Why think step by step? Reasoning emerges from the locality of experience

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Abstract

Humans have a powerful and mysterious capacity to reason. By working through a series of purely mental steps, we can make inferences we would not be capable of making directly—despite the fact that we get no additional data from the world. Similarly, when large language models generate a series of intermediate steps (a chain of thought) before answering a question, they often produce better answers than they otherwise would. We investigate why and how chain-of-thought reasoning is useful in language models, testing the hypothesis that reasoning is effective when training data consists of local clusters of variables that influence each other strongly. These training conditions enable the chaining of accurate local inferences in order to estimate relationships between variables that were not seen together in training. We prove that there will exist a "reasoning gap", where reasoning through intermediate variables improves inference, for the simple case of an autoregressive density estimator trained on local samples from a chain-structured probabilistic model. We then test our hypothesis empirically in more complex models, training an autoregressive language model on samples from Bayes nets but only including a subset of variables in each sample. We test language models' ability to match conditional probabilities with and without intermediate reasoning steps, finding that intermediate steps are only helpful when the training data is locally structured with respect to dependencies between variables and that the combination of locallystructured observations and reasoning is much more data-efficient than training on all variables. Our results illustrate how the effectiveness of reasoning step by step is rooted in the local statistical structure of the training data.

1 Introduction

The human mind is a ship – the immediate inferences we make from instinct keep us afloat, but reason is the compass that brings us to the shore of wisdom. Many tasks that we find hard to do immediately – solving math problems, planning vacations, understanding our relatives – become much easier when we talk ourselves through a reflective reasoning process. Likewise, by considering thought experiments or "intuition pumps" in science we can form strong beliefs – such as that the rate at which an object falls should not depend on its mass – purely by thinking through a set of steps

[1, 2]. It is not *a priori* obvious that step-by-step reasoning should be helpful. Reasoning does not give us any new data from the world, yet it can still improve our inferences. In investigating the origins of human reasoning, we must thus ask, why does reasoning help?

Large language models have been shown capable of performing a wide variety of tasks by immediately answering a question. However, they struggle with some complex tasks like math word problems [3, 4]. A recent line of work has demonstrated that inducing language models to produce a "chain of thought" consisting of intermediate steps toward a solution, before giving an answer, leads to better performance than prompting them to produce an answer directly [5–7]. Other work has built on these findings, showing that providing worked solutions in context is helpful across many tasks, including logical and common sense question-answering [8, 9]. These findings raise an important question: why is chain-of-thought reasoning useful? Exploring this question may also provide insight into the origins of human reasoning.

We hypothesize that chain-of-thought reasoning is useful in language models due to *local* structure in the training data. Human experience is governed by our first-person perspective: we see and hear aspects of the world that are near to us in time and space. Yet our reasoning transcends these local bounds, supporting plans and conclusions that span distance and years. Similarly, language models are trained on documents in natural language, which have a topic structure. A document is usually about a few topics that are closely interconnected [10, 11]. When concepts co-occur frequently in experience or training data, estimating the effect of one on the other is easy to do directly with simple statistical estimators. However, when we need to infer the effect of one piece of information on another, but have not encountered them together, we must make a series of inferences, jumping between pairs of concepts that connect what we know to what we want to infer. We posit that chain-of-thought reasoning becomes useful exactly when the training data is structured locally, in the sense that observations tend to occur in overlapping neighborhoods of concepts. To illustrate, we may know the value of some variable A and want to know about another variable C, so we would try to estimate P(C|A). However, if we need to estimate probabilities from samples and we have not often seen A and C together, we would struggle to estimate P(C|A) directly from experience. Instead, we might estimate it by reasoning through intermediate variables. If conditioning on an intermediate variable B renders A and C independent of each other, we can compute the conditional probability by marginalizing over B, using the fact that $P(C|A) = \sum_{B} P(C|B)P(B|A)$.

Our hypothesis is similar to that advanced by Chan et al. [12] to explain why in-context learning (generalizing from examples shown in context) occurs. They show that "burstiness," the tendency of the same classes to be clustered close together, in the training data is important for language models to learn to infer tasks based on examples in the context window. Burstiness and locality are two different statistical properties of training data that could arise from topic structures in language models or an ego-centered perspective in humans.

In this work, we train language models on samples from Bayesian networks while varying observation structures and evaluate their ability to match conditional probabilities. Our theoretical and experimental results show that performing conditional inference by first generating intermediate variables improves the ability of a language model to match true conditional probabilities only when the training data is structured locally with respect to strong dependencies and the intermediate variables are relevant to the relationship between the variables of interest. Allowing the model to *generate* intermediate variables and their values is similarly helpful to being given ideal intermediate variables to reason through. This suggests that chain-of-thought reasoning is useful for language models because:

1) Direct prediction is inaccurate for some inferences because the relevant variables are rarely seen together in training; 2) Chain-of-thought reasoning improves estimation because it can incrementally chain local statistical dependencies that are frequently observed in training. Furthermore, we find that the combination of locally-structured training data and reasoning with self-generated intermediate variables yields much greater data-efficiency than training on data containing all variables.

2 Task setup

Our theory and experiments take place in the context of conditional inference in joint distributions, as represented by Bayesian networks. In our framing, a learner sees samples from the Bayes net and needs to accurately estimate conditional probabilities. However, the learner may not see all variables together, having access only to locally-structured observations instead.

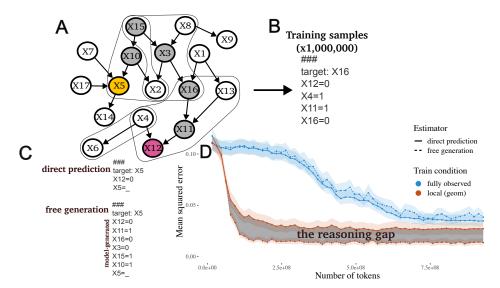


Figure 1: Overview of our training and estimation setup. A: visualization of a Bayes net. The pink variable is an example observed variable and the yellow variable is an example target variable. Grey variables are examples of useful intermediate variables for reasoning. Lines show examples of local neighborhoods from which training samples are drawn. B: format of the training samples. C: illustration of direct prediction and free generation estimators as prompts. We prompt the model to either immediately predict the target variable (direct prediction), or do so after generating intermediate variables and their values (free generation). We then compute mean squared errors between estimated and true conditional probabilities. D: mean squared error by number of training tokens for each train condition and estimator.

We describe our framework formally. First, we assume there is some underlying Bayes net with random variables $\{Y_i\}_{i=1}^N$ taking support in some finite set \mathcal{X} . We denote the distribution defined by the Bayes net as p_d , the *data distribution*. Our training data is a sequence of *variable indices* $i \in \{1, \dots N\}$, and *variable values* $v_i \in \mathcal{X}$. Variable values always follow variable indices.

2.1 Observation distribution

One important notion in our experiments and theory is the observation distribution p_{obs} , which is a distribution over subsets of the variable indices. Observation distributions take support on a set $\mathcal{Y}_{obs} \subseteq \mathcal{P}(\{1,\ldots,N\})$. As a consequence, our learner will only see samples from the joint distribution over certain subsets of random variables in the Bayes net. The generative process for our sequence consists of two steps. First, we sample a set of variable indices $\{i_t\}_{t=1}^K$ according to p_{obs} ; the variable indices appear in random order. These indices correspond to some set of random variables $\{Y_{i_t}\}_{t=1}^K$ in the Bayes net. We then sample the variable values $\{v_{i_t}\}_{t=1}^K$ of these variable indices according to the distribution $p_d(Y_{i_1},\ldots,Y_{i_K})$. Importantly, p_d and p_{obs} together define a distribution p on training sequences.

We are particularly interested in local observation distributions as they enable the learning of strong dependencies and reflect some of the statistical structure of human experience. In local observation distributions, the learner observes a subset of variables that are close together in the Bayes net graph. Figure 1A shows several local neighborhoods on an example Bayes net.

2.2 Estimators

Given an autoregressive conditional probability estimation model q that is trained to predict variable indices and values, we can use one of three different estimators for the conditional probabilities. The estimators differ in what sequence gets produced before estimating the target variable. If we want to compute the conditional probability of a target variable Y_i being some value y_i given some observed variable Y_j known to be y_j , we can use one of the following estimators.

Direct prediction The direct prediction estimator is the baseline without any reasoning: it is the probability directly output by q.

$$\hat{q}_D(Y_i = y_i | Y_j = y_j) = q(Y_i = y_i | Y_j = y_j). \tag{1}$$

We simply use the model to directly estimate the probability of the target variable given the value of the observed variable.

Scaffolded generation The scaffolded generation estimator represents ideal reasoning if we knew the best set of steps to work through. A scaffold is an ordered set S consisting of variables that were each observed with another scaffold variable and collectively d-separate the observed variable from the target variable. In the case of a chain, the scaffold consists of all variables between Y_i and Y_j . Variables are ordered by their distance from the observed variable in the Bayes net. We estimate each variable given the observed variable and previously-generated scaffold variables using q before estimating the target probability. We approximately marginalize over the scaffold variables' values using M Monte Carlo samples from the conditional distributions.

$$\hat{q}_S(Y_i = y_i | Y_j = y_j) = \frac{1}{M} \sum_{k=1}^M q(Y_i = y_i | \{Y_s = y_s^{(k)}\}_{s \in S}, Y_j = y_j)$$
(2)

where
$$y_s^{(k)} \sim q(Y_s | \{Y_t = y_t^{(k)}\}_{t \in S | t \prec s}, Y_j = y_j)$$
 (3)

We will denote the distribution defined by the sampling procedure in 2 by q_S .

Free generation The free generation estimator is similar to scaffolded generation in that it generates intermediate variables before the target, but free generation uses the model to choose which variables to instantiate rather than just to estimate their values. We simply sample variable indices and values from q until it generates the index of the target variable. At that point, we compute the probability of the target variable. We average over M such samples. This estimator tests whether trained models spontaneously generate useful intermediate variables.

3 Theoretical results

In order to understand the range of situations in which reasoning might be useful, we study the conditions under which a risk-minimizing sequence model q benefits from reasoning through intermediate variables. In particular, we analyze a simplified version of our task in which the training data consists of pairs of adjacent variables from a directed chain. In this setting, we prove that the minimizer of a risk consisting of cross entropy with entropy regularization exhibits a *reasoning gap* in which the bias of direct conditional probability estimates between non-adjacent pairs of random variables is higher than indirect estimates that chain together conditional probabilities of intermediate random variables.

We assume that a risk minimizer q is trained on a sequence of alternating variable indices $i_t \in \{1,\ldots,N\}$ and variable values $Y_i \in \mathcal{X}$ where the Y_i s take support in some finite set \mathcal{X} . In the sequence, variable values always follow variable indices. We assume that the joint distribution p_d over Y_1,Y_2,\ldots,Y_N factorizes as $p_d(Y_1,\ldots Y_N)=p_d(Y_1)\prod_{i=1}^N p_d(Y_{i+1}|Y_i)$. The observation distribution p_{obs} only assigns non-zero probability to non-adjacent variable pairs, i.e. $p_{\text{obs}}(\{i,j\})=0$ if |i-j|>1 and $p_{\text{obs}}(X)=0$ if $|X|\neq 2$. The training set consists of i.i.d. samples from p, which is the distribution over complete sequences of variable indices and values defined by p_{obs} and p_d .

We show that when our data has the locality structure as described, marginalizing over intermediate random variables by using the learned conditional probabilities between adjacent variables leads to lower bias estimates than using the learned estimate directly:

Theorem 3.1. Let S be the space of possible sequences consisting of variable indices followed by variable values. Let u be the uniform distribution over S. Let H(p,q) denote the cross entropy between distributions p and q. We consider the following risk:

$$R(q) = H(p,q) + H(u,q) \tag{4}$$

Let $q^* = \arg \min_q R(q)$ be a minimizer of the risk over all possible probability distributions. Then, for all non-adjacent random variables Y_i and Y_j , reasoning through the intermediate variables has

lower bias than direct prediction. That is, for any $y_i, y_j \in \mathcal{X}$:

$$|\mathbb{E}_{q_s^*}[\hat{q}_S(Y_i = y_i|Y_j = y_j)] - p_d(Y_i = y_i|Y_j = y_j)|^2$$

$$< |\hat{q}_D(Y_i = y_i|Y_j = y_j) - p_d(Y_i = y_i|Y_j = y_j)|^2$$

Here, the expectation is over the randomness in the Monte Carlo samples of intermediate variables.

Proof sketch. We characterize q^* in terms of p_d and u by analyzing the risk, which decomposes into a sum of cross-entropy terms, either between $q(\cdot)$ and $p(\cdot)$ or between $q(\cdot)$ and $q(\cdot)$ and q(

We consider two cases. For any adjacent pairs Y_i and Y_{i+1} , $q^*(Y_{i+1}|Y_i)$ will interpolate between the conditional probability $p_d(Y_{i+1}|Y_i)$ and the uniform distribution. This is because the risk will contain a term of the form $\mathbb{E}_{p_d(Y_{i+1}|Y_i)}[\log q(Y_{i+1}|Y_i)]$ and a term of the form $\mathbb{E}_u[\log q(Y_{i+1}|Y_i)]$. As we show in the appendix, the minimizer of the sum of these terms is a mixture between $p_d(Y_{i+1}|Y_i)$ and the uniform distribution. On the other hand, for non-adjacent pairs Y_i and Y_j , $q^*(Y_i|Y_j) = \frac{1}{|\mathcal{X}|}$. As a consequence of the observation distribution p_{obs} , Y_i and Y_j will never appear together. Therefore, we will only find a term of the form $\mathbb{E}_u[\log q(Y_i|Y_j)]$ in the risk and minimizing the risk for Y_i and Y_j is equivalent to minimizing the entropy regularization term since the risk does not penalize $q^*(Y_i|Y_j)$ for not matching $p_d(Y_i|Y_j)$.

Given q^* , we can calculate the bias of the scaffolded estimator \hat{q}_S , where we approximately marginalize over the intermediate random variables by sampling from the conditional probability distributions $q^*(Y_{i+1}|Y_i)$. By the argument above, the scaffolded estimator is a mixture between $p(Y_{i+1}|Y_i)$ and u with mixture weight $\lambda \in (0,1)$. Therefore, its bias can be expressed as $(1-\lambda)^2|p(Y_{i+1}|Y_i)-\frac{1}{|\mathcal{X}|}|$. The second term in the product is exactly the bias of the direct estimator and $(1-\lambda)^2 < 1$. The desired inequality immediately follows. Intuitively, the bias of the scaffolded estimator is lower because it leverages the dependency structure of the data, chaining together local conditional probabilities of variables it has seen together in training to estimate conditional probabilities for unseen pairs. \square

We note that a similar theorem holds without entropy regularization, but with some additional assumptions about training sequences. Full details of the theorem, alternative formulations, and proofs can be found in Appendix A. In the next section, we explore whether the reasoning gap occurs in practice for transformer language models in situations with more complex dependency and observation structures.

4 Experimental methods

We test our hypothesis that locally-structured training data leads to a reasoning gap by training a language model (i.e., an autoregressive density estimator with a transformer architecture) and testing conditional inference accuracy. We manipulate the structure of the training data and measure the effectiveness of different estimators. The key question is whether there are training conditions under which scaffolded or free generation out-perform direct prediction. Code and data are available at https://github.com/benpry/why-think-step-by-step.

4.1 Training data

The first step in generating our training data is to create Bayes nets. We generate a random topology for the networks, incrementally adding 100 random edges between pairs of variables. After generating a topology, we create conditional probability tables for each variable. We design the conditional probability tables, and select among generated Bayes nets, to maximize the mutual information between distant variable pairs. (If we did otherwise, the conditional probabilities would be very close to the marginal probabilities of the target variables and a language model could come very close to matching true conditional probabilities without learning the relationships between variables.) The probability of a variable being 1 for each setting of its parents is randomly sampled from $\text{Beta}(\frac{1}{5},\frac{1}{5})$, which favors nearly deterministic relationships. We generate 100 Bayes nets according to this process, then compute the mutual information between each pair of variables. We select the 50 pairs of non-adjacent variables that have the highest mutual information, then randomly sample 25 of those pairs to hold out from the training set. Finally, we select the 10 Bayes nets, out of the initial 100, for

which the 25 held-out pairs of variables have the highest mean mutual information. Pseudocode for Bayes net generation is shown in Algorithm 1 of Appendix B.

For each of the 10 selected Bayes nets, we generate a training set consisting of 1 million samples formatted as strings. The strings consist of the name of each variable followed by its value; variables are ordered randomly. Variable names are the letter 'X' followed by a number from 0 to 99. For example, if the variable 'X42' has value 1, the string would include the line "X42=1". We mention the name of the last variable in the sample in the beginning of the string, marking it with the word "target." We also include '###' before the sample to indicate where it begins. A schematic example of a formatted sample string is shown in Figure 1B and a full example is shown in Appendix C.

From each complete sample from the Bayes net, we select a subset of sampled variables according to the *observation distribution*, which is a distribution over subsets of variables. Pseudocode for getting a subset of variables from an observation distribution is shown in Algorithm 2 in Appendix B. At a high level, observation distributions have three important properties:

Locality Observed samples contain only variables from a local neighborhood, consisting of a central variable along with all variables of distance at most k from it. To sample from the observation distribution, we sample the central variable uniformly randomly and then sample k from some distribution that controls the local neighborhood size. In our experiments, we draw k either from a geometric distribution with a parameter of 0.5 or a Zipfian distribution with a parameter of 2.

Variable dropout Even within a local subset of the world, we may not see everything at once. Certain variables may be missing or go unnoticed. We formalize this intuition with *variable dropout*. With some probability (0.2 in our experiments), variables are dropped from a local neighborhood and the learner does not see them. Variable dropout may also help a model generalize to pairs of variables that were unseen in training as more unique subsets of variables appear in the training set.

Held-out pairs Finally, target pairs of variables are held out across all training data. Performance at matching conditional probabilities for these pairs is our main performance metric. If a local neighborhood, after variable dropout, would include a pair of variables we decided to hold out, we randomly remove one of the two variables in the pair from the sample.

We also create two **control conditions** to demonstrate the importance of a local observation distribution. As one control, we consider training data made up of local neighborhoods from the wrong Bayes net. This maintains the co-occurrence distribution structure, but the co-occurrences do not reflect the structure of which variables influence each other. As another control, we use a *fully-observed* condition where each sample contains almost all of the variables in the Bayes net. One of the two variables in each held-out pair is randomly dropped, but all other variables are included. These controls enable us to test whether local structure in the training data drives the value of reasoning.

4.2 Estimation

Each of the estimators in Section 2.2 is implemented via a combination of sampling from and scoring with the language model. For instance, in free generation the model is prompted with the target variable name and initial observation (as in training data) and sampled from until the target variable is generated. The probabilities for different values are then examined. Figure 1C illustrates how we implement direct prediction and free generation as prompts and Appendix D contains examples of each estimator. For estimators that rely on Monte Carlo estimation, we use 10 samples.

We also introduce *negative scaffolded generation* as a control estimator that generates irrelevant intermediate variables. For each pair of variables, we select a random set of variables equal in size to the scaffold, but which does *not* include any of the scaffold variables. We prompt the language model to generate values for the negative scaffolds in the same way as in scaffolded generation.

4.3 Model architecture

We use a smaller version of the GPT-2 autoregressive transformer architecture [13], as implemented by the HuggingFace transformers library [14]. Our model has 512-dimensional embeddings, 10 layers, and 8 attention heads. Data is tokenized via a Byte Pair Encoding tokenizer fit to data in our format [15]. We trained this architecture with randomly-initialized weights for 300,000 gradient

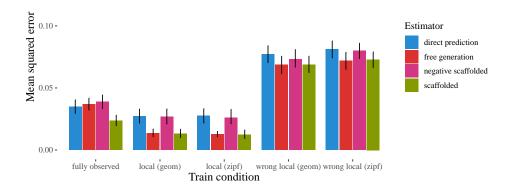


Figure 2: Mean squared errors between estimated and true conditional probabilities for held-out pairs with high mutual information. Error bars denote 95% confidence intervals. Both free and scaffolded generation significantly out-perform direct prediction when the training data is locally structured.

Table 1: Mean squared errors with 95% confidence intervals between direct prediction probabilities and either true or marginal probabilities for non-held-out pairs with high mutual information. In the local training conditions, direct prediction is close to perfect at matching the conditional probabilities.

	fully observed	local (geom)	local (zipf)	wrong local (geom)	wrong local (zipf)
true	. , ,	.004 [.003, .005]	.003 [.003, .004]	.052 [.046, .060]	.056 [.050, .062]
marginal		.114 [.105, .121]	.112 [.105, .120]	.047 [.042, .051]	.033 [.029, .038]

steps on batches containing 3,072 tokens each, for a total of 921,600,000 tokens of training. We trained our model using the Adam optimizer [16]. Each language model's training set consisted of 1,000,000 samples from a single Bayes net. The models achieved near-perfect performance on the training task. Further training details are provided in Appendix E.

5 Results

We measure a language model's ability to accurately estimate conditional probabilities for held-out pairs by computing the mean squared error (MSE) between the estimated and true probabilities. Each held-out pair gives four data points: if we hold out the pair X1, X2 we can compute p(X1|X2=0), p(X1|X2=1), p(X2|X1=0), and p(X2|X1=1). Pooling across the 10 Bayes nets we trained models on gives us 1,000 data points per train condition and estimator. Figure 1D shows our main result: free generation performs better (lower MSE) than direct prediction and performs strongly with less training when the data is structured locally. The MSEs for all estimators and training conditions after 921.6 million tokens (300,000 gradient steps) of training are shown in Figure 2.

5.1 When reasoning helps

We find a benefit to reasoning when the observation distribution has the correct locality structure. When the training data is structured locally with respect to strong dependencies, both scaffolded and free generation perform significantly better than direct prediction—the *reasoning gap*. Scaffolded and free generation also perform significantly better than negative scaffolded generation, indicating that relevant intermediate variables help in predicting the target variable, but irrelevant intermediate variables do not. Furthermore, the success of free generation demonstrates that a model trained on local subsets of a Bayes net can self-generate helpful intermediate variables.

In free generation, the model continues generating variables until it produces the target variable. This results in reasoning traces of varying length, including many long traces. One might expect long traces to distract the model, but this did not occur in our experiments: the length of the reasoning

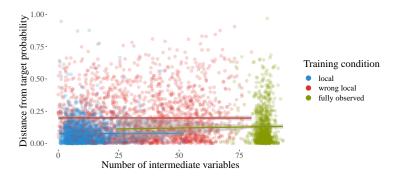


Figure 3: Number of intermediate variables generated in free generation vs. absolute distance between true and estimated conditional probabilities for each training condition. Lower dots indicate more accurate estimation, while dots further to the right indicate more intermediate variables generated.

trace does not relate strongly to the accuracy, as is shown in Figure 3. However, free generation does not out-perform direct prediction substantially when the training data is fully observed.

It is also of note that training on locally-structured data reduces the average length of reasoning traces (Fig. 3). In local training conditions, free generation usually produces a set of variables that *d*-separates the observed variable from the target variable – 71% of the time in the local neighborhood conditions. In contrast, the training conditions with the wrong locality structure only lead to *d*-separating reasoning traces 34% of the time. The fully-observed training condition also usually created *d*-separating reasoning traces (69%), likely because it generated a large number of variables. *d*-separation is important because it ensures that all the influence that the observed variable has on the target variable is captured by the intermediate variables. These results suggest that training on local clusters of variables is valuable because it helps free generation produce intermediate variables that are relevant to the relationship between the observed and target variables. Still, chain-of-thought reasoning can be helpful even if the reasoning trace does not completely *d*-separate the two variables. In the local training conditions, the model does not generate a *d*-separating trace 29% of the time, yet there is virtually no performance difference between free and scaffolded generation.

5.2 Data complexity and reasoning

The combination of locally-structured training data and step-by-step reasoning can also lead to accurate conditional probability estimates with much less training than would be required if a model were trained on fully-observed data. To demonstrate this difference, we run both direct prediction and free generation on checkpoints from our models that are generated after every 5000 gradient steps (15.3 million tokens) of training. Part D of Figure 1 shows the results of this analysis.

When data is fully observed, direct prediction and free generation performances improve slowly but consistently. There is no reasoning gap, as both estimators perform almost identically. When the model is trained on data from geometrically-sized local neighborhoods, direct prediction performance improves quickly, then plateaus. There is a substantial reasoning gap where free generation outperforms direct prediction. Free generation matches the true conditional probabilities very closely after about 120 million training tokens, achieving the best performance of any combination of training data type and estimator. Still, a sufficiently large transformer can eventually memorize the relationships in its training corpus with enough training. We evaluated the data complexity of direct learning by training a language model of the same architecture on fully-observed data without any held-out pairs. Direct prediction in this case takes over 3 times as much training to achieve the same performance as local training with free generation, despite the model seeing the relevant pairs in training (see Appendix F for detailed results). Training language models on datasets consisting of local neighborhoods with strong dependencies and performing chain-of-thought reasoning at inference time can therefore be more data-efficient than training on more complete data.

Table 2: Mean squared errors between estimated conditional probabilities and marginal probabilities of target variables with 95% confidence intervals. Lower values indicate closer matches.

	fully observed	local (geom)	local (zipf)	wrong local (geom)	wrong local (zipf)
direct prediction	.086 [.079, .092]	.115 [.107, .123]	.116 [.108, .124]	.029 [.025, .033]	.022 [.018, .025]
scaffolded	.107 [.099, .114]	.132 [.124, .140]	.131 [.123, .140]	.048 [.043, .053]	.040 [.035, .046]
free generation	.120 [.112, .129]	.123 [.116, .130]	.127 [.119, .134]	.049 [.044, .055]	.043 [.038, .049]
negative scaffolded	.089 [.082, .095]	.116 [.108, .123]	.115 [.107, .123]	.035 [.031, .040]	.026 [.022, .030]

5.3 When reasoning is unnecessary

Table 1 shows MSEs between direct prediction estimates and true probabilities for the 25 high-mutual-information variable pairs that were *not* held out from the training set. In the local training conditions (and to a lesser extent fully-observed), direct prediction matches the true conditional probabilities almost perfectly. This indicates that our language models learn to match conditional probabilities directly when the observed and target variables co-occur in the training distribution. Observing these variables together frequently obviates the need for step-by-step reasoning.

5.4 When reasoning fails

We test the hypothesis that language models match the *marginal* probabilities of the target variables when they fail to predict the true conditional probabilities by comparing models' estimates against the true marginal probabilities. The mean squared errors between the estimated conditional probabilities and marginal probabilities of the relevant target variables are shown in Table 2. We can see the opposite of the trend for true probabilities: the worse a training condition does at matching the true conditional probability, the better it matches the marginal. The language models trained on data with the wrong locality structure generated estimates that were particularly close to the marginal probabilities. When the variables that co-occur with each other frequently are not local in the Bayes net, they often have very little influence on each other. This means that the joint distribution over co-occurring variables is usually very close to the product of the marginal probabilities, i.e. $P(X_1, X_2, X_3) \approx P(X_1)P(X_2)P(X_3)$ for non-local X_1, X_2, X_3 . Without the ability to estimate conditional probabilities accurately, there are no reliable 'steps' for step-by-step reasoning to use.

6 Discussion

Our theoretical and empirical results demonstrate that estimating conditional probabilities by reasoning through intermediate variables can out-perform direct prediction when the training data has local structure. When the training data includes all the variables, free generation does not lead to better performance than direct prediction. When the training data has the wrong locality structure, the models do not reliably learn conditional probabilities that can be chained together. Our results demonstrate a minimal case in which chain-of-thought reasoning is helpful and suggest important conditions under which it is likely to be helpful in more naturalistic settings: we can expect chain-ofthought reasoning to help when a model is tasked with making inferences that span different topics or concepts that do not co-occur often in its training data, but can be connected through topics or concepts that do. Furthermore, chain-of-thought reasoning enables greater data efficiency: a model trained on locally-structured data with chain-of-thought reasoning at inference time can accurately match conditional probabilities with less training than a model trained on all the data. This result can provide insight into why humans are more data-efficient than language models. Since humans experience the world from a first-person perspective, the information we encounter is structured in small clusters of entities that are tightly coupled with each other. This idea could also be relevant to data curation for the training of language models. Constructing datasets with tightly-correlated observation neighborhoods that collectively cover the space of relevant concepts may amplify language models' ability to perform chain-of-thought reasoning while reducing their data needs.

Future work should explore the structure of the observation distribution for human learners to understand whether and how the information we observe facilitates reasoning. Using modern language models as toy models in which we can study reasoning is a promising direction for computational cognitive science to study long-standing problems in reasoning and problem solving, such as the

value of thought experiments. Finally, we plan to explore questions of how language models might learn to reason more effectively through fine-tuning, in-context learning, and reinforcement learning.

Limitations Of the many forms of chain-of-thought prompting that exist in the literature, our findings are most relevant to zero-shot prompting [e.g. 5] where a model instantiates intermediate variables on the way to an answer without any other examples of reasoning traces in its context window. It is less applicable to methods that involve giving the model examples of reasoning [e.g. 7]. Our results are also in the context of simple propositional worlds. Reasoning in rich worlds with more structure may require more expressive languages with which to reason and specify hypotheticals. Our theoretical results do not predict the empirical phenomenon that transformers revert to the marginal distributions for held-out pairs. We leave it to future work to explore how the inductive biases of transformers might induce this behavior on unseen data.

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A Theoretical analysis

In this section, we theoretically analyze chain-of-thought reasoning when the underlying data distribution can be represented as a directed chain. We prove that the minimizer of a risk consisting of a cross entropy term and an entropy regularization term will exhibit a "reasoning gap" when the data has a particular locality structure.

A.1 Problem Setup

We assume that we observe a sequence of variable indices $i_t \in \{1, \dots, N\}$ and variable values $v_t \in \mathcal{X}$ for some finite set \mathcal{X} . In the sequence, variable values always follow variable indices. Note that, since our results concern estimators that are only ever conditioned on a single variable, it suffices to consider sequences of length two. However, our setup can be interpreted as assuming we observe independent local neighborhoods of size 2 with token separators.

Factorization of data distribution We assume that the joint distribution p_d over Y_1, Y_2, \dots, Y_N factorizes as

$$p_d(Y_1, \dots Y_N) = p_d(Y_1) \prod_{j=1}^N P_d(Y_{j+1}|Y_j)$$

and that Y_1, Y_2, \dots, Y_N take support in some finite discrete set \mathcal{X} . Note that the variable indices index particular random variables in p_d .

Local observation distribution We will consider a setting where only adjacent variables in the graphical model can appear adjacent in the sequence. More formally, let \mathcal{Y} refer to the set of all variable identifiers. Let \mathcal{Y}_{obs} be the set of all allowed pairs of variable indices. Then, $\mathcal{Y}_{\text{obs}} \subseteq \mathcal{P}(\{1,\ldots,N\})$ and \mathcal{Y}_{obs} consists of pairs of the form (i,i+1). We will define the distribution over these valid subsets of variable indices as p_{obs} ; in particular, p_{obs} takes support only on \mathcal{Y}_{obs} and assigns equal probability to all of its pairs. The two distributions p_d and p_{obs} define a distribution p over the sequence of variable indices and variable values.

That is, for any non-adjacent pairs Y_i and Y_j and for any variable values y_i and y_j ,

$$p(i_1 = i, v_1 = y_i, i_2 = j, v_1 = y_j) = 0$$
(5)

For adjacent pairs Y_{i+1} and Y_i and for variable values y_{i+1} and y_i ,

$$p(i_1 = i, v_1 = y_i, i_2 = i + 1, v_1 = y_{i+1}) \propto p_d(Y_i = y_i, Y_j = y_j)$$
(6)

Intuitively, this property will imply that the risk minimizer only gets to see a small subset of local statistical dependencies in the graphical model. This key property of the observation distribution will induce a reasoning gap.

A.2 Preliminaries

We begin with a proposition that will be useful in the main theorem. The proposition concerns the minimizer of the sum of two cross-entropy terms.

Proposition 1. Let
$$\alpha_1 \geq 0$$
, $\alpha_2 \geq 0$. Let $R(q) = \alpha_1 \mathbb{E}_{p_1(x)}[-\log q(x)] + \alpha_2 \mathbb{E}_{p_2(x)}[-\log q(x)]$. Then $q^* = \arg \min R(q) = \frac{\alpha_1}{\alpha_1 + \alpha_2} p_1(x) + \frac{\alpha_2}{\alpha_1 + \alpha_2} p_2(x)$

Proof. We assume the probability distributions are discrete. The Lagrangian is given by

$$\mathcal{L}(q, \lambda_0) = -\alpha_1 \sum_{x} p_1(x) \log q(x) + -\alpha_2 \sum_{x} p_2(x) \log q(x) + \lambda_0 (\sum_{x} q(x) - 1)$$
 (7)

The first order conditions are

$$\frac{\partial \mathcal{L}}{\partial q(x)} = -\alpha_1 \frac{p_1(x)}{q(x)} + -\alpha_2 \frac{p_2(x)}{q(x)} + \lambda_0 = 0 \tag{8}$$

$$\frac{\partial \mathcal{L}}{\partial \lambda_0} = \sum_{x} q(x) - 1 = 0 \tag{9}$$

(10)

The first condition allows us to write $q(x) = \frac{\alpha_1 p_1(x) + \alpha_2 p_2(x)}{\lambda_0}$. We can substitute this for q into the other first order condition (*i.e.*, q normalizes) to obtain

$$\sum_{x} \frac{\alpha_1 p_1(x) + \alpha_2 p_2(x)}{\lambda_0} = 1$$

This implies $\lambda_0 = \alpha_1 + \alpha_2$ and the desired result follows immediately.

A.3 Main Theorem

Our main result is that the minimizer of the risk q^* under the distribution p defined by $p_{\rm obs}$ and p_d and a cross-entropy loss function with entropy regularization will exhibit a "reasoning gap". We begin with a characterization of q^* . For simplicity, in the result below, we'll use x_t to denote elements of the sequence that correspond either to variable values i_t or variable indices i_t .

Theorem A.1. Let u be the uniform distribution. Let p be the distribution over variable indices and variable values defined by p_{obs} and p_d . Let H(p,q) denote the cross entropy between distributions p and q. We consider the following risk: Then $q^* = \arg\min_q R(q)$ satisfies the following properties.

- For all pairs of adjacent random variables Y_i and Y_{i+1} , $q^*(Y_i|Y_j) = \lambda p_d(Y_{i+1}|Y_i) + (1 \lambda)\frac{1}{|\mathcal{X}|}$ for some $\lambda \in (0, 1)$.
- For all pairs of non-adjacent random variables, $q^*(Y_i|Y_j) = \frac{1}{|\mathcal{X}|}$.

Proof. We can write the risk as a sum across timesteps.

$$R(q) = \sum_{t=1}^{T} \mathbb{E}_{p(x_{1:t})} \left[-\log q(x_t|x_{1:t-1}) \right] + \sum_{t=1}^{T} \mathbb{E}_{u(x_{1:t})} \left[-\log q(x_t|x_{1:t-1}) \right]$$
(11)

(12)

Let us consider the left sum. By the law of iterated expectations, we can decompose the fourth term in the sum where x_4 is a variable value as

$$\mathbb{E}_{p(i_{1:2},v_{1:2})}[-\log q(v_2|i_{1:2},v_1)] \tag{13}$$

$$= \mathbb{E}_{p(i_{1:2},v_1)} [\mathbb{E}_{p(v_2|i_{1:2},v_1)} [-\log q(v_2|i_{1:2},v_1)]]$$
(14)

$$= \sum_{i_1} \sum_{v_1} \sum_{i_2} \mathbb{E}_{p(v_2|i_{1:2},v_1)} [-\log q(v_2|i_{1:2},v_1)] p(i_{1:2},v_1)$$
(15)

$$= \sum_{i_1, i_2 \in \mathcal{Y}_{obs}} \sum_{v_1} \mathbb{E}_{p(v_2|i_{1:2}, v_1)} [-\log q(v_2|i_{1:2}, v_1)] p(i_{1:2}, v_1)$$
(16)

Importantly, notice that the outer sum over the variable indices i_1, i_2 is over \mathcal{Y}_{obs} due to the observation distribution.

On the other hand, consider the right sum.

$$\mathbb{E}_{u(i_{1:2},v_{1:2})}[-\log q(v_2|i_{1:2},v_1)] \tag{17}$$

$$= \mathbb{E}_{u(i_{1:2},v_1)} \left[\mathbb{E}_{u(v_2|k_{1:2},v_1)} \left[-\log q(v_2|i_{1:2},v_1) \right] \right]$$
 (18)

$$= \sum_{i_1} \sum_{v_1} \sum_{i_2} \mathbb{E}_{u(v_2|i_{1:2},v_1)} [-\log q(v_2|i_{1:2},v_1)] u(i_{1:2},v_1)$$
(19)

$$= \sum_{i_1, i_2 \in \mathcal{Y} \times \mathcal{Y}} \sum_{v_1} \mathbb{E}_{u(v_2|i_{1:2}, v_1)} [-\log q(v_2|i_{1:2}, v_1)] u(i_{1:2}, v_1)$$
(20)

(21)

We consider two different cases. Suppose the variable indices are adjacent so that $i_2 = i + 1$ and $i_1 = i$ for some i. In addition, fix some value for v_1 . Then, we can take exactly two terms, one from the left and right sum.

$$\frac{1}{2} \mathbb{E}_{p(v_2|i_{1:2},v_1)} [-\log q(v_2|i_{1:2},v_1)] p(i_{1:2},v_1)
+ \frac{1}{2} \mathbb{E}_{u(v_2|i_{1:2},v_1)} [-\log q(v_2|i_{1:2},v_1] u(i_{1:2},v_1)$$
(22)

The expectations that appear in Eq 22 are either 1) a cross entropy between either $q(Y_i|Y_j)$ and $p_d(Y_i|Y_j)$ or 2) a cross entropy between $q(Y_i|Y_j)$ and the uniform distribution. By an application of Proposition 1, the sum of these two terms is minimized by taking $q^*(Y_i|Y_j) = \lambda_{i,j} \frac{1}{|\mathcal{X}|} + (1 - \lambda_{i,j})p(Y_i|Y_j)$ for $\lambda_{i,j} = \frac{u(i_{1:2},v_1)}{u(i_{1:2},v_1)+p_d(Y_i|Y_j)}$. The result holds for any adjacent pairs.

Finally, we consider non-adjacent pairs Y_i and Y_j . By construction, we can never have $i_2 = i, i_1 = j$ in the left sum. We will only have one cross entropy between $q^*(Y_i|Y_j)$ and $u(Y_i)$. Therefore, minimizing the risk is equivalent to minimizing the entropy regularization term and taking $q^*(Y_i|Y_j) = \frac{1}{|\mathcal{X}|}$.

In the following corollary we will show that squared bias of the scaffolded generation estimator, which explicitly reasons through intermediate variables, is less than the squared bias of the direct estimator.

Theorem A.2. For all $y_i, y_j \in \mathcal{X}$ with |i - j| > 1,

$$|\mathbb{E}[\hat{q}_{S}^{*}(Y_{i}=y_{i}|Y_{j}=y_{i})] - p(Y_{i}=y_{i}|Y_{j}=y_{i})|^{2} < |\hat{q}_{D}^{*}(Y_{i}=y_{i}) - p(Y_{i}=y_{i}|Y_{j}=y_{i})|^{2}$$

Proof. We will calculate both sides of the inequality. Here the expectation is understood to be taken with respect to $y_i \sim q^*(Y_i|Y_{i-1}=y_{i-1}), y_{i-1} \sim q^*(Y_{i-1}|Y_{i-2}=y_{i-2})\dots y_{j+1} \sim q^*(Y_{j+1}|Y_j=y_j)$. We begin by showing that $\mathbb{E}[\hat{q}_S^*(Y_j=y_j|Y_i=y_i)] = \lambda p(Y_i|Y_j) + (1-\lambda)\frac{1}{|\mathcal{X}|}$ for some $\lambda \in (0,1)$. We prove this result for the case where $Y_i=Y_3$ and $Y_j=Y_1$ but the same calculation applies for any other i,j with |i-j|>1, and when we sample from the intermediate conditional probabilities $q^*(Y_k|Y_{k-1})$ for i< k< j.

$$\begin{split} \mathbb{E}_{y_2 \sim q^*(Y_2|Y_1)}[q^*(Y_3 = y_3|Y_2 = y_2)] \\ &= \sum_{y_2} q^*(Y_3 = y_3|Y_2 = y_2)q^*(Y_2 = y_2|Y_1 = y_1) \\ &= \mathbb{E}_{y_2 \sim q^*(Y_2|Y_1)}[(1 - \lambda_{3,2})p(Y_3 = y_3|Y_2 = Y_2) + \lambda_{3,2}\frac{1}{|\mathcal{X}|}] \qquad \text{by Theorem 3.1} \\ &= \lambda_{3,2}\frac{1}{|\mathcal{X}|} + (1 - \lambda_{3,2})\mathbb{E}_{y_2 \sim q^*(Y_2|Y_1)}[p(Y_3 = y_3|Y_2 = Y_2)] \\ &= \lambda_{3,2}\frac{1}{|\mathcal{X}|} \\ &+ (1 - \lambda_{3,2})(1 - \lambda_{2,1})\sum_{y_2} p(Y_3 = y_3|Y_2 = y_2)p(Y_2 = y_2|Y_1 = y_1) \\ &+ (1 - \lambda_{3,2})(\lambda_{2,1})\sum_{y_2} \frac{1}{|\mathcal{X}|}p(Y_2 = y_2|Y_1 = y_1) \\ &= (1 - \lambda)\frac{1}{|\mathcal{X}|} + \lambda p(Y_3 = y_3|Y_1 = y_1) \end{split}$$

Here $\lambda = (1 - \lambda_{3,2})(1 - \lambda_{2,1})$. Importantly, the expected value is a strict convex combination of the marginal and conditional probabilities.

The bias of direct estimator can be computed as $\left|\frac{1}{|\mathcal{X}|} - p(Y_i = y_i|Y_j = y_j)\right|^2$.

Finally, we show that these results imply the desired inequality. By the previous results, $\mathbb{E}[\hat{q}_S^*(Y_i = y_j|Y_i = y_i)] = \lambda p(Y_i|Y_j) + (1-\lambda)\frac{1}{|\mathcal{X}|}$ for some $\lambda \in (0,1)$.

$$\begin{split} |\mathbb{E}_{y_{i} \sim q_{S}^{*}(Y_{i}|Y_{j}=y_{j})} [\hat{q}_{S}^{*}(Y_{i}|Y_{j}=y_{j})] - p(Y_{i}=y_{i}|Y_{j}=y_{j})|^{2} \\ &= |\lambda p(Y_{i}=y_{i}|Y_{j}=y_{j}) + (1-\lambda)\frac{1}{|\mathcal{X}|} - p(Y_{i}=y_{i}|Y_{j}=y_{j})|^{2} \\ &= |\lambda p(Y_{i}=y_{i}|Y_{j}=y_{j}) + \frac{1}{|\mathcal{X}|} - \lambda\frac{1}{|\mathcal{X}|} - p(Y_{i}=y_{i}|Y_{j}=y_{j})|^{2} \\ &= |(\lambda-1)p(Y_{i}=y_{i}|Y_{j}=y_{j}) + (1-\lambda)\frac{1}{|\mathcal{X}|}|^{2} \\ &= (1-\lambda)^{2}|(\frac{1}{|\mathcal{X}|} - p(Y_{i}=y_{i}|Y_{j}=y_{j})|^{2} \\ &< |\frac{1}{|\mathcal{X}|} - p(Y_{i}=y_{i}|Y_{j}=y_{j})|^{2} \end{split}$$

We note that we can obtain a reasoning gap in a setting without the entropy regularization assumption by replacing it with the assumption that held-out pairs can appear adjacent but are sampled from their marginal distributions.

B Pseudocode for data generation

This section contains pseudocode for the algorithms we use to generate Bayes nets and choose a subset of variables to include according to an observation distribution.

First, Algorithm 1 is used to create Bayes nets. This algorithm takes the number of nodes and edges to create and defines a directed acyclic graph by randomly adding edges between pairs of nodes. Next, it assigns conditional probability tables to the nodes given the values of their parents to create a Bayes net.

Algorithm 1 Algorithm for generating a Bayes net

```
Input: Number of nodes N, number of edges M
G = (E, V) \leftarrow \text{empty graph}
for i \in \{1, \dots, N\} do V \leftarrow V \cup \{Xi\}
end for
for i \in \{1, \ldots, M\} do
   v_1, v_2 \leftarrow \text{random pair of vertices} \in V
   while (v_1, v_2) \in E or (v_1, v_2) would create a cycle do
      v_1, v_2 \leftarrow another random pair of vertices \in V
   end while
   E \leftarrow E \cup (v_1, v_2)
end for
T \leftarrow \{\}
for v \in \text{TOPOLOGICALSORT}(G) do
   t \leftarrow empty conditional probability table
   for c \in \text{possible configurations of } v's parents do
      p \leftarrow \text{BETA}(\frac{1}{5}, \frac{1}{5})
      t[c] \leftarrow p
   end for
   T \leftarrow T \cup \{(v,t)\}
end for
D \leftarrow \text{Bayes net defined by graph } G \text{ and conditional probability tables } T
return D
```

For each sample, we only show a subset of all the variables according to an observation distribution. Algorithm 2 shows the procedure we use to select which variables to display in a given sample. We first sample central variable c (uniformly) and a distance k (according to a geometric or Zipfian distribution), then get all the variables within distance k of c in the graph. Next, we drop each variable with probability 0.2. If any of the held-out pairs remain, we randomly remove one variable from each pair. In the wrong locality structure training conditions, we use a graph G that does not correspond to the net from which our samples are drawn, but has the same variable names. In the fully observed condition, we start with all variables, but still remove held-out pairs according to the final for loop.

Algorithm 2 Algorithm for selecting variables to include based on an observation distribution

```
Input: Bayes net graph G = (V, E), set of held-out pairs P, size distribution D
c \leftarrow \mathsf{random} \; \mathsf{variable} \in V
k \leftarrow \text{SAMPLE}(D)
R \leftarrow \{\}
for v \in V do
   if v is within distance k of c in G then
      R \leftarrow R \cup \{v\}
   end if
end for
for v \in R do
  if Sample(Bernoulli, 0.2) = 1 then
      R \leftarrow R \setminus \{v\}
   end if
end for
for (v_1, v_2) \in P do
  if v_1 \in R and v_2 \in R then
      if Sample(Bernoulli, 0.5) = 1 then
         R \leftarrow R \setminus \{v_1\}
      else
         R \leftarrow R \setminus \{v_2\}
      end if
   end if
end for
return R
```

C Full sample of training data

The following is an example of a sample from a local neighborhood of a Bayes net in string format, as used in training our models:

```
###
target: X5
X17=0
X92=0
X13=0
X52=1
X24=1
X26=1
X91=0
X36=0
X34=0
X12=1
X20=0
X5=1
```

The full training set consists of 1,000,000 samples like this concatenated together.

D Formatting estimators as prompts

D.1 Direct prediction

In direct prediction, we create a simple prompt that specifies the name and value of the observed variable, then states the name of the target variable. For example, if we wanted to estimate $p(X_2|X_1=0)$ we would create the following prompt:

target: X2 X1=0 X2=

We would then take the softmax of the log-probabilities the language model assigns to '1' and '0' being the next token and use the resulting probability of '1' as the estimate.

D.2 Scaffolded generation

In scaffolded generation, we pre-compute a sequence of intermediate variables, then use the language model to estimate their values. For example, if we wanted to estimate $p(X_4|X_1)$ and we knew X_2 and X_3 were scaffold variables, we would start with the following prompt:

```
###
target: X4
X1=0
X2=
```

We would then sample the next token from the language model and append it along with the next scaffold variable to the prompt. For example, if we got a value of 1 from the language model, we would give it the following prompt:

```
###
target: X4
X1=0
X2=1
X3=
```

We repeat this process until all scaffold variables have values, then compute the probability assigned to the target variable at the end, in the same way we do for direct prediction. The final prompt we use to estimate the probability might look like this:

```
###
target: X4
X1=0
X2=1
X3=0
X4=
```

We repeat this process 10 times to produce a Monte Carlo estimate over the values of the scaffold variables and average the probabilities assigned to the target variable over samples.

D.3 Free generation

Free generation is similar to scaffolded generation, but we let the model choose which intermediate variables to instantiate, rather than sample only their values. For example, if we are trying to infer $p(X_4|X_1=0)$ we would first prompt it like this:

```
###
target: X4
X1=0
```

We then sample the next two tokens from the model, which is exactly enough for one variable name. We add an equals sign, then sample the value of the variable in the same way as other conditions. For example, this might be what our prompt looks like after generating one intermediate variable and its value

###
target: X4
X1=0
X5=1

We repeat this process until the model outputs the name of the target variable. At that point, we have a prompt that might look like this

###
target: X4
X1=0
X5=1
X2=0
X7=0
X3=1
X4=

We then extract the probability of the target variable in the standard way. Again, we average target variable probabilities over 10 samples of the intermediate variables.

E Training Details

Our model is a smaller version of the GPT-2 architecture, with 512-dimensional embeddings, 10 layers, and 8 attention heads. This gives us a total of 32,573,440 parameters. We fit a Byte Pair Encoding tokenizer to data from our samples, which produced 356 unique tokens.

Our text was grouped into chunks of 1024 tokens and batches of 3, for a total of 3072 tokens per gradient step. We used the Adam optimizer, with an initial learning rate of 10^{-3} and Beta values of 0.9 and 0.999.

All models were trained on Nvidia Titan Xp GPUs. They were trained for 300, 000 gradient steps, which took approximately 20 hours each.

F Data efficiency of fully-observed training with no held-out pairs

To supplement our data efficiency analyses, we ran a version of the fully-observed training without any held-out pairs. In this setting, the transformer can directly memorize the true conditional probabilities, but it takes a long time for direct prediction to perform as well as free generation with locally-structured data. Figure 4 compares the performance of direct prediction and free generation for locally-structured training data with held-out pairs and for fully-observed training data with no held-out pairs. Direct prediction with fully-observed training data can out-perform free generation with locally-structured training data, but it takes approximately 650 million tokens worth of training to reach the same performance. In contrast, free generation with geometric locally-structured training data converges after about 200 million tokens of training.

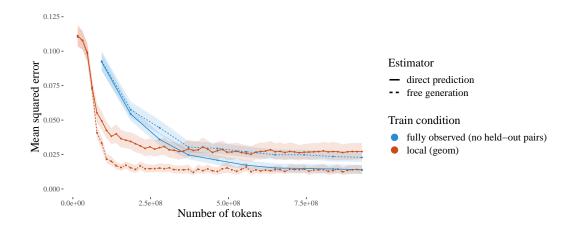


Figure 4: Learning curves comparing mean squared error on held-out pairs, estimated using free and direct prediction for training data consisting of either geometrically-sized local neighborhoods or the full set of variables. Unlike the version reported in the main text, no pairs of variables are held out in this fully-observed condition. Even though the model is trained directly on the held-out pairs in the fully-observed condition, there is a substantial data efficiency advantage to using locally-structured training data and free generation at inference time.