}^{N} \log p(z_n; f(w_n)). \end{aligned} \tag{1}$$

The minimization term here is important: the shortest program is the one in which p_w, W, and f are jointly selected so as to minimize the total program length. We describe one possible strategy for doing this optimization in Appendix B. While some assumptions have gone into this framework for estimating $K(Z)$, we justify them in Appendix C. Now that $K(Z)$ has been fully defined, we can provide some more intuition for its components.

$K(p_w)$ is the complexity of the language used to describe the representation. For instance, a language in which each word is independent of the others would be simpler than a language in which each word is highly context-sensitive.

$K(W|p_w)$ is the complexity of the sentences needed to describe the representation using the language p_w. If sentences tend to be typical utterances with high probability under the language, they will have low complexity. If instead sentences tend to be uncommon utterances with low probability (e.g., from rare tokens), they will have high complexity.

$K(f)$ is the complexity of the semantics that define how sentences (discrete token sequences) map to their meanings (high-dimensional vectors). This term is central to the definition of compositionality that we will introduce in Section 3.

$K(Z|W, f)$ arises from imperfect reconstructions of Z, such as errors due to continuous parts of Z that can't be modeled as a function of discrete inputs. From a cognitive science perspective, this can be thought of as the "ineffability" of a representation, which is the part of it that we cannot describe in language (Ji & Elmoznino et al., 2024).

3 Representational compositionality: a formal definition of compositionality

Our definition of compositionality is a ratio of constituent terms appearing in the decomposition of $K(Z)$ in Equation (1):

Definition 2 (*Representational compositionality*)

The compositionality of a representation, denoted by $C(Z)$, is:

$$C(Z) = \frac{K(Z)}{K(Z|W)} = \frac{K(p_w) + K(W|p_w) + K(f) + K(Z|W,f)}{K(f) + K(Z|W,f)}, \tag{2}$$

where p_w, W, and f are jointly obtained from the shortest program that compresses Z in Equation (1).

Crucially, p_w, W, and f are *not* free parameters: they are intrinsic to the representation in that they best compress Z (see the minimization in Equation (1)). Like Kolmogorov complexity, then, $C(Z)$ is intractable to compute because it requires an exponentially-large search over all possible tuples (p_w, W, f). However, like Kolmogorov complexity, $C(Z)$ can still be tractably estimated using efficient compression and optimization methods. While the primary contribution of this work is theoretical and aimed at justifying Definition 2, we outline a strategy for finding (p_w, W, f) and estimating $C(Z)$ in Appendix B. We will also later introduce a complementary definition for the compositionality of a *language* as opposed to a *representation* in Section 3.1 that is easier to estimate in certain cases, as we show in our experiments.

We now unpack Definition 2 to see how it accounts for the problems of the colloquial Definition 1 and explains computational properties typically associated with compositionality.

Expressivity and compression Effectively, representational compositionality says that the compositionality of a representation is a compression ratio that depends on two things: (1) the complexity of the representation, which appears in the numerator, and (2) the complexity of the semantics which construct the representation from its constituent parts, which appears in the denominator. When a representation is highly expressive (high $K(Z)$) but can nevertheless be compressed as a *simple* function of constituent parts (low $K(Z|W)$), representational compositionality says that the representation is highly compositional. Representational compositionality therefore formalizes a hypothesis in cognitive science that compositionality emerges from competing pressures for expressivity and compression (e.g., Kirby, 1999; Kirby et al., 2008, 2004, and references therein).

Constituent "parts" are intrinsic to Z Note that unlike the colloquial Definition 1, representational compositionality makes it clear where the "constituent parts" (tokens in W), "complex expressions" (W), and "structure" (f) associated with a representation come from: they are intrinsic properties of the representation. Compositional representations are those that are compressible *in principle* as simple functions of constituent parts, regardless of whether or not we know what that optimal compression scheme is.

Systematicity and generalization Representational compositionality formalizes the intuition that the constituent parts of a compositional representation determine the meaning of the whole in a *systematic* way (Szabó, 2012, 2022). For instance, if f arbitrarily maps sentences w to their representations z in a way that does not take the structure or words of the sentence into account (as in the case of idioms), then its complexity $K(f)$ is necessarily high and compositionality is low (we demonstrate this through experiments in Section 4.1). In addition, if f is inaccurate in how it maps sentences to their representations, the error $K(Z|W,f)$ is high and the compositionality low. A representation that is highly compositional according to our definition thus benefits from the generalization ability of simple functions (low $K(f)$) that fit their data well (low $K(Z|W,f)$). Crucially, this ability of f to generalize to novel sentences and representation samples explains the fundamental relationship between compositionality and notions of systematicity from cognitive science (Szabó, 2022).

Structure-preserving semantics Representational compositionality explains the widely-held intuition that semantics functions f which are compositional are structure-preserving in how they map $w \rightarrow z$ (Montague et al., 1970). As explained in Ren et al. (2023), structure-preserving maps have lower Kolmogorov complexity, and thus higher compositionality according to our definition. In a structure-preserving map, each word in the sentence w independently affects a different subspace of the representation z so that pairwise-distances are similar in sentence-space and representation-space.

Modularity & compositionality Representational compositionality explains the precise relationship between compositionality and structural modularity, which has been taken for granted in past work but is difficult to formally articulate (Goyal and Bengio, 2022; Lepori et al., 2023; Mittal et al., 2022). A modular semantics function f is simple because it

decomposes knowledge into smaller reusable components that are algorithmically independent, and thus contributes to high compositionality under our definition. This also explains why natural language is highly compositional. Linguists typically model language using context-free grammars (Chomsky, 1956), in which a sentence hierarchically decomposes into a parse tree with a "production rule" applied at each node. The recursive application of these production rules, akin to a small number of modules in f, is then thought to determine the meaning of the sentence as a whole.

Ultimately, a formal definition of compositionality should be judged based on whether it agrees with our intuitions, generalizes them in meaningful ways, and is quantitatively consistent. Based on the properties listed above, we argue that representational compositionality satisfies all of these desiderata. To provide further intuition for representational compositionality and its implications, we describe some concrete illustrative examples in Appendix D.

3.1 Special case: compositionality of language systems

In Definition 2 of representational compositionality, W is not a free parameter, but rather a collection of sentences intrinsic to Z that minimize its description length. However, we can also consider the special case of languages in which the sentences are fixed to some W^L that is external to the representation. Such cases are common in the real world; in a natural language such as English, W^L are the sentences that a person may utter while Z are the underlying neural activity patterns (thoughts) that those sentences elicit. We could then ask to what degree this *language system* composed of thoughts Z and given sentences W^L is compositional. Expressing each thought with an arbitrary sentence would result in a non-compositional language system, whereas using sentences that accurately describe thoughts through simple semantics would be highly compositional. We define the compositionality of a language system as:

Definition 3 (*Language system compositionality*)

The compositionality of a language system L that maps sentences W^L to their representation Z, denoted by $C^L(Z)$, is:

$$C^L(Z) = \frac{K(Z)}{K(Z|W^L)} = \frac{K(Z)}{K(f^L) + K(Z|W^L, f^L)}, \tag{3}$$

where f^L is obtained from the shortest program that compresses Z given W^L.

This definition opens the door to comparisons between the compositionalities of different real-world language systems, such as French and Japanese, which we attempt in Section 4.3.

4 Empirical results

In this section, we evaluate our compositionality definitions, $C(Z)$ and $C^L(Z)$, on both synthetic and real-world datasets to see if they agree with intuitions.

While no other formal definition of representational compositionality has been proposed, a heuristic commonly used to measure language system compositionality is *topological similarity*. For some language system (W^L, Z), topological similarity computes a pairwise distance matrix between rows in W^L and another distance matrix for Z, then correlates the two flattened matrices. Intuitively, if the pairwise distances of Z are preserved in W^L, topological similarity scores the language system as compositional because the two spaces share structure. Throughout our experiments, we compare our definitions to topological similarity. As an aside, we note that our definition explains why topological similarity is a reasonable heuristic: simple semantics functions f (e.g., identity, linear) tend to preserve the structure of their inputs.

4.1 Synthetic representations

Our first set of experiments consider representations Z that are generated synthetically using known rules through: $z \sim p(z; f(w)), w \sim p_w(w)$. Since we know the underlying programs that generated the representations in this case, we know the ground truth complexity terms $K(p_w)$, $K(W|p_w)$, $K(f)$, and $K(Z|W, f)$ needed to compute $C(Z)$ exactly. These experiments are therefore less about empirically estimating compositionality in practice and more about validating whether the definition matches with intuitions. The high-level methodology used to generate representations is described below, with additional details (such as derivations of complexity terms) provided in Appendix F.

Lookup table representations The simplest way to construct a representation from sequences of discrete tokens is to assign each token in the vocabulary a fixed embedding in a lookup table, and then concatenate these embeddings across the sequence (Figure 2a). Alternatively, the lookup table could assign each unique n-gram an embedding and we could concatenate the embeddings for consecutive n-sized chunks in the sequence. We call n the "disentanglement" factor

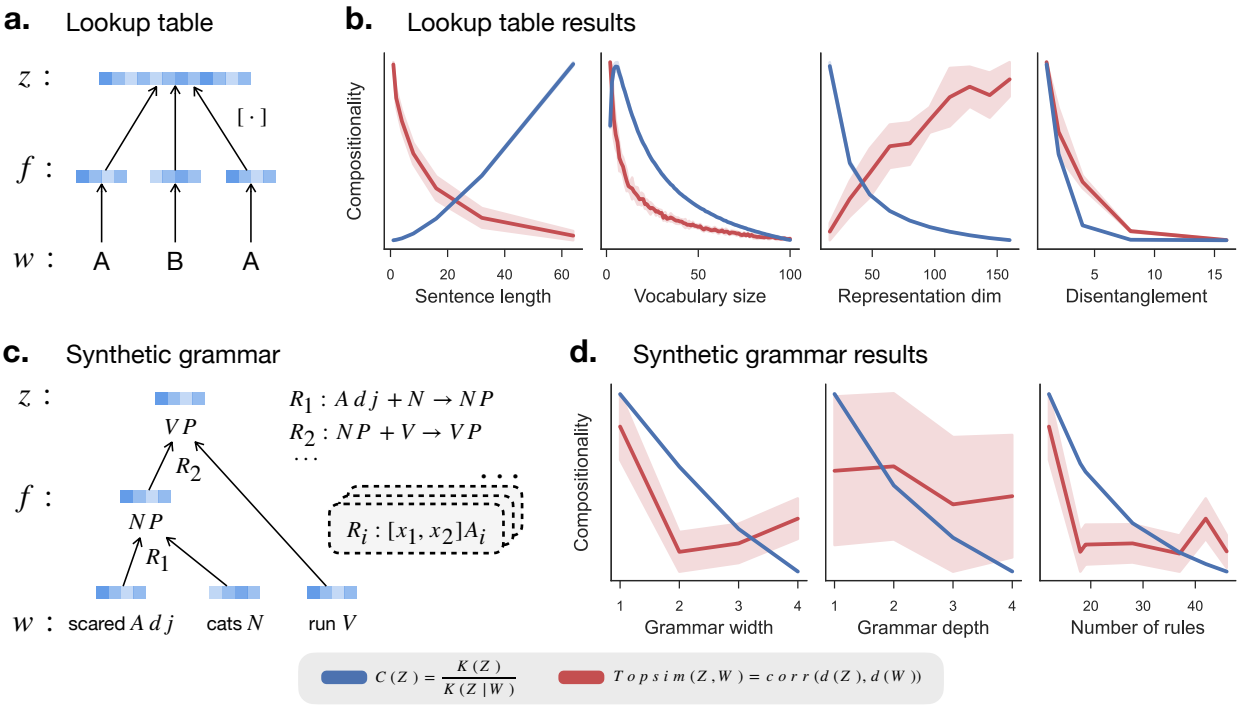


Figure 2: Compositionality of synthetically-generated representations. Representational compositionality $C(Z)$ is shown in blue, topological similarity is shown in red. $C(Z)$ is consistent with intuitions about compositionality across all experiments, whereas topological similarity is not. **a.** Lookup table representations are generated by uniformly sampling sentences of a particular length and vocabulary size, and mapping individual words or n-grams to vectors in a lookup table, followed by concatenation. **b.** $C(Z)$ and topological similarity as a function of ground-truth representation properties. "Disentanglement" refers to varying n-gram size. **c.** Synthetic grammar representations are generated by first sampling sentences using some transition matrix $p(w_{i+1}|w_i)$ and parsing them according to a pre-defined context-free grammar. Parses produce a binary tree with words as the leaves and grammar rules as the nodes. Words are mapped to vector embeddings in a lookup table, and rule application linearly projects concatenated inputs using rule-specific weights. The representation is constructed by first embedding the words and then hierarchically applying the correct rule's linear projection at each node until the root is reached. **d.** Compositionality and topological similarity as a function of ground-truth properties of the grammar. All error bars show standard deviations across 10 random seeds.

because $n = 1$ corresponds to a representation that is perfectly disentangled: each word fully determines a subset of dimensions in the representation, with no context sensitivity. We generate representations by varying certain parameters of the generative program while keeping others constant, and observe the effects on compositionality in Figure 2b.

Sentence length: As representation dimensionality is held constant and sentence length increases, compositionality should intuitively increase. For instance, if sentences are of length 1, we are not tempted to call the representation compositional. The more the representation decomposes according to parts, the more compositional it should be. We see empirically that representational compositionality matches this intuition. This is because $K(Z)$ increases with sentence length (there are more possible z values, for instance) and $K(f)$—proportional to the size of the lookup table—is smaller (same number of table entries, each with lower-dimensional embeddings as sentence length grows). In contrast, topological similarity shows the opposite trend by decreasing with sentence length, thus violating intuitions.

Vocabulary size: Vocabulary size has a more complex relationship to compositionality. If the vocabulary is too small relative to sentence length, then expressivity and compositionality are limited (e.g., with only one word in the vocabulary, nothing can be expressed). On the other hand, if the vocabulary is too large relative to sentence length, then compositionality is low because expressivity doesn't come from combining constituent parts (e.g., with one-word sentences and a large vocabulary, there is no notion of parts). For a given sentence length, then, compositionality should peak at some intermediate vocabulary size. This is precisely what we observe empirically with representational compositionality: a sharp increase in compositionality early on followed by a monotonic decrease as vocabulary size increases further. While topological similarity also shows a decrease in compositionality as a function of increased vocabulary size, it does not show the early increase, and is in fact largest for a vocabulary size of 1.

Representation dimensionality: For a fixed sentence length and vocabulary, how does compositionality relate to representation dimensionality? We implemented this by increasing the dimensionality of the word embeddings that are

concatenated to form the representation. As these embeddings increase in dimensionality, the representation grows more expressive, but only due to increased word complexities rather than their combinations. We should therefore expect compositionality to decrease. Representational compositionality empirically captures this phenomenon. This is because the only thing increasing in this scenario is the size of the lookup table $K(f)$, which is present in both the numerator and denominator of $C(Z)$, so that $C(Z)$ decreases. Topological similarity, in contrast, shows the opposite trend and increases as a function of representation dimensionality.

Disentanglement: Intuitively, the more the meanings of words are context-dependent, the less compositional we consider them (e.g., idioms like "he kicked the bucket" are not considered compositional). Therefore, as a function of disentanglement, compositionality should decrease. We observe this empirically with representational compositionality. This is because the size of the lookup table—and therefore the complexity of the semantics $K(f)$—grows exponentially as a function of disentanglement. Topological similarity also decreases as a function of disentanglement.

Context-free grammar representations While our lookup table experiments provide intuitions for representational compositionality, they are unlikely to reflect the structure of representations in DNN and brains. For instance, The Language of Thought hypothesis (Fodor, 1975) posits that representations underlying human thought have a hierarchical structure akin to context-free grammars in natural language (Chomsky, 1956). In such grammars, the meanings of sentences decompose according to parse trees, where children merge into parents through *production rules* and leaves correspond to words. For instance, the sentence "scared cats run" decomposes according to "$\texttt{ADJECTIVE}\ (scared) + \texttt{NOUN}\ (cats) \rightarrow \texttt{NOUN-PHRASE}\ (scared\ cats)$" followed by "$\texttt{NOUN-PHRASE}\ (scared\ cats) + \texttt{VERB}\ (run) \rightarrow \texttt{VERB-PHRASE}\ (scared\ cats\ run)$", where symbols such as NOUN-PHRASE are *parts of speech* (similar to data types) and functions between parts of speech such as $\texttt{NOUN} + \texttt{VERB} \rightarrow \texttt{VERB-PHRASE}$ are *production rules*.

To model such systems using representational compositionality, we generated representations using simple synthetic grammars (Figure 2c). First, we assigned each word in the vocabulary an embedding and a part of speech tag, and we defined a grammar with a set of production rules. We then generated a dataset of sentences and parsed them using the grammar. Finally, the semantics were defined by embedding each word in the sentence and then applying a rule-specific function at every node in the parse tree until the root was reached, who's value we defined to be the representation. The rule-specific functions concatenated children embeddings and applied a linear projection with rule-specific weights.

We generated many synthetic representations in this way and measured their resulting representational compositionality (Figure 2d). For representational compositionality to match intuition, the complexity of the grammar and the number of rules needed to define it should be inversely proportional to compositionality. For example, in a natural language like English, we can express an infinite number of possible ideas using a relatively small set of grammatical rules and vocabulary, and this is why we believe natural language is compositional. We thus varied two properties of the grammar: its "width" and its "depth". Width refers to the number of rules that are defined for each level of the parse tree's hierarchy. Depth refers to the number of levels in the parse tree's hierarchy with unique rules prior to solely recursive application (analogous to how sentences in natural language can be recursively embedded within others).

As both width and depth increase the complexity of the grammar, we should expect compositionality to decrease as a function of both. We see empirically that representational compositionality is consistent with this intuition. This is because $K(f)$ (and therefore $K(Z|W)$) increase as a function of the number of rules, each of which was associated with its own linear projection matrix. Topological similarity, on the other hand, only loosely correlates with intuitions about compositionality, and has far more noise with different draws of Z from the same grammar.

4.2 Emergent languages from multi-agent training

Next, we further validate our compositionality metric by applying it to real-world representations. To avoid having to solve the difficult optimization problem involved in measuring $C(Z)$ (which requires a minimization of $K(Z)$ w.r.t. p_w, W, f) we instead consider language systems in which $W = W^L$ is fixed and measure $C^L(Z)$ (see Section 3.1).

One interesting case of real language systems is those that emerge in multi-agent settings where agents must learn to communicate. We consider the setting of Li and Bowling (2019); Ren et al. (2020) in which a speaker and a listener learn to communicate in a simple object reference game, where objects have symbolic attributes analogous to color, size, shape, etc. Agents trained using reinforcement learning typically communicate successfully, but often learn non-compositional language systems that arbitrarily map sentences to objects. However, Li and Bowling (2019); Ren et al. (2020) have shown that compositionality can emerge through a multi-generation process called *iterated learning* (Kirby et al., 2015), where the agents' parameters are periodically reset and retrained on sentence/object pairs from the previous generation (see Figure 3a). Kirby et al. (2015) hypothesize that this occurs because iterated learning places an inductive bias for simple language systems that are more easily learnable across subsequent generations.

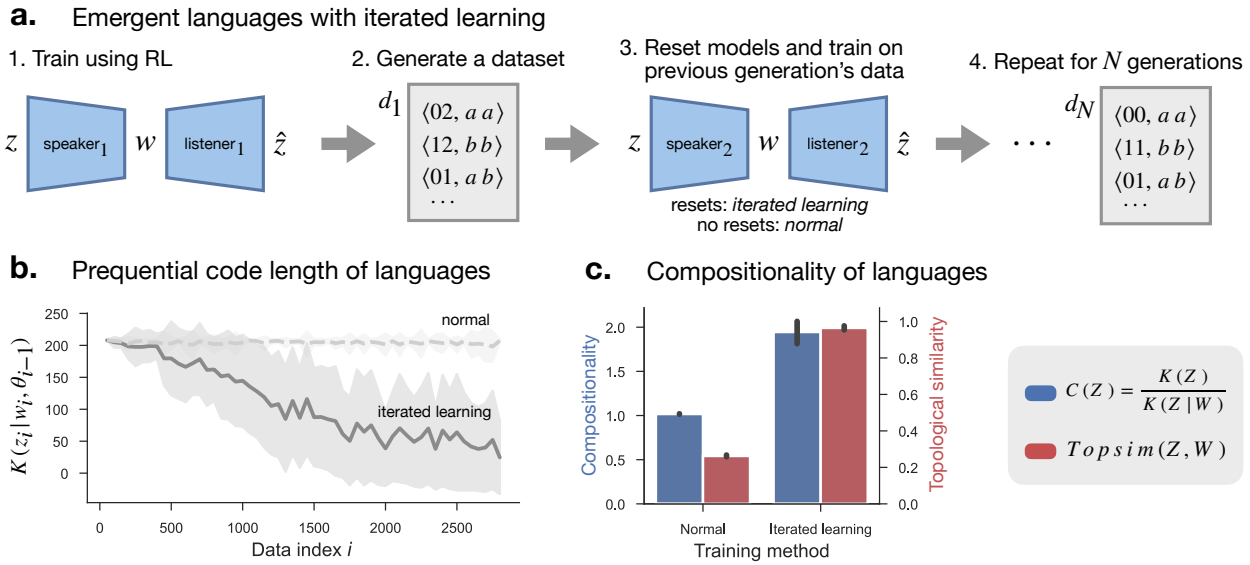


Figure 3: Compositionality of language systems that emerge in multi-agent settings with and without iterated learning. a. We consider language systems in which W^L and Z emerge from agents trained to communicate in an object reference game. Iterated learning is an inductive bias for compositionality in which periodically resetting model parameters creates simpler languages across generations. We trained models with and without iterated learning to compare their compositionalities using our definition. **b.** We used prequential coding to measure $K(Z|W^L)$ for the emergent languages, where the area under the curve is the "prequential code length" estimating compression size. W^L for models trained using iterated learning achieved a much lower prequential code length than those trained normally without iterated learning, meaning the semantics f mapping W^L to Z were simpler. **c.** Our language system compositionality metric $C^L(Z)$ (blue) agrees with topological similarity (red) on the ordering of models trained with and without iterated learning, but the numerical values provided by $C^L(Z)$ provide more theoretical insight (see main text). All error bars show standard deviations across 5 random seeds.

We trained agents both with and without iterated learning and measured $C^L(Z)$ for the resulting language systems. Training details are provided in Appendix G. After N generations, we obtain a dataset consisting of all possible objects Z and the sentences output by the speaker W^L when given those objects as input. To measure $C^L(Z)$, we need both $K(Z)$ and $K(Z|W^L)$. Since Z consists of a set of symbolic objects sampled uniformly, $K(Z)$ is simply equal to $|\mathcal{O}|\log_2(|\mathcal{O}|)$, where $\mathcal{O}$ is the set of all possible objects. To measure $K(Z|W^L)$, we used a compression method called prequential coding (Blier and Ollivier, 2018) that provides good estimates in practice (see Appendix E). Intuitively, prequential coding compresses Z given W by incrementally encoding individual datapoints $z_{<i}$ and fitting a model θ_{i-1} to predict them using $w_{<i}$ as input. The more datapoints are encoded, the better the model becomes by having seen more training data, and the more accurately it can predict the next datapoint z_i. Since prediction error is equivalent to complexity, $K(z_i|w_i, \theta_{i-1})$ will decrease as a function of i, which means that every subsequent datapoint takes fewer bits to encode. The total complexity $K(Z|W)$ is estimated by summing all of these terms.

In Li and Bowling (2019) and Ren et al. (2020), compositionality was measured using topological similarity. Using $C^L(Z)$, we find that we are able to reproduce their results (see Figure 3b,c): iterated learning produces language systems that are more compositional. However, a desirable property of our definition is that the absolute quantities of the metric are meaningful and interpretable. In particular, the "normal" language system trained without iterated learning obtains the lowest possible compositionality score, $C^L(Z) = K(Z)/K(Z|W^L) = 1$, meaning that the mapping from sentences to representations is entirely arbitrary. In contrast, topological similarity can at best only be used as a relative metric for comparing different language systems, as its theoretical link to compositionality is not well understood.

4.3 Natural languages

While it is commonly accepted that all natural languages are roughly equal in their expressive power (their ability to express ideas and thoughts), a highly debated question in linguistics is whether or not they are all equally compositional (Joseph and Newmeyer, 2012). For instance, while one camp suggests that high compositionality in one respect is generally balanced by low compositionality in another, other evidence suggests that languages which undergo significant outside contact experience a pressure for easier learnability and thus higher compositionality, such as in the case of English being exposed to non-native speakers. This question has been difficult to answer definitively, partly due to the absence of a principled and quantitative definition of compositionality.

To investigate the compositionalities of natural language systems using our definition, we first collected a dataset of English sentences describing natural images (COCO, 2024), which we then translated into French, Spanish, German, and Japanese using a large open source model (Costa-jussà et al., 2022). To obtain proxies of "meanings" Z for these sentences, we encoded them using a multilingual sentence embedding model that outputs a dense fixed-size vector (Reimers and Gurevych, 2020). More experimental details as well as limitations of this approach can be found in Appendix H. Using these datasets of sentence/representation pairs, we measured the compositionalities of each natural language system $C^L(Z)$ using the same prequential coding approach as in Section 4.2.

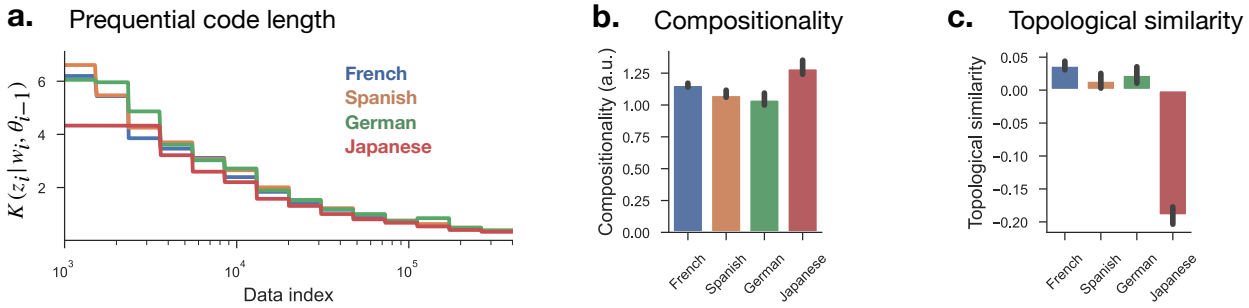


Figure 4: Compositionality of natural language systems. We consider language natural systems in which W^L are sentences in some language and Z are sentence embedding vectors obtained from a pretrained multilingual model. **a.** We used prequential coding to measure $K(Z|W^L)$ for these natural languages, where the area under the curve is the "prequential code length" estimating compression size. Languages have highly similar prequential code lengths, with Japanese having the lowest among them. **b.** Assuming all languages have equivalent expressivity $K(Z)$, their relative compositionalities measured using our definition $C^L(Z)$ are similar. **c.** Using topological similarity as a measure of compositionality gives counter-intuitive results, with most languages having near-zero topological similarity and Japanese being a strong outlier with a topological similarity of -0.2. All error bars show standard deviations across 3 random seeds.

Our results are shown in Figure 4. We find that the prequential code lengths of all languages are highly similar, indicating that they have semantics f of roughly equal complexity (Figure 4a). Assuming that these natural languages are all equally expressive in their abilities to express ideas and identify referents (i.e., equal $K(Z)$; a common assumption in linguistics), their compositionalities as measured by our definition $C^L(Z)$ are roughly equivalent, with Japanese having slightly higher relative compositionality (Figure 4b). Using topological similarity as an alternative definition of compositionality gives counter-intuitive results that contradict our own: most languages have a near-zero topological similarity, except for Japanese which is a strong outlier with a topological similarity of -0.2 (Figure 4c).

5 Conclusion

We introduced a novel definition of compositionality, representational compositionality, that is grounded in algorithmic information theory. Through theoretical arguments and empirical experiments, we showed that this simple definition not only accounts for our many intuitions about compositionality, but also extends them in useful ways.

In virtue of being quantitatively precise, representational compositionality can be used to investigate compositionality in real-world systems. We demonstrated this in the case of emergent and natural language representations, but in a limited way that only considered *language systems* where the sentences describing a representation are externally defined. Measuring the compositionalities of *representations* requires the development of additional machine learning tools, who's overall architecture we sketch out in Appendix B. The development of such tools is an important direction for future work, as it will allow us to investigate the compositionalities of representations that emerge from different learning objectives, neural architectures, inductive biases, and brain regions. These insights can be used to validate or reject hypotheses about compositionality, such as the Language of Thought hypothesis (Fodor, 1975).

Representational compositionality can also play an important role in the design and validation of machine learning models with principled inductive biases for compositionality. Namely, in addition to supporting a given task, a compositional representation must be easily describable as a simple function of constituent parts. There are both direct and indirect ways to achieve this that are grounded in our definition, both of which we intend to pursue in future work.

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Appendix A Background on Kolmogorov complexity

Kolmogorov complexity was independently developed in the 1960s by Kolmogorov (1965), Solomonoff (1964), and Chaitin (1966), and defines a notion of "information quantity".

Intuitively, the Kolmogorov complexity of an object is the length of the shortest program (in some programming language) that outputs that object. Specifically, given some finite string x, $K(x)$ is the length $l(r)$ (in bits) of the shortest binary program r that prints x and halts. Let U be a universal Turing machine that executes these programs. The Kolmogorov complexity of x is then:

$$K(x) = \min_r \{l(r) : U(r) = x, r \in \{0,1\}^*\}, \tag{4}$$

where $\{0,1\}^*$ denotes the space of finite binary strings. A related notion is the conditional Kolmogorov complexity of a string x given another string y, which is the length of the shortest program that takes y as input and outputs x:

$$K(x|y) = \min_r \{l(r) : U(r(y)) = z, r \in \{0,1\}^*\}, \tag{5}$$

where $r(y)$ denotes a program taking y as input. Finally, we can also define a "joint" Kolmogorov complexity $K(x,y)$, which denotes the length of the shortest program that jointly outputs both x and y. Surprisingly, joint Kolmogorov complexity is related to conditional Kolmogorov complexity (up to an additive logarithmic term, which we will ignore) by the Symmetry of Information theorem (Li et al., 2008):

$$K(x,y) = K(y|x) + K(x) = K(x|y) + K(y). \tag{6}$$

Kolmogorov complexity has many intuitive properties that make it attractive as a measure of information quantity, and although it is less common than notions from Shannon information theory (Shannon, 2001), it is strictly more general (as we will show later below). The smaller and the more "structure" an object has—regularity, patterns, rules, etc.—the more easily it can be described by a short program and the lower its Kolmogorov complexity. Kolmogorov complexity therefore is deeply rooted in the idea of compression. For instance, a sequence with repeating patterns or a dataset that spans a low-dimensional subspace can be significantly compressed relative to its original size, and this results in low Kolmogorov complexity. In contrast, a random string devoid of any structure cannot be compressed at all and must in effect be "hard-coded", making its Kolmogorov complexity equal to its original size in bits.

While powerful, Kolmogorov complexity has certain limitations. First and foremost, Kolmogorov is intractable to compute exactly because it requires a brute force search over an exponentially large space of possible programs. It is therefore often of conceptual rather than practical value, although it can nevertheless be upper-bounded using more efficient compression strategies. Second, Kolmogorov complexity depends on the programming language of choice. For instance, if a programming language has a built-in primitive for the object being encoded, Kolmogorov complexity is trivially small. This concern, however, is often overblown: given any two Turing-complete programming languages, the difference in Kolmogorov complexity that they assign to an object is upper-bounded by a constant that is independent of the object itself, because any Turing-complete programming language can simulate another (Fortnow, 2000; Grünwald and Vitányi, 2003). In practice, we can simply consider "reasonable" Turing-complete programming languages that don't contain arbitrary object-specific primitives, in which case this simulation constant will be relatively small and the particular programming language of choice will have little effect. Finally, Kolmogorov complexity is only defined for discrete objects because no terminating program can output a continuous number with infinite precision. This concern is also less consequential in practice, because we can always represent continuous objects using finite (e.g., floating-point) precision.

Important properties for machine learning In ML, we are often concerned with datasets and probabilistic models. Kolmogorov complexity relates to these two concepts in several interesting ways. First, we can ask about the Kolmogorov complexity of a finite dataset $X = (x_1, ..., x_n)$ where each sample is drawn *iid* from a distribution $p(x)$. It turns out that if we have access to the true distribution $p(x)$, optimal algorithms such as arithmetic coding (Witten et al., 1987) can encode each sample using only $\log_2 p(x_i)$ bits. Intuitively, this is because samples that occur more frequently can be encoded using shorter codes in order to achieve an overall better compression. We thus have that:

$$K(X|p) = -\sum_{i=1}^{n} \log_2 p(x_i). \tag{7}$$

If instead of access to the true distribution $p(x)$ we only have a probabilistic model of the data $p_\theta(x)$, we have that:

$$K(X|p) \leq K(X|p_\theta) \leq -\sum_{i=1}^{n} \log_2 p_\theta(x_i), \tag{8}$$

where we have equality on the LHS when $p_\theta = p$ and equality on the RHS when the cost of improving p_θ (in bits of written code) would be greater than the benefits from more accurate modeling. In practice, if p_θ is close to p, we can say that $K(X|p_\theta) \approx -\sum_{i=1}^{n} \log_2 p_\theta(x_i)$.

This insight is significant. Notice that $-\sum_{i=1}^{n} \log_2 p_\theta(x_i)$ is the negative log-likelihood of the data under the model, which is a common loss function used in ML. This tells us that models with lower error better compress their data, and directly relates Kolmogorov complexity to optimization in ML. However, what if we do not have a model? What is the Kolmogorov complexity of the data itself? Intuitively, if the dataset is sufficiently large, the optimal method for encoding it should be to first specify a model and then encode the data using that model as in Equation (8). Specifically, using identities in Fortnow (2000), we have:

$$K(X) \leq K(X|p_\theta) + K(p_\theta). \tag{9}$$

This encoding scheme on the RHS is referred to as a 2-part code (Grünwald, 2007). For large datasets, we have equality when the model's description length and error are jointly minimized, which occurs when the model $p_\theta(x)$ is equivalent to the true distribution $p(x)$:

$$K(X) = \arg\min_{p_\theta} K(X|p_\theta) + K(p_\theta) = \arg\min_{p_\theta} -\sum_{i=1}^{n} \log_2 p_\theta(x_i) + K(p_\theta) \tag{10}$$

$$= K(X|p) + K(p) = -\sum_{i=1}^{n} \log_2 p(x_i) + K(p). \tag{11}$$

Again, we can draw important connections to ML. Equation (9) says that the Kolmogorov complexity of a dataset is upper-bounded by the a model's error and complexity. In addition, Equations (10) and (11) tell us that the simplest model that explains the data is most likely to be the true one, which draws a theoretical link between compression, maximum likelihood training, model complexity, and generalization (Goldblum et al., 2023).

Relation to Shannon information In Shannon information theory (Shannon, 2001), the notion of information quantity is entropy. Given a random variable $X \sim p(x)$, entropy is defined as: $H(X) = \mathbb{E}_{x\sim p(x)} - \log_2(p(x))$. Notice that the $-\log_2(p(x))$ inside the expectation is equal the quantity inside the sum of Equation (7), which specified the minimum number of bits needed to encode a sample from a dataset given the distribution that sample was drawn from. This is no accident: entropy can be seen as the average number of bits needed to compress events from a distribution using an optimal encoding scheme when the distribution $p(x)$ is known. If we simply sum these bits for a finite number of samples instead of taking an expectation, we get exactly $K(X|p)$ as defined in Equation (7).

As we have seen, though, the assumption about a known distribution $p(x)$, need not be made in the Kolmogorov complexity framework. In this sense, Kolmogorov complexity is a strict generalization of Shannon information theory: $K(X)$ as defined in Equation (11) is equivalent to summed entropy plus the complexity of the distribution $p(x)$, which is unknown and needs to be encoded. In the Shannon framework, it is difficult to derive a meaningful notion for the information quantity in the distribution $p(x)$ because it is an individual object—a function, in particular—and Shannon information is only defined for random variables (Grünwald and Vitányi, 2003). A second drawback of Shannon information is that entropy is a measure of statistical determinability of states; information is fully determined by the probability distribution on states and unrelated to the representation, structure, or content of the individual states themselves (Grünwald and Vitányi, 2003). For this current work, we require a notion of complexity that can account for representations and functions, making Kolmogorov complexity better suited to the task.

Appendix B Compressing a representation using discrete auto-encoders

To measure compositionality as defined in Definition 2, we must first compress $K(Z)$ using the program form in Section 2. This involves finding a p_w, W, and f that jointly minimize:

$$K(Z) = \min_{p_w, W, f} K(p_w) + K(W|p_w) + K(f) + K(Z|W, f) \tag{1 revisited}$$

$$= \min_{p_w, W, f} K(p_w) - \sum_{n=1}^{N} \log p_w(w_n) + K(f) - \sum_{n=1}^{N} \log p(z_n; f(w_n)).$$

While this is an intractable search problem, it can be turned into an easier optimization problem using modern deep learning tools. In particular, we can minimize at least some of the terms in Equation (1) by fitting a discrete auto-encoder

to Z using a learned prior in the latent W-space, as illustrated in Figure B.1. This auto-encoder consists of an encoder $w = e(z)$ that maps the representation to a discrete latent space of sentences, a latent prior $p_w(w)$, and a decoder $p(z; f(w))$ that outputs the sufficient statistics of a Gaussian distribution in order to evaluate the likelihood of the original representation. In practice, the latent prior $p_w(w)$ can be parameterized using an auto-regressive model such as a causal Transformer, which tends to work well on language data. We can then train this discrete auto-encoder using the following loss function:

$$\mathcal{L}(Z; e, p_w, f) = \sum_{z \in Z} -\log p_w(e(z)) - \log p(z; f(e(z))). \tag{12}$$

The first term in this loss ensures that W has high prior likelihood, and optimizes both the prior model p_w as well as the encoder e that produces the latent sentences. The second term in the loss ensures that Z has high likelihood given W, and optimizes the decoder f as well as the encoder e so that they preserve information about Z. Recall from Equation (7) that the negative likelihood of an object under some probability distribution is equal to its conditional Kolmogorov complexity given that distribution. As a result, minimizing the loss in Equation (12) is equivalent to finding a p_w, W, and f that jointly minimize $K(W|p_w) + K(Z|W, f)$.

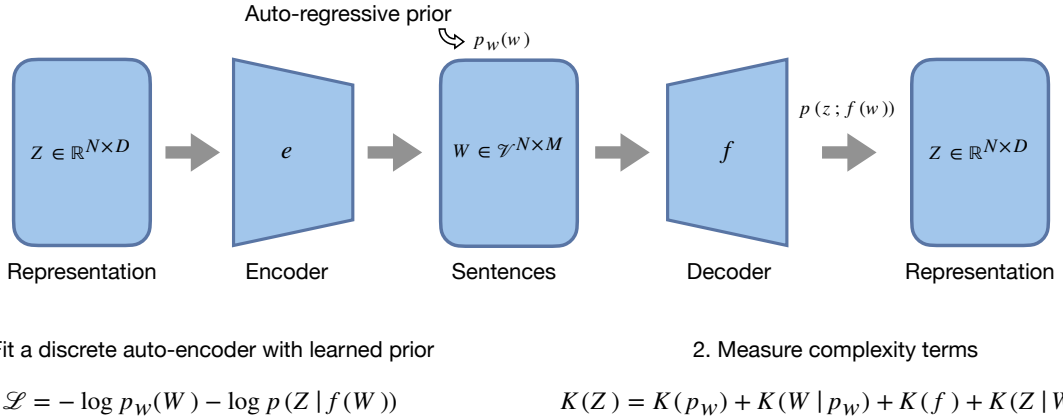

Figure B.1: Estimating the complexity of a representation $K(Z)$ by fitting a discrete auto-encoder with learned latent prior. The encoder, prior, and decoder are jointly trained with a loss that maximizes the likelihood of Z using sentences that have high prior likelihood $p_w(W)$. If p_w and f are also regularized to be simple functions, fitting this discrete auto-encoder is equivalent to finding a p_w, W, and f that jointly minimize $K(Z)$.

To measure $K(Z)$, we also need to minimize $K(p_w)$ and $K(f)$. For this, two options present themselves:

1. Hope that the implicit simplicity bias of DNNs trained using SGD does a good enough job on its own of finding solutions with low complexity (Blier and Ollivier, 2018).
2. Use additional regularization techniques that implicitly minimize the complexities of the models, such as simple architectures, L1 or L2 weight penalties, modularity (Goyal and Bengio, 2022), dropout (Hinton et al., 2012), periodic resetting Zhou et al. (2021), etc.

Regardless of which method is used, the complexities of the final trained models can be estimated using a method called prequential coding (Blier and Ollivier, 2018), which we describe in Appendix E. Thus, we are able to estimate all of the constituent complexity terms of $K(Z)$ in Equation (1). The main challenge in this overall approach then becomes how to successfully train a discrete auto-encoder with a prior in latent space, in a way that is both stable and scalable.

VQ-VAE The most popular method for training discrete auto-encoders is the Vector-Quantized Variational Auto-Encoder (VQ-VAE) (Van Den Oord et al., 2017). While the latent prior in a VQ-VAE is generally trained post-hoc, some work has managed to train the prior end-to-end along with the rest of the model (Cohen et al., 2022; Jones and Moore, 2020; Yasuda et al., 2021). The main challenge with VQ-VAEs is that they explicitly discretize in the latent space during training—which is an inherently non-differentiable operation—and then attempt to approximate gradients using imperfect estimators (Bengio et al., 2013; Jang et al., 2016). As a result, training is often unstable and fraught with degenerate solutions that collapse in the latent space (Łańcucki et al., 2020).

Simplicial embeddings Another option, which avoids the difficulty of training with hard-discretization, is to use so-called *simplicial embeddings* in the latent space (Lavoie et al., 2023). Simplicial embeddings amount to soft attention:

each vector "chunk" representing a word in the latent space is projected onto $|\mathcal{V}|$ word embeddings followed by a softmax, and the weighted word embeddings are then summed at each sentence position. The temperature of the softmax can then be gradually decreased over the course of training such that the operation approaches a hard-discretization in the limit. As the operation is entirely continuous and deterministic, it is easier to train using end-to-end gradient descent methods (although it may become numerically unstable at low softmax temperatures). One challenge becomes how to define and train the prior p_w in this case, where W is in fact a sequence of continuous word embedding mixtures as opposed to a sequence of discrete tokens. One possibility is to perform a hard-discretization of the latent before it is passed to the prior, along with relevant gradient estimators (e.g. Bengio et al., 2013; Jang et al., 2016). While this could make training more difficult, the encoder-decoder part of the model would at least remain entirely continuous and deterministic. Another option is to define p_w in continuous space, where the input is a sequence of word embedding mixtures and the "next-token" targets are categorical distributions over words.

GFlowNets If we still wish to perform hard-discretization, but do not want to resort to imperfect gradient estimators required for end-to-end training, Generative Flow Networks (GFlowNets) could be a promising alternative (Bengio et al., 2021, 2023). GFlowNets can learn to sample some compositional discrete object in proportion to a reward function. The reward function and GFlowNet can also be conditioned on some input, and the reward function can be learned in alternation with the GFlowNet using expectation-maximization (GFlowNet-EM) (Hu et al., 2023). In the case of a discrete auto-encoder, the encoder would be a GFlowNet, while the decoder and prior would be the reward function. While this approach has been used to train a discrete auto-encoder before (Hu et al., 2023), it comes with its own challenges. First, GFlowNet-EM is not an end-to-end training procedure (no gradients flow from the decoder to the encoder), which makes it more difficult to train. Second, while GFlowNets sample proportionally to their reward, our ultimate goal is to *maximize* the reward (i.e., find sentences W that maximize the prior and reconstruction). To do this, we will ultimately have to decay the temperature of the reward over the course of training in order to settle to a final solution that minimizes the loss in Equation (12). Training GFlowNets with a sparse reward, however, is more difficult due to exploration challenges (Atanackovic and Bengio, 2024).

Appendix C Assumptions in compressing a representation

In laying out our framework for measuring $K(Z)$ in Section 2, we made several key assumptions.

First, we assumed that the shortest program that outputs Z has a particular form. If it does not, then the estimated $K(Z)$ can be far greater than the true one. However, we argue that the assumed program form is safe for the kinds of representations that we are interested in and the kinds of insights we wish to gain from estimating $K(Z)$. Namely, we are interested in seeing if given neural representations share similar properties to conscious human thought, which is believed to have a symbolic structure where each thought is a composition of discrete concepts (Fodor, 1975). If a representation does not have this kind of structure, then our method would detect it in the form of a high estimated $K(Z)$, even if this is an overestimate of the true Kolmogorov complexity due to incorrectly assuming the program form in Section 2.

Second, actually estimating $K(Z)$ using Equation (1) requires a minimization over p_w, W, and f. This optimization approach assumes that the p_w and f which minimize $K(Z)$ are DNNs. While this can seem unintuitive at first given the significant number of parameters in DNNs, it has been found that they converge to solutions that are remarkably simple and compressible (Blier and Ollivier, 2018; Goldblum et al., 2023; Rae, 2023; Sutskever, 2023), which likely explains their strong generalization abilities. We therefore believe that for neural representations with sufficient complexity, the assumption that they can be best compressed using DNNs is justified.

Appendix D Examples of compositional representations

To supplement and clarify the arguments in Section 3, it is easiest to gain further intuition for our definition of compositionality through concrete examples of different hypothetical representations. For each, we have strong intuitions about whether or not the representation is compositional, and we will see that our definition agrees with—and indeed extends—these intuitions.

Example 1, $\downarrow C(Z)$: f is a lookup table from w to z Consider a representation Z that is sampled from a mixture of Gaussians, where the centroids are far apart but their locations lack any kind of structure (i.e., they are randomly distributed). To simplify things, let us assume that there are as many unique centroids as there are possible sentences. In such a case, the semantics function f would identify each centroid with a unique sentence and the resulting error $K(Z|W, f)$ would be low. However, because these centroids lack any structure, f would have to define an *arbitrary* mapping from each sentence to its corresponding centroid. In other words, f would function as a lookup table from

w to z that does not leverage the internal structure (i.e., words and their ordering) in the sentence to achieve a more compressed mapping. The resulting description length of f would be equal to the size of the lookup table, which would grow exponentially with the sentence size. f would be, in effect, a complex "hard-coded" mapping (in fact, the most complex possible) with $\mathcal{O}(K(f)) = |\mathcal{V}|^M$, where M is the sentence length and $|\mathcal{V}|$ is the vocabulary size. The resulting compositionality $C(Z)$ would be extremely low.

Example 2, $\downarrow C(Z)$: Z is a smooth continuous function The above example considered a case where the representation had discrete structure that could be accurately modeled by sentences, and the source of low compositionality came from a high $K(f)$. However, the compositionality can also be low if Z is inherently continuous, in which case modeling it using a discrete W is at best an approximation via quantization. In such a case, the error $K(Z|W, f)$ would be high and the corresponding compositionality would be low. Note that it might be possible to compress Z using a low-dimensional continuous code rather than discrete sentences, from which an equivalent (perhaps even identical) definition of continuous compositionality could be derived, but in this work we consider only compositions of discrete parts.

Example 3, $\downarrow C(Z)$: Z is simple Most of the discussion thus far has focused on the denominator of $C(Z)$ in Definition 2. However, a representation can also lack compositionality if the complexity of the numerator, $K(Z)$, is low. If Z were very low—say it were a constant, for instance—then it could be modeled using a simple f that achieves low error $K(Z|W, f)$. However, we would certainly not be tempted say that the representation is compositional. In fact, it would be best compressed using a single word and an f that outputs a constant, rather than using complex sentences and simple compositional rules. Compositionality must therefore also increase with the expressivity of the representation, which is captured by the numerator $K(Z)$.

Example 4, $\uparrow C(Z)$: f assigns an embedding to each word followed by a simple operation We now turn to paradigmatic examples of high compositionality, beginning with the most intuitive. Consider once again a representation Z that is sampled from a mixture of Gaussians like in *Example 1*, but this time imagine that the centroids are arranged in a structured way. In particular, imagine that they are structured such that each can be described as a concatenation of subcomponents that are shared across all centroids. Now, the simplest f would be one that first assigns a vector embedding to each word such that it represents a possible subcomponent of the centroid, and then concatenates the embeddings for all words in the sentence. The complexity of f would then scale only linearly as a function of the number of words in the vocabulary (assuming they are all necessary), because concatenation is a simple operation that takes a constant number of lines of code. We would have $\mathcal{O}(K(f)) = |\mathcal{V}|$, which is independent of the sentence length, in contrast to the arbitrary mapping in *Example 1* that scaled as $\mathcal{O}(K(f)) = |\mathcal{V}|^M$. This is a substantial reduction in complexity and increase in compositionality, and it comes from the fact that the words contribute independently to the representation. This is a case of a perfectly disentangled representation, which in our theory is simply an extreme case of compositionality, but intermediate cases are possible as well. For instance, the representation could be determined by interactions between pairs of words in the sentence, or it might be the case that words largely contribute independently to the representation but that there is some small degree of context-sensitivity, as in human language. Our theory unifies all of these cases under a single, succinct definition.

Example 5, $\uparrow C(Z)$: f is modular As already explained in Section 2, a modular f is simpler to describe and thus implies higher compositionality. This accounts for intuitions about the relationship between compositionality and models that exhibit structural modularity (Goyal and Bengio, 2022; Lepori et al., 2023).

Example 6, $\uparrow C(Z)$: f has many equivariances The connection between equivariance and compositionality is perhaps less obvious (Gordon et al., 2020), but it is a natural and intuitive consequence of our definition. Equivariance (and invariance) is a source of structure that decreases the complexity of a function (Immer et al., 2022; van der Ouderaa and van der Wilk, 2022; Wilk et al., 2018). For instance, convolutional layers have local connectivity and reuse weights across spatial locations, which both reduces their description length and makes them equivariant to spatial translations. We can also consider linear equivariance as a special case that is easy to illustrate. If f is linearly equivariant to a particular operation g in sentence-space, it means that $f(g(w)) = f(w) + v_g$, where v_g is a constant vector that corresponds to the equivariant change in the representation output by f. The difference in the function's behaviour for two different inputs, w and $g(w)$, can therefore be compactly described by a single vector, whereas in the general non-equivariant case the change in the function's behaviour can be arbitrarily complex. In an extreme case, if f can be completely described by a set of linear equivariances, then each w corresponds to a set of g_i's applied to a constant "default" sentence, and f merely needs to encode a single vector for each of these g_i's then sum those that apply to a particular input. The resulting function is very similar to the one described in *Example 4*, where f applied a simple operation to a sequence of word embeddings in a sentence (in this case vector addition). The function also bears similarities to the one described in *Example 5* if we view the equivariances as modules. Similar arguments can be made

for non-linear equivariance, where the complexity $K(f)$ would still be reduced, but to a lesser extent. In general, the more equivariances a function has and the simpler those equivariances are, the lower the complexity $K(f)$ and the higher the compositionality $C(Z)$.

Appendix E Prequential coding

While the Kolmogorov complexity of a model $K(p_\theta)$ is difficult to measure directly, it turns out that we can jointly estimate $K(D|p_\theta) + K(p_\theta)$ in cases where the model was fit to the data using a learning algorithm, as is the case in ML. From Equation (6), we have that:

$$K(D|p_\theta) + K(p_\theta) = K(D, p_\theta). \tag{13}$$

Instead of trying to estimate the terms on the LHS directly, we can estimate the RHS by finding the shortest program that jointly compresses both the dataset and the model, which we turns out to be easier through a compression algorithm called *prequential coding* illustrated in Figure E.1 and described below.

a.

```
# Prequential coding to compress D
def construct_D_and_p(T):
  D = []   # Starting off without any data
  for _ in range(0, N):
    # Train a model on all the data so far
    p = T(D)

    # Specify the (encoded) next datapoint
    D_next_encoded = [...]  # K = -log(p(D_next))

    # Extend the dataset after decoding with p
    D += decode(D_next_encoded, p)

  return D, T(D)
```

b.

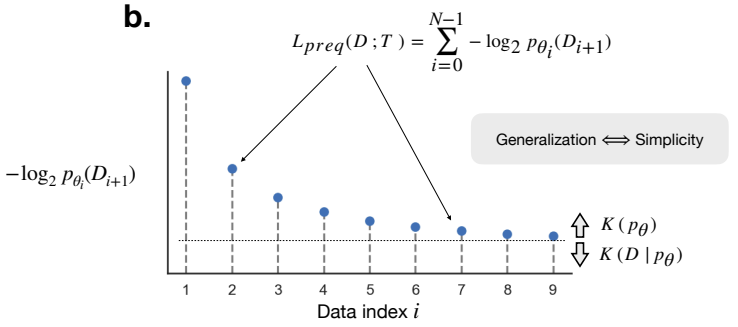

Figure E.1: Illustration of prequential coding, a method for estimating $K(D, \theta) = K(D|p_\theta) + K(p_\theta)$ using p_θ's learning algorithm T. a. Pseudocode of the prequential coding program that outputs both D and p_θ. The program jointly compresses D and p_θ by incrementally training a model using T on increasingly more data, each time efficiently encoding the next datapoint using the model obtained from all previous ones. The primary sources contributing to total program length come from specifying each next datapoint D_{i+1} in compressed form using the current model p_{θ_i}, which takes $-\log_2 p_{\theta_i}(D_{i+1})$ bits. **b.** A visual illustration of the number of bits needed to specify each next datapoint given the model that was trained on all previous ones. As the learner T sees more data, it outputs models that assign a higher likelihood to new observations, and can thus better compress them. The total prequential code length $L_{preq}(D;T)$ is given by the area under the curve. The area underneath the curve's last point is equal to the number of bits needed to encode the entire dataset given the final model, $K(D|p_\theta)$. Since $L_{preq}(D;T) = K(D|p_\theta) + K(p_\theta)$, the area above the curve's last point is equal to $K(p_\theta)$. Prequential coding formalizes the intuition that simple models generalize better, thus quickly decreasing their prediction error for the next datapoint.

Prequential coding first assumes that we have access to a learning algorithm T which was used to fit the model p_θ. For instance, $p_\theta = T(D)$ might correspond to a randomly initialized DNN architecture fit to D using SGD with some set of hyperparameters. Then, consider an ordering of *iid* datapoints $D = \{D_1, ..., D_N\}$, and denote $D_{1:i} = \{D_1, ..., D_i\}$. In prequential coding, the first datapoint D_1 is hard-coded in an uncompressed form, which takes a large number of bits. The learning algorithm T is then used to train a model $p_{\theta_1} = T(D_1)$ on this single observation. Because the model is trained on only one datapoint, it will not be very accurate; however, it should be better than a random model that has seen no data at all. Because of the relationship between probabilistic generative models and compression described in Appendix A, we can use this model to specify the next datapoint D_2 in a compressed form using only $-\log_2 p_{\theta_1}(D_2)$ bits. At this point, we have encoded 2 datapoints, on which we can train a new model $p_{\theta_2} = T(D_{1:2})$. Having seen more data, this model should assign a higher likelihood to a new datapoint D_3, which we can specify in compressed form using $-\log_2 p_{\theta_2}(D_3)$ bits. This process repeats until the entire dataset has been generated. At this point, the model p_θ can be obtained simply by applying the learning algorithm to the complete dataset $p_\theta = T(D)$, since we assumed by construction that this was where the model came from.

The total number of bits that it takes to jointly compress D and p_θ using prequential coding is the sum of how many bits it takes to specify each next datapoint using a model that was trained on all previous ones. Visually, it is the area under the *prequential coding curve* shown in Figure E.1b. We can call the total length of this compression program the

prequential code length $L_{preq}(D;T)$ (Blier and Ollivier, 2018):

$$L_{preq}(D;T) = \sum_{i=0}^{N-1} -\log_2 p_{\theta_i}(D_{i+1}) \tag{14}$$

$$L_{preq}(D;T) \geq K(D, p_\theta) = K(D|p_\theta) + K(p_\theta). \tag{15}$$

Strictly speaking, $L_{preq}(D;T)$ is an upper-bound on $K(D, p_\theta)$: the prequential coding algorithm is *one* way to jointly compress the data and model, but it is not necessarily the optimal way. The upper-bound is tight in practice, however, if (a) the final model p_θ does a good job of compressing the data (i.e., $K(D|p_\theta) \ll K(D)$) and (b) passing data to the learner T through the prequential coding algorithm is an effective strategy for compressing the model. Regarding this second point, consider how the model is obtained through prequential coding. Data is gradually transmitted to the learner T, with each additional datapoint requiring fewer bits to encode. If the speed of improvement in predicting the next datapoint is fast as a function of the amount of data observed, it means that the learner is effectively able to converge to the final model using only a small amount of data that takes few bits to encode, and thus that the model has low complexity. Concretely, when prequential coding is a good algorithm for jointly compressing the data and model, then $L_{preq}(D;T) \approx K(D, p_\theta)$ and the model complexity is given by (Blier and Ollivier, 2018):

$$\begin{aligned} L_{preq}(D;T) &\approx K(D|p_\theta) + K(p_\theta) \\ K(p_\theta) &\approx L_{preq}(D;T) - K(D|p_\theta). \end{aligned} \tag{16}$$

Assuming that the model's error decreases monotonically with the size of the training dataset, $K(D|p_\theta)$ is equal to the area under the lowest point of the prequential coding curve in Figure E.1b. The area above this point is therefore the complexity of the model $K(p_\theta)$. This relates Kolmogorov complexity to intuitions about generalization in ML: the simpler a model is, the quicker it generalizes from limited amounts of training data.

Appendix F Synthetic representations — experimental details

F.1 Lookup table representations

Generating the representations We generated our synthetic lookup table representations Z (and their ground-truth sentences W) according to the program summarized in Algorithm 1. In short, the program does the following:

- **Generate a lookup table:** We begin by constructing a lookup table from words (or n-grams) to their embeddings. This table has dimensions $(K^q, \frac{D}{M \times q})$, where K is the vocabulary size, q is our disentanglement factor (i.e., the size of the n-grams), and D is the desired dimensionality of Z. We use the Skellam distribution to generate lookup table entries, which is a discrete approximation of a Gaussian distribution with precision λ. This discretization is necessary because a continuous distribution would cause the correction term $K(Z|W, f)$ to be infinite.
- **Sample W:** We generate random integer sentences uniformly with shape (N, L), where N represents the number of samples and L denotes the number of words per sentence. Each integer in W corresponds to a word from our vocabulary of size K.
- **Decode W to get Z:** For each sentence $w \in W$, we perform the following steps to obtain the corresponding representation sample $z \in Z$:
  - We divide the sentence into consecutive L/q subsequences, each representing an n-gram (or a word if $q = 1$).
  - For each subsequence, we retrieve the corresponding embedding from the lookup table.
  - We concatenate these embeddings to form the complete representation sample z for the sentence.
- **Add noise:** We then add Gaussian noise (discretely approximated by a Skellam distribution with mean 0 and standard deviation r for the same reason as above) to the representation. This introduces stochasticity to our representations that cannot easily be modeled with discrete parts. The final representation Z has shape (N, D).

Calculating the compositionality To compute representational compositionality $C(Z)$ according to Definition 2, we need to calculate the following terms: $K(p_w)$, $K(W|p_w)$, $K(f)$, and $K(Z|W, f)$. We show how to do this below for a lookup table representation:

Algorithm 1: Sampling Z using a lookup table program

Input:
number of samples N
sentence length M
vocabulary size K
embedding dimension D
disentanglement factor q
quantization precision λ
noise ratio r

// Generate lookup table:
lookup_table $\leftarrow$ skellam_sample($\mu = 0, \sigma = 1, \lambda = \lambda$, shape $= (K^q, \frac{D}{M/q})$)

// Sample W:
$W \leftarrow$ random_integer$(0, K-1,$ shape $= (N, \mathrm{M}))$

// Decode W to get Z:
$Z \leftarrow []$
for each w **in** W **do**
  $z \leftarrow []$
  for position $= 0$ **to** $(M/q) - 1$ **do**
    entry $\leftarrow (w[\text{position} \times q : \text{position} \times q + q - 1])$
    z.append(self.lookup_table[entry])
  end for
  $z \leftarrow$ concatenate(z)
  Z.append(z)
end for
$Z \leftarrow$ stack(Z)

// Add noise:
if $r > 0$ **then**
  noise $\leftarrow$ skellam_sample$(\mu = 0, \sigma = r, \lambda = \lambda,$ shape $= Z$.shape$)$
  $Z \leftarrow Z +$ noise
end if
return Z

- $K(p_w)$: The language p_w in this case a uniform categorical distribution over integers in range $(0, K-1)$ at each sentence position $l \in \{0..(M-1)\}$, where K is the vocabulary size and M is the sentence length. To specify an integer u, we need $\log_2 u$ bits, so we have $K(p_w) = \log_2 K + \log_2 M$. There is also a complexity term associated with describing the function for the uniform distribution itself, but we ignore this because it is a small constant.
- $K(W|p_w)$: As described in Section 2, $K(W|p_w)$ is simply equal to $-\sum_{i=1}^{N} \log_2 p_w(w_i)$. To derive $p_w(w_i)$ for each sentence $w_i \in W$, we notice that each w_i is composed of L words, each sample from a uniform categorical distribution over $(0, K-1)$. Thus $p_w(w_i) = \frac{1}{K^M}$ for each sentence w_i. In total, then, $K(W|p_w) = -\sum_{i=1}^{N} \log_2 p_w(w_i) = -\sum_{j=i}^{N} \log_2 \frac{1}{K^M} = NM \log_2 K$ bits.
- $K(f)$: In this case, the function that maps sentences to their meanings is mainly composed of the lookup table, with some additional small constant complexity to describe how to use the lookup table. To describe each number a in the lookup table, we need $-\log_2 p(a)$ bits, where p is the PMF of the distribution these numbers were sampled from. In our case, this distribution is the Skellam distribution with a mean of 0, a standard deviation of 1, and a precision of λ. We therefore have $K(f) = -\sum_{a \in \text{lookup table}} \log_2 p(a)$. Given that the size of the lookup table is $(K^q \times \frac{D}{M/q}))$, the complexity of the semantics $K(f)$ grows linearly in D, polynomially in K, and exponentially in q.
- $K(Z|W, f)$: This term comes from imperfect reconstructions of Z. It can be thought of as the number of bits needed to correct the errors in these imperfect reconstructions. In these lookup table representations, these imperfect reconstructions come from the noise added to Z when it is sampled, which cannot be recovered

since the lookup table does not contain it. To describe the corrections, we therefore just need to describe this noise. Each noise sample ϵ can be described using $-\log_2 q(\epsilon)$ bits where q is the PMF of the distribution the noise was sampled from. In our case this is a Skellam distribution with a mean of 0, standard deviation of r, and precision of λ. If we let E be the matrix of all noises added form Z, we have that $K(Z|W, f)$ is equal to $-\sum_{\epsilon \in E} \log_2 q(\epsilon)$.

Combining these complexity terms together, the final expression for $C(Z)$ following Definition 2 is:

$$C(Z) = \frac{K(Z)}{K(Z|W)} = \frac{K(p_w) + K(W|p_w) + K(f) + K(Z|W, f)}{K(f) + K(Z|W, f)}$$
$$= \frac{\log_2 K + \log_2 M + NM \log_2 K - \sum_{a \in \text{lookup table}} \log_2 p(a) - \sum_{\epsilon \in E} \log_2 q(\epsilon)}{-\sum_{a \in \text{lookup table}} \log_2 p(a) - \sum_{\epsilon \in E} \log_2 q(\epsilon)}$$

Experiment parameters We used the following parameter values to generate representations (except when sweeping one parameter while keeping the others constant): $N = 1000$, $M = 16$, $K = 10$, $D = 64$, $q = 1$, $\lambda = 0.01$, $r = 0.01$. To sweep over sentence length, we varied M from $(1, D)$, only keeping values where D was divisible by M. To sweep over vocabulary size, we varied K from $(2, 100)$. To sweep over representation dimensionality, we varied D from $(M, 2M, ..., 10M)$. To sweep over disentanglement, we varied q from $(1, M)$, only keeping values where M was divisible by q. For each setting of experiment parameters, we generated representations across 10 different random seeds.

F.2 Context-free grammar representations

Generating the representations We generated our context-free grammar representations Z (and their ground-truth sentences W) according to the following procedure:

- **Generate a context-free grammar:** Our context-free grammars consist of exclusively binary production rules that combine two child non-terminals into a parent non-terminal. We define a vocabulary of size K and evenly assign each word to one of T possible base part of speech types that serve as the first non-terminal symbols in the context-free grammar. We call these T first non-terminals "terminal parts of speech". We algorithmically generate the grammar in a way that depends on two parameters: the `width` and the `depth`. The `depth` refers to the number of levels in the parse tree (above the parts of speech) that have unique non-terminal symbols which can only exist at that level. The `width` refers to the number of unique non-terminal symbols defined at each level of depth. At any given level of depth, we generate a production rule for all possible combinations of non-terminals at that level, each of which produces one of the possible non-terminals at the next level (we evenly distribute outputs across these possible non-terminals at the higher level). For arbitrarily long sentences to still have valid parses despite the finite depth of our grammar, we define additional recursive production rules that take non-terminals at the highest level of the grammar and produce one of those same non-terminals. To provide additional clarity for how we generated these grammars, we give an example below for $T = 5$, `width` $= 2$, and `depth` $= 5$ (we exclude the vocabulary for brevity). In this grammar, the terminal parts of speech are denote by the prefix "T_" and other non-terminals are denoted by the prefix "r[depth level]_".

```
start: r2_1 | r2_2
r0_1: T_1 " " T_2 | T_2 " " T_3
    | T_3 " " T_4 | T_4 " " T_5 | T_5 " " T_1
r0_2: T_1 " " T_3 | T_2 " " T_4
    | T_3 " " T_5 | T_4 " " T_1 | T_5 " " T_2
r1_1: r0_1 " " r0_1 | r0_2 " " r0_1
r1_2: r0_1 " " r0_2 | r0_2 " " r0_2
r2_1: r1_1 " " r1_1 | r1_2 " " r1_1
    | r2_1 " " r2_1 | r2_2 " " r2_1
r2_2: r1_1 " " r1_2 | r1_2 " " r1_2
    | r2_1 " " r2_2 | r2_2 " " r2_2
```

- **Sample W:** We generate random integer sentences of length M based on a transmission sentence defined over terminal parts of speech. Denote a terminal part of speech by $t \in 1..T$. A sentence w always randomly starts from a word that has either $t = 1$ or $t = 2$ with equal probability. Permissible transitions to the next word's terminal part of speech are $t_{i+1} \leftarrow t_i + 1$ or $t_{i+1} \leftarrow t_i + 2$, which we sample between with equal probability (we also wrap t_{i+1} so that it remains in range $1..T$). Given a sampled terminal part of speech at a location in w, we randomly sample a word that has been assigned that terminal part of speech.

- **Semantics f:** The representation is assigned a dimensionality D. Each word in the vocabulary is given a D-dimensional embedding by sampling from a Skellam distribution, which is a discrete approximation of a Gaussian distribution, using $\mu = 0$, $\sigma = 1$, and quantization precision λ. For each production rule i in the grammar, we define a linear mapping $A_i \in \mathbb{R}^{2D \times D}$ with values sampled from a Skellam distribution using $\mu = 0$, $\sigma = 1$, and quantization precision λ. Given a sentence w, the semantics function f is defined by the following steps:
  - Parse w using Earley parser (Earley, 1970) implemented with the `Lark` Python package.
  - Retrieve the embedding for each word in w.
  - Hierarchically apply the function $[x_1, x_2]A_i$ at each node in the parse tree to obtain a node embedding, where $[x_1, x_2]$ are the concatenated embeddings of the child nodes and A_i is the linear transform of the production rule at the node. The embedding of the root node is taken to be z for the sentence.
- **Add noise:** We then add Gaussian noise (discretely approximated by a Skellam distribution with mean 0 and standard deviation r) to the representation. This introduces stochasticity to our representations that cannot easily be modeled with discrete parts. The final representation Z has shape (N, D).

Calculating the compositionality To compute representational compositionality $C(Z)$ according to Definition 2, we need to calculate the following terms: $K(p_w)$, $K(W|p_w)$, $K(f)$, and $K(Z|W, f)$. We show how to do this below for a context-free grammar representation:

- $K(p_w)$: The language p_w in this case is defined by a terminal part of speech for each vocabulary item and a binary matrix of permissible transitions between terminal parts of speech. Defining the terminal part of speech for each vocabulary item takes $\log_2 T$ bits, and we have K vocabulary items. The binary transition matrix is of shape $(T + 1) \times T$ (where the $+1$ is for the grammar's `start` symbol), and so takes $T(T + 1)$ bits to define. The total Kolmogorov complexity of the language (ignoring code of a constant complexity that doesn't scale with K or T) is therefore $K(p_w) = K \log_2 T + T(T + 1)$.
- $K(W|p_w)$: As described in Section 2, $K(W|p_w)$ is simply equal to $-\sum_{i=1}^{N} \log_2 p_w(w_i)$. Since p_w is defined by a transition matrix over terminal parts of speech, and for each terminal part of speech each word having that terminal part of speech has equal probability, we have that $p_w(w_i) = \prod_{m=1}^{M} \frac{1}{|t(w_{i,m-1})|}$ where $t(\cdot)$ is the set of all permissible next words $w_{i,m}$ that the previous word $w_{i,m-1}$ can lead to based on the transition matrix between terminal parts of speech, and $w_{i,0}$ denotes the grammar's `start` symbol. We therefore have that $K(W|p_w) = -\sum_{i=1}^{N} \log_2 p_w(w_i) = -\sum_{j=i}^{N} \sum_{m=1}^{M} \log_2 \frac{1}{|t(w_{i,m-1})|}$ bits.
- $K(f)$: The semantics are defined by the parser, the production rule operations (linear maps), and the word embeddings. Both the parsing algorithm and the production rule operations scale in complexity as a function of the number of production rules in the grammar, so we ignore the parsing algorithm's complexity and only consider the production rules and word embeddings as the scaling behaviour is the same. To describe each number in the word embedding table a, we need $-\log_2 p(a)$ bits, where p is the PMF of the distribution these numbers were sampled from. In our case, this distribution is the Skellam distribution with a mean of 0, a standard deviation of 1, and a precision of λ. The complexity of the embedding table is therefore $-\sum_{a \in \text{embedding table}} \log_2 p(a)$. Given that the size of the embedding table is $(K \times D))$, the complexity of the embedding table grows linearly in both K and D. To describe each production rule i, we must describe a matrix of shape $2D \times D$. Each number in this matrix takes $-\log_2 p(v)$ bits to encode, where p is the PMF of the distribution these numbers were sampled from. In our case, this distribution is the Skellam distribution with a mean of 0, a standard deviation of 1, and a precision of λ. The total complexity of all production rules is therefore $-\sum_{i \in \text{num rules}} \sum_{(r,c) \in 2D \times D} \log_2 p(A_{i,(r,c)})$. We therefore have that $K(f) = -\sum_{a \in \text{embedding table}} \log_2 p(a) - \sum_{i \in \text{num rules}} \sum_{(r,c) \in 2D \times D} \log_2 p(A_{i,(r,c)})$ bits.
- $K(Z|W, f)$: This term comes from imperfect reconstructions of Z. It can be thought of as the number of bits needed to correct the errors in these imperfect reconstructions. In these lookup table representations, these imperfect reconstructions come from the noise added to Z when it is sampled, which cannot be recovered since the lookup table does not contain it. To describe the corrections, we therefore just need to describe this noise. Each noise sample ϵ can be described using $-\log_2 q(\epsilon)$ bits where q is the PMF of the distribution the noise was sampled from. In our case this is a Skellam distribution with a mean of 0, standard deviation of r, and precision of λ. If we let E be the matrix of all noises added form Z, we have that $K(Z|W, f)$ is equal to $-\sum_{\epsilon \in E} \log_2 q(\epsilon)$.

Combining these complexity terms together, the final expression for $C(Z)$ following Definition 2 is:

$$C(Z) = \frac{K(Z)}{K(Z|W)} = \frac{K(p_w) + K(W|p_w) + K(f) + K(Z|W,f)}{K(f) + K(Z|W,f)}$$
$$= \frac{\begin{array}{c} K \log_2 T + T(T+1) - \sum_{j=i}^{N} \sum_{m=1}^{M} \log_2 \frac{1}{|t(w_{i,m-1})|} \\ - \sum_{a \in \text{embedding table}} \log_2 p(a) - \sum_{i \in \text{num rules}} \sum_{(r,c) \in 2D \times D} \log_2 p(A_{i,(r,c)}) - \sum_{\epsilon \in E} \log_2 q(\epsilon) \end{array}}{- \sum_{a \in \text{embedding table}} \log_2 p(a) - \sum_{i \in \text{num rules}} \sum_{(r,c) \in 2D \times D} \log_2 p(A_{i,(r,c)}) - \sum_{\epsilon \in E} \log_2 q(\epsilon)}$$

Experiment parameters We used the following parameter values to generate representations (except when sweeping one parameter while keeping the others constant): $N = 1000$, $M = 16$, $K = 100$, $D = 10$, $T = 5$, $\texttt{width} = 3$, $\texttt{depth} = 2$, $\lambda = 0.01$, $r = 0.01$. To sweep over sentence length, we varied M from $(1, D)$, only keeping values where D was divisible by M. To sweep over grammar width, we varied `width` from $(1, 4)$. To sweep over grammar depth, we varied `depth` from $(1, 4)$. For each setting of experiment parameters, we generated representations across 10 different random seeds.

Appendix G Emergent languages — experimental details

Dataset construction To obtain emergent languages from multi-agent reinforcement learning in a simple object reference game, both with and without iterated learning, we used the code base from Ren et al. (2020), found at `https://github.com/Joshua-Ren/Neural_Iterated_Learning`. Objects consisted of 2 attributes with 8 possible discrete values each, for a total of $8^2 = 64$ possible objects. Sentences similarly were of length 2 and had a vocabulary size of 8. We used the default values in Ren et al. (2020) for all model and training hyperparameters (refer to their associated code base for details), but reserved no held-out objects for separate validation. After training, we generated 50 sentences from the speaker agent for each unique object, giving us W^L and Z, respectively. The resulting size of these datasets were thus $50 \times 8^2 = 3200$.

Estimating compositionality Estimating the compositionalities of these different emergent language systems $C^L(Z)$ requires estimates of the numerator $K(Z)$ and denominator $K(Z|W^L)$. Both with and without iterated learning, Z consisted of the same enumeration over all possible discrete symbolic objects $\mathcal{O}$. Each $z \in Z$ can therefore be represented using a single integer indexing the object, where these integers range from $\{1..|\mathcal{O}|\}$ and therefore each require $\log_2(|\mathcal{O}|)$ bits to encode. Summing these bits over all objects gives a total of $K(Z) = |\mathcal{O}| \log_2(|\mathcal{O}|)$.

We estimated $K(Z|W^L)$ for each language using prequential coding (see Appendix E). The model architecture used for prequential coding was an MLP with 2 hidden layers of size 256. Each word in W^L embedded into a 64-dimensional vector, and these concatenated embeddings were the input to the MLP. The MLP output logits over object values for each attribute. To estimate prequential code lengths more efficiently and avoid having to retrain the model N times (where N is the dataset size), we incremented the size of the dataset by chunks of size 50 at a time. We used the Adam optimizer with a learning rate of 1×10^{-3} to train the model at each iteration of prequential coding. We reserved 400 datapoints for a separate validation set that was used for early stopping at each iteration of prequential coding.

Appendix H Natural languages — experimental details

Dataset construction We obtained English sentences from captions that were used to describe images in the Common Objects in Context (COCO) dataset (COCO, 2024), downloaded from Hugging Face. The reason for using a dataset of image captions was that we expected these captions to use common words and simple sentence structures, given their grounding in visual stimuli. For each image, the dataset contained two independent captions, and we kept only the first. This gave us a total of $414,010$ English sentences. We then translated each sentence to French, Spanish, German, and Japanese using a large open-source language model with 3.3 billion parameters (Costa-jussà et al., 2022). We visually inspected several of the French, German, and Japanese sentences (no authors spoke Spanish) to make sure the translations were reasonable, and we found them to be of high quality. These sentences constituted the W^L's for our experiments. We obtained proxies for the "meanings" Z of these sentences by passing them through a large, pretrained, multilingual sentence embedding model that output a fixed-size vector for each sentence (Reimers and Gurevych, 2020). Both the translation model and the sentence embedding model were obtained from Hugging Face.

Estimating compositionality Estimating the compositionalities of these different language systems $C^L(Z)$ requires estimates of the numerator $K(Z)$ and denominator $K(Z|W^L)$. While we did not estimate $K(Z)$, we assumed that it was approximately equal among languages. This is a common assumption in linguistics, where languages appear

to be equivalent in their expressive power to express ideas, refer to objects, etc. Fixing the numerator $K(Z)$ to some (unknown) constant shared among languages allowed us to assess their *relative* compositionalities by estimating only the denominator $K(Z|W^L)$. We estimated $K(Z|W^L)$ for each language using prequential coding (see Appendix E).

The model architecture used for prequential coding was the same as the one used to generate Z (Reimers and Gurevych, 2020). Learning a significant number of word embeddings from only $\approx 400,000$ samples would have been difficult however. We therefore used the original model's pretrained word embeddings and only computed prequential code length by resets of the model's downstream weights, which encode the semantics of the grammar rather than the word meanings. Strictly speaking, then, we only estimated $K(Z|embeddings(W^L))$. To estimate prequential code lengths more efficiently and avoid having to retrain the model $\approx 400,000$ times, we incremented the size of the dataset in chunks. Chunk boundaries were selected on a base-10 logarithmic scale from $1,000$ to N datapoints (the full size of the dataset), with 15 interval boundaries. A logarithmic scale was used because we observed that next-datapoint prediction error as a function of dataset size changed more quickly in low-data regimes and more slowly in high-data regimes. We could therefore more accurately estimate the true prequential coding curve using a logarithmic chunking scale that had higher resolution in low-data regimes. We used the Adam optimizer with a learning rate of 1×10^{-4} to train the model at each iteration of prequential coding. We reserved $10,000$ datapoints for a separate validation set that was used for early stopping at each iteration of prequential coding.

Limitations Our approach for measuring the compositionalities of real-world language systems has several limitations that should be taken into account when judging the results. First, the translation model that we used may not have been trained on equal amounts of text from the different languages we studied, which could have lead to lower quality translations for some languages compared to others. Similarly, the multilingual sentence embedding model that we used may have not been trained on equal amounts of data from the different languages, leading to lower quality embeddings for some languages compared to others which could have impacted the quantity and accuracy of "true" sentence meaning captured in Z. Indeed, for these reasons we did not include the original English language sentences and embeddings in our experiments (we thought it very likely that the sentence embedding model had been trained on far more English text compared to other languages). Finally, the use of pretrained sentence embeddings as a proxy for sentence meaning Z is likely flawed. The sentence embedding model that we used is trained with invariance-based self-supervised methods, and the resulting representations are unlikely to capture the full scope meaning that would be represented in human brains processing these sentences.