LEARNING EXTRAPOLATIVE SEQUENCE TRANSFORMA-TIONS FROM MARKOV CHAINS

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Paper under double-blind review

ABSTRACT

Most successful applications of deep learning involve similar training and test conditions. However, for some generative tasks, samples should improve desirable properties beyond previously known values, which requires the ability to generate novel hypotheses that *extrapolate* beyond training data. While large language models have been successfully extended to a variety of sequence modeling problems, greedy autoregressive sampling can struggle to explore the solution space sufficiently to extrapolate, especially when the properties of interest are global to the sequence. On the other hand, sequence-level sampling methods such as Markov chain Monte Carlo (MCMC) offer theoretical guarantees about capturing the distribution of interest, but suffer from the curse of dimensionality in discrete structured spaces. We propose a new approach that bridges the gap between MCMC and autoregressive sampling, which may be viewed as off-policy reinforcement learning. Our approach uses selected states from Markov chains as a source of training data for an autoregressive inference network, which is then able to generate novel sequences at test time that extrapolate along the sequence-level properties of interest. The proposed approach is validated on three problems: protein sequence design, text sentiment control, and text anonymization. We find that the learned inference network confers many of the same (and sometimes better) generalization benefits compared to the slow sampling process, but with the additional benefit of high sample efficiency.

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1 INTRODUCTION

033 034 035 036 037 038 039 040 041 042 043 044 In creative tasks such as scientific discovery, a key requirement is the ability to *extrapolate* beyond existing knowledge. For example, automating the generation of novel hypotheses is central to mathematical discovery, biological sequence design, molecular optimization, and the creation of new materials [\(Romera-Paredes et al., 2024;](#page-15-0) [Fu et al., 2023;](#page-12-0) [Jain et al., 2022;](#page-13-0) [Trabucco et al., 2022;](#page-16-0) [Gao](#page-12-1) [et al., 2022\)](#page-12-1). Beyond scientific discovery, extrapolation is necessary in many creative applications, such as writing assistants for creative writing [\(Swanson et al., 2021;](#page-16-1) [Gómez-Rodríguez & Williams,](#page-12-2) [2023\)](#page-12-2). It is natural to wonder if large-scale generative training affords extrapolation as an emergent ability [\(Schaeffer et al., 2024\)](#page-15-1). Unfortunately, prior work has found that state-of-the-art foundation models can struggle on tasks requiring extrapolation [\(Dziri et al., 2023;](#page-12-3) [Chakrabarty et al., 2024\)](#page-10-0). Notably, [Lu et al.](#page-13-1) [\(2024\)](#page-13-1) compare different reasoning and inference strategies, finding that the only strategy to successfully increase sample diversity is Monte Carlo search, which typically suffers from low sample efficiency and can produce degenerate samples in high-dimensions [\(Holtzman et al.,](#page-12-4) [2019\)](#page-12-4).

045 046 047 048 049 050 051 052 053 How can we *efficiently* extrapolate beyond the training data? We build on a recent approach which leverages the de-noising ability of masked language models (MLM) to extrapolate [\(Padmakumar](#page-15-2) [et al., 2023\)](#page-15-2). The idea is to generate many sequence transformations that improve the target objective as evaluated by a trained scorer model, and then to supply these transformations as training data for a greedy extrapolative model. To search for suitable transformations to create this augmented training set, [Padmakumar et al.](#page-15-2) [\(2023\)](#page-15-2) apply a random mask to sequences in the training data, which are then in-filled by sampling from an MLM. Samples are kept if the improvement in the objective between the sampled sequence and the original sequence is within a fixed range. This process is repeated for a fixed number of steps with the goal of identifying transformations that make incremental improvements to the objective. A key assumption is that, after training a sequence-to-sequence

069 070 071 072 073 074 075 Figure 1: The sentiment extrapolation task [\(§4.2,](#page-5-0) [Padmakumar et al.](#page-15-2) [\(2023\)](#page-15-2)) requires generating reviews with ratings beyond the range observed at training time. Here, we illustrate the search process using a toy 1D representation of the features (x-axis) and rating (y-axis). Monte Carlo exploration can produce reviews that extrapolate, but many steps are required. However, once good state sequences have been discovered, we can sub-sample the transitions that decrease the rating $(A \rightarrow C \rightarrow N)$ and use them to learn an extrapolative model. The reviews shown to the right for states B, C, and N are actual reviews generated by our method, while A is a genuine review from the validation data.

model on the selected transformations, composing more than one transformation can lead to effective extrapolation. However, although this approach was found to be successful in extrapolating beyond the training region for some tasks, its success is critically dependent on the choice of a number of sensitive hyper-parameters, including a threshold on the relative improvement from different transformations and a fixed number of iterative decoding steps.^{[1](#page-1-0)}

082 083 084 085 086 087 088 089 090 091 092 093 094 In this paper, we first seek to better understand how generative models, in particular models trained using in-filling objectives [\(Bavarian et al., 2022;](#page-10-1) [Tay et al., 2022\)](#page-16-2), implicitly capture knowledge that can be leveraged for extrapolative generation. To do so, we formalize the process of searching for sequences that score highly under the target sequence-level objective as approximate inference in an energy-based model (EBM) [\(LeCun et al., 2006\)](#page-13-2). This model is specified via an unnormalized score (negative energy), which can incorporate multiple criteria via a product-of-experts [\(Hinton, 2002;](#page-12-5) [Mireshghallah et al., 2022\)](#page-13-3). The experts will typically include a measure of fluency or faithfulness along with a task-specific sequence-level objective for extrapolation. While exact inference in EBM is intractable, the MLM provides a convenient and effective *proposal distribution* for a Metropolis-Hastings (MH) sampler, which under mild assumptions approximates the distribution over sequences defined by the EBM [\(Goyal et al., 2021\)](#page-12-6). Beyond providing a conceptual framework for understanding the search process, we find this formulation also provides practical benefits in terms of improved generalization and robustness [\(§4\)](#page-4-0).

095 096 097 098 099 100 101 102 103 104 105 However good the proposal distribution, MH still suffers from all the aforementioned limitations. Therefore, we fine-tune a model using the Markov chains resulting from MH as training data. Our objective in doing so is to generate sequences that achieve scores in the extrapolation range in *as few steps as possible*. This is illustrated in [Figure 1](#page-1-1) for the controlled task of review generation [\(§4.2\)](#page-5-0). Using every transition in the Markov chains is clearly undesirable, since some transitions may fail to improve the score or result in *worse* scores. As a result, we explore several strategies to sub-sample state sequences from the complete chains, including adaptive schemes based on the relative improvement in energy. While the model we fine-tune has an autoregressive parametrization [\(§3\)](#page-2-0), by selecting a variable number of transitions from the Markov chains, we implicitly learn a nonautoregressive model that transforms an initial sequence (token-by-token) a variable number of times to improve the score beyond the training range. By further incorporating the sequence-level score at each step of generation—similar to reward-to-go in sequence modeling approaches to reinforcement

¹In a personal communication, the authors report that their procedure exhibits large variance, and indeed we are unable to reproduce published results using the code released by [Padmakumar et al.](#page-15-2) [\(2023\)](#page-15-2).

108 109 110 learning [\(Janner et al., 2021\)](#page-13-4)—the model can learn to incorporate this feedback, for example to help determine when to stop generating.

111 112 113 114 115 116 117 118 119 120 121 Summary of contributions We propose a framework to extrapolate beyond a given training dataset given an arbitrary scoring function. Our approach leverages existing components, namely pre-trained language models trained using de-noising objectives, to explore the space of sequence-to-sequence transformations and their impact on the target objective. We formalize this process as MCMC, and consider a variety of strategies to select training data from the resulting Markov chains to fine-tune a model to generate novel sequences. In particular, we propose a multi-step generative process in which, starting from an initial state, the properties of interest are optimized in multiple rounds, similar to non-autoregressive generation. We evaluate our model on three tasks: protein engineering, sentiment style transfer, and anonymization.^{[2](#page-2-1)} In some cases, we find that our model, q_{θ} , can achieve competitive results with MCMC and other baselines, but using a significantly smaller number of steps [\(§4\)](#page-4-0). In other cases, specifically [§4.1,](#page-4-1) we find that the fine-tuned model achieves significantly better extrapolation.

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2 PROBLEM STATEMENT

126 127 128 129 130 131 132 133 134 135 136 137 138 139 140 141 We consider sequence-level search problems where the task is to generate novel sequences $x \in \mathcal{X}$ that satisfy one or more properties of interest $y \in \mathcal{Y}$. Given a candidate sequence x, we assume that an oracle $o(x) \in Y$ may be consulted to assess x, but that it may be expensive to consult. For example, assessing a novel candidate may involve conducting physical experiments or running expensive simulations (as in the protein task described in [§4.1\)](#page-4-1), and therefore we wish to minimize the number of evaluations of $o(x)$ when searching for new sequences. At training time, we observe sequences $x \in \mathcal{X}^{\text{train}}$ with properties taking values in the training range $o(x) \in \overline{\mathcal{Y}}^{\text{train}}$, and our objective is to fit a generative model q_θ such that samples $x' \sim q_\theta$ successfully extrapolate beyond the training data for the property of interest: $o(x') \notin \mathcal{Y}^{\text{train}}$. For example, for the sentiment task, the training range consists of ratings between 2 and 4 stars, and the extrapolation range consists of ratings that are highly negative (less than 2-stars) or highly positive (greater than 4-stars). If the oracle is expensive to consult at training time, we instead assume access to a *guide* $s(x)$ that provides a computationally tractable estimate $s(x)$ of the oracle score $o(x)$. For example, $s(x)$ may be a neural network trained to predict properties of x based on a database of previous experiments with hypothesized sequences x and measured outcomes $o(x)$. At test time, we generate $x' \sim q_\theta$ and then evaluate performance under the oracle $o(x')$. Overall, the central problem is how to fit q_θ without overfitting the training data and in such a manner as to enable extrapolation.

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3 METHOD

145 146 147 148 149 150 151 152 153 154 155 156 Extrapolative generation We are interested in generating novel sequences that extrapolate beyond a given training distribution for one or more attributes of interest. Since the attributes of interest may be properties of the complete sequence, we consider the family of energy-based models (EBM) [\(LeCun](#page-13-2) [et al., 2006\)](#page-13-2), where the log-probability of an event is proportional to a sequence-level score $s(x)$. Similar to rewards in reinforcement learning (RL), this parametrization affords considerable flexibility in choosing appropriate scoring functions for the task. The scoring function may be fast (for instance, a small neural classifier) or slow (such as using a slow evaluation process to calculate the folding energy of a protein). However, in either case, exact sampling from an EBM is intractable since the partition function Z involves a sum over all possible sequences. In our experiments, we often include multiple terms in our energy, which are combined in a product of experts $\ln p(x) =$ $\alpha_1s_1(x) + \alpha_2s_2(x) + \ldots - \ln Z$, weighted with scalar hyperparameter α . For example, for the sentiment task, we include Hamming distance to the original review in addition to the sentiment rating.

158 159 160 Masked-infilling language models In general, while MCMC can be used to (approximately) draw samples from EBMs, the algorithm suffers from the curse of dimensionality which can manifest as slow mixing and in failures to identify modes of the energy landscape. These issues can be mitigated

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²We additionally include a minimal demonstration of the key idea on a toy task in [Appendix H.](#page-21-0)

162 163 164 165 166 167 168 169 170 in part by choosing effective proposal distributions. Crucially for our method, language models trained with mask-infilling objectives can serve as effective proposal distributions [\(Goyal et al.,](#page-12-6) [2021;](#page-12-6) [Mireshghallah et al., 2022\)](#page-13-3).^{[3](#page-3-0)} This fact allows us to obtain proposals using existing pre-trained language models. Specifically, we use the Metropolis-Hastings (MH) algorithm which uses a proposal distribution $q(x' | x)$ to draw candidate states x' given the current state x. These proposals are then either accepted, in which case x' is taken as the new state, or rejected in which case $x' = x$, according to the standard MH acceptance criterion. To implement q , we mask at random subset of the current state x, and then *infill* the masked sequence based on a self-supervised pre-training process [\(Devlin](#page-10-2) [et al., 2019;](#page-10-2) [Lewis, 2019;](#page-13-5) [Raffel et al., 2023\)](#page-15-3).

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172 173 174 175 176 177 178 179 180 181 182 183 184 185 186 Training q_{θ} Although an effective proposal distribution can improve the mixing time of MCMC, the amount of iterations required to identify modes of the distribution may still be prohibitive. Our approach will therefore be to fine-tune a separate model q_θ from which it is efficient to draw samples that ideally extrapolate beyond the scores explored during MCMC (see [Appendix H](#page-21-0) for a simple demonstration of this idea). This is similar to off-policy RL, where we use MCMC as a particular kind of exploration policy to generate training episodes. We imbue q_{θ} with specific inductive biases to encourage extrapolation beyond the training data. In particular, rather than sampling $x \sim q_\theta$ directly, we allow generation to proceed via multiple intermediate states x_1, x_2, \ldots, x_N . The intuition for this strategy, which is borne out in our experiments [\(§4\)](#page-4-0), is that it is easier to learn a conditional transformation $q_{\theta}(x_n | x_1, x_2, \dots, x_{n-1})$ than directly sample the structured objects x. Unlike the state-to-state transitions in MCMC however, q_θ is biased to be greedy: it aims to continually improve the energy from state-to-state and in general may avail of information from the complete history of previous states x_1, x_2, \ldots , *as well as associated scores* $s(x_1), s(x_2), \ldots, s(x_{n-1})$, when producing the next state x_n . By conditioning on the scores, the policy has the ability to incorporate these into planning, not unlike the sequence model RL formulations proposed by [Janner et al.](#page-13-4) [\(2021\)](#page-13-4); [Chen](#page-10-3) [et al.](#page-10-3) [\(2024\)](#page-10-3).

187 188 189 190 Autoregressive refinement To fit q_θ , we assume access to a training dataset providing one or more initial states, from which we sample state trajectories using MCMC. We then create *training episodes* $(x_1, s_1), (x_2, s_2), \ldots, (x_N, s_N)$ by sub-sampling state sequences from the complete trajectories. We discuss several strategies for this in [§3.1.](#page-3-1) The training episodes are encoded as a sequence of tokens:

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x_0 <seq0> x_1 <seq1> s_1 x_2 <seq2> s_2 ... x_n s_n <stop>

193 194 195 196 197 198 Above, $\langle \text{seq} \rangle$ and $\langle \text{stop} \rangle$ are distinguished symbols encoded either as special vocabulary terms or as strings in a pre-trained model, s_i are scalar scores, and x_i are token sequences of possibly variable length. Then q_{θ} is trained using teacher forcing to generate each token of each intermediate state x_i (for $i > 0$) conditioned on all previous states $x_0, x_1, \ldots, x_{i-1}$. As previously mentioned, the concrete advantage to formulating inference in this way is that revisions can condition on previously generated sequences and energy scores. As an ablation, we also experiment with a Markov variation that only conditions on the previous state, which performs well in certain settings.

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Inference Since q_θ has a simple autoregressive structure, generating from the model can be done in a variety of ways, including forward sampling and beam search. We note that in principle constrained decoding techniques could be used to enforce adherence to the structure above, but we did not find this necessary in practice. After generating each intermediate state x_i , the sequence is either scored using $s(x_i)$ and the result deterministically appended to the sequence, or q_θ learns to *predicts* the sequence score.^{[4](#page-3-2)} When \lt stop> is generated from the model, the final state x_n is taken to be the sample.

3.1 CREATING TRAINING EPISODES

210 211 212 Creating training episodes consisting of the *entire* Markov chain, which could include hundreds or thousands of states, is undesirable. Ideally, q_θ should be computationally efficient at inference time, only generating a small number of intermediate states before producing the <stop> symbol. As a

²¹³ 214 ³See [Wang & Cho](#page-16-3) [\(2019\)](#page-16-3) for further context on this approach and [Hennigen & Kim](#page-12-7) [\(2023\)](#page-12-7) for some analysis and extensions.

⁴Another possibility is to consult the oracle at *intermediate* states of generation, although we do not directly evaluate this version in our experiments.

216 217 218 219 result, we require relatively short training episodes. Note also that the sampling method might explore high-energy regions of the state space, and it may be sub-optimal to include such exploration in the training episodes; therefore, we ideally want to select state transitions from the complete sample that result in a decreased energy. We examine several strategies for selecting states.

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221 222 223 224 225 226 227 228 229 Uniform thinning If the sampling chain tends to monotonically improve the energy, the simple strategy of sub-sampling the states at regular intervals can be expected to result in a state sequence with incremental progress towards a local optimum. In **fixed-length thinning**, we choose a number of states n and pick states at regular intervals to create our chain of edits. Choosing the number of states to add to the chain may disadvantage the model in cases where there are different numbers of states in each unthinned sequence; for instance, collapsing sequences with 10 edits and 100 edits to 5 states each might lead to intense variability in scope of edits seen in the data. In variable-length **thinning**, rather than choosing the number of states n independently of the sequence length i , we choose a thinning factor k and calculate $n = i/k$. This dynamically allocates each edit change a number of states based on the entire edit sequence length.

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232 233 234 235 First and best If the task is sufficiently simple, a single step should be adequate to extrapolate. By taking the initial and lowest energy states of the Markov chain, we create single-step training examples. This can be considered a special case of uniform thinning where the training episode length is two.

236 237 238 239 240 241 242 243 244 245 246 Changes in energy Ideally, we would like the states chosen for training episodes to be governed by properties of states in the chain, such as the relative improvements in energy from state to state, particularly if the energy does not monotonically decrease. A simple way to incorporate this idea into the selection of training episodes is to identify state transitions that most improve the energy. In fixed-length Δ energy, we cache the energy for each state while running MCMC, then select the n states that most improve energy from the previous step to construct our training episode. However, forcing a model to select a certain number of states may result in unoptimal behavior. For example, if an edited state x_1 is unlikely to significantly improve, the model ideally should learn to immediately emit the \langle stop> symbol, rather than continuing to generate minute improvements. Rather than selecting *n* states, **variable-length** Δ energy selects any states which improve energy by a particular threshold, e.g. 10%.

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4 EXPERIMENTS

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250 251 252 253 254 255 256 257 258 259 To address whether q_{θ} has the capacity for sample-efficient extrapolation, we apply our method to two tasks from [Padmakumar et al.](#page-15-2) [\(2023\)](#page-15-2) which require extrapolation: protein engineering and sentiment extrapolation. To demonstrate that q_{θ} retains the capacity to "interpolate" (i.e., generalize well in a non-extrapolative task), we evaluate on a complex task solely requiring interpolation, namely text anonymization. In all experiments, to demonstrate method efficiency, we show the number of "iterations" each method takes—we consider "iterations" to loosely correspond to the computational work of passing the sequence through the inference model once. Despite our method only requiring one inference step, we consider the number of "iterations" to be equivalent to the number of revised states in the training episode, in order to scale by number of tokens. In variable-length methods, we report the average number of iterations.

4.1 PROTEIN ENGINEERING

262 263 264 265 266 267 268 269 We replicate the ACE2 stability task from [Padmakumar et al.](#page-15-2) [\(2023\)](#page-15-2). The goal is to generate mutants of the human angiotensin-converting enzyme 2 (ACE2) with higher stability than the wildtype, measured with lower free energy compared to the wildtype(ddG). Lower ddG corresponds to more stable mutants. The protein is represented as a sequence of 83 amino acids, from a vocabulary of 20 amino acids in total. We finetune a ProtBert model [\(Elnaggar et al., 2020\)](#page-12-8) to predict ddG from a mutated ACE2 sequence. We use the ACE2 dataset from [Chan et al.](#page-10-4) [\(2021\)](#page-10-4), restricting the training data to only examples with ddG between -4 and 10. The objective is to generalize to sequences with ddG beyond the training range (i.e. below -4). We describe our experimental procedure in detail in [§D.1.](#page-18-0)

270 271 272 273 274 275 276 Baselines We compare our generated sequences to results from [Padmakumar et al.](#page-15-2) [\(2023\)](#page-15-2); specifically, we consider their reported scores for masking and infilling, iteratively masking and infilling with ranked outputs (Iterative sampling), Genhance by [Chan et al.](#page-10-4) [\(2021\)](#page-10-4) and Iterative Controllable Extrapolation (ICE) by [Padmakumar et al.](#page-15-2) [\(2023\)](#page-15-2). In both cases, we report the variant *with scorer*, where at each step the model generates multiple options and chooses the best of these options using the training-time scorer. We also report the scorer-free variant of ICE, which generates a single output at each step, similar to q_{θ} .

277 278 279 280 281 Metrics We evaluate the stability of the generated proteins using FoldX [Schymkowitz et al.](#page-15-4) [\(2005\)](#page-15-4), which calculates the ddG for each protein. We report the proportion of generated mutants which fall below certain thresholds: -1 and -2.5, which are within the training region, and -5, -6, and -7, which are within the extrapolation region.

Results Our results with q_{θ} trained on training episodes constructed using fixed-length Δ energy can be found in [Table 1.](#page-5-1) Despite the fact that MCMC fails to outperform the baselines taken from [Padmakumar et al.](#page-15-2) [\(2023\)](#page-15-2), we find that in the extrapolation range q_θ significantly outperforms our baselines and MCMC.

296 297 298 299 300 Table 1: Overall ACE2 stability results. Each cell represents the percentage of generated sentences lower than the threshold. Lower ddG is more stable; -1 and -2.5 are in the training range, -5 and below is in the extrapolation range. While MCMC does not approach the success of the baseline, the best variant of q_θ , trained on training episodes created using fixed-length Δ energy to select states, significantly outperforms the baseline.

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4.2 SENTIMENT EXTRAPOLATION

304 305 306 307 308 309 310 311 312 313 Given a training dataset of Yelp reviews [\(Zhang et al., 2015\)](#page-16-4) with moderate sentiment, ranging from 2-stars to 4-stars, the goal is to learn to generate reviews that extrapolate beyond the training region to the highly negative (1-star) or highly positive (5-star) reviews. Following [Padmakumar et al.](#page-15-2) [\(2023\)](#page-15-2), we fit two regression models, a training-time scorer and an oracle scorer used for evaluation. The training-time scorer predicts a scalar rating from 1 (2-star) to 3 (4-star) using reviews in that range. The oracle scorer uses all of the training data and predicts the complete range of ratings given input text. Prior work considers a simple version of this task where success is measured only in how well generated texts extrapolate beyond the training region. We introduce a variation where success is also explicitly measured by the change in fluency after editing, to prevent our models from greedily optimizing only a single metric at the expense of fluency. Details of our procedure can be found in [§D.2.](#page-19-0)

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315 316 317 318 319 320 Baselines We report results from [Padmakumar et al.](#page-15-2) [\(2023\)](#page-15-2), namely the ICE and ICE with scorer methods. ICE with scorer was previously described in [§4.1;](#page-4-1) without the scorer, the model simply generates a single option for the output sequence. We also report results using our implementation of Genhance [\(Chan et al., 2021\)](#page-10-4). Finally, we report results using an FUDGE [\(Yang & Klein, 2021\)](#page-16-5), an autoregressive classifier-guided method not specifically designed for extrapolation. We describe our implementation of FUDGE in [§D.2.](#page-19-0)

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322 323 Metrics To evaluate sentiment, we use the oracle scorer as described in [\(Padmakumar et al., 2023\)](#page-15-2). When editing in the positive direction, we consider a 4-star review or above to be in the training region, and a 5-star review to be in the extrapolation region; when editing in the negative direction,

324 325 326 we consider a 2-star review or below to be in the training region, and a 1-star review to be in the extrapolation region. We report the proportion of all sentences in these regions.

327 328 329 330 We also introduce a fluency metric, the median percentage change in perplexity as measured by GPT-2 large [\(Radford et al., 2019\)](#page-15-5). Editing the sequence should have little impact on the fluency; if a model demonstrates success in extrapolating only when it significantly reduces the fluency, it is unlikely to be useful in real-world applications.

331 332 333 334 335 As the Yelp review dataset does not have a premade validation split [\(Zhang et al., 2015\)](#page-16-4), we use the first thousand examples of the test set as a validation set. [Padmakumar et al.](#page-15-2) [\(2023\)](#page-15-2) report their test results on a random subset of 1831 reviews from the test set, all of which fall in the training range of 2-, 3-, and 4-star reviews. We report the FUDGE results on a 1500-sentence subset of the test set, and for MCMC and q_{θ} , we create three 2000-sentence subsets of the test set and report the average of each of these three runs in our results, finding that there is little variation regardless of the test set.

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Results We show our results with q_θ trained on first/best training episodes in [Table 2](#page-6-0) alongside results from [Padmakumar et al.](#page-15-2) [\(2023\)](#page-15-2). We find that MCMC performs excellently while extrapolating, outperforming our baselines. Our trained q_{θ} outperforms our baselines in extrapolative capacity, and outperforms MCMC in efficiency (as measured by number of iterations) and fluency. Example generations can be found in [§G.1.](#page-21-1)

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Table 2: Comparing our methods to the [Padmakumar et al.](#page-15-2) [\(2023\)](#page-15-2) results on the extrapolative sentiment task. We report the proportion of sentences below a threshold for the favorable training range (2 stars for negative sentiment, 4 stars for positive sentiment) and a threshold for the extrapolation range (1 star for negative sentiment, 5 stars for positive sentiment). MCMC performs well on those metrics, but moderately decreases fluency while requiring nearly 500 iterations. We compare this to q_θ trained using first/best training episodes. q_{θ} decreases fluency less and requires only a single inference-time iteration. We provide 95% confidence intervals over three different test sets.

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4.3 ANONYMIZATION

361 362 363 364 365 366 367 368 369 370 Writing can exhibit a wide range of stylometric features that can be used to identify the author of a document. In cases where anonymity is desired, there is a need to automatically remove personally-identifying features. Since stylometric features are typically extracted at the documentlevel [\(Rivera-Soto et al., 2021\)](#page-15-6), it is appealing to tackle this problem using sequence-level objectives. Similar to previous tasks, we first extract training episodes from an MCMC driven sampler. We adapt the style transfer method proposed by [Khan et al.](#page-13-6) [\(2024\)](#page-13-6) to generate training episodes making one key change: rather than using a specific target style, we parameterize the energy function such that *any* style different from the initial style is desirable. Given some text x , the system results in a series of states $y_1, y_2, \ldots y_n$, these episodes are then used to train our anonymization system. Details on our adaptation of [Khan et al.](#page-13-6) [\(2024\)](#page-13-6) can be found in [Appendix F.](#page-20-0)

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372 373 374 Baselines We consider four baseline anonymization systems: GPT3.5, GPT4 [\(OpenAI et al., 2024\)](#page-14-0), DIPPER [\(Krishna et al., 2023\)](#page-13-7), and Round Trip Machine Translation (MT). Implementation details for each of these systems can be found in [§F.1.](#page-20-1)

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376 377 Metrics To evaluate the quality of anonymization outputs we consider two metrics measuring author verification Equal Error Rates (EER), and semantic similarity between original and anonymized text. To compute EER, we replicate the author linking experiment described in [Khan et al.](#page-13-8) [\(2021\)](#page-13-8). **378 379 380 381 382 383 384 385** Our evaluation set consists of 50 authors, each with 16 posts that have been paraphrased. Given the first 8 *original* posts from an author's history as a 'query', we are interested in correctly identifying the 2nd set of 8 *anonymized* posts as a match, and all other author posts as negatives. We use a pre-trained author embedding ^{[5](#page-7-0)} to encode each set of 8 messages into a vector and use cosine similarities between two candidates as a score. If we successfully circumvent the detection system, we expect the EER to rise. For semantic similarity, we use a publicly released checkpoint to encode original and anonymized documents^{[6](#page-7-1)}. A successful systems maintains a high similarity under this metric.

Table 3: Comparing our methods with anonymization baselines. MCMC achieves improved results over baselines, but takes significantly more iterations than any other method; our best variant of q_{θ} , trained using variable-length Δ energy, achieves reasonable performance on both metrics in significantly fewer iterations than MCMC.

Results We find that baseline systems do a poor job at maintaining semantic similarity, or in the case of Round Trip MT, do so at the cost of not introducing enough changes to circumvent author verification. While the iterative MCMC sampler proposed by [Khan et al.](#page-13-6) [\(2024\)](#page-13-6) does perform well under both of these metrics, it is very costly to run, with an average of 4498 iterations to yield an anonymized sample. Our system, with q_θ trained on variable-length Δ energy, is able to distil this sampling procedure and return an anonymized sample with just a few in-context iterations.

5 ANALYZING EPISODE CREATION STRATEGY

Tables [4,](#page-7-2) [5](#page-8-0) and [6](#page-8-1) show the effects of different methods of creating training episodes to train q_θ as described in [§3.1;](#page-3-1) we also analyze the impact of other features of the training episodes in [Appendix B](#page-17-0) and [Appendix C.](#page-18-1)

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> Table 4: Varying training episode creation for the ACE2 stability task. We find that fixed-length Δ energy outperforms our other training episode creation strategies when extrapolating.

We find that the procedure used to sub-sample states from the Markov chains influences the model's success. When selecting multiple states from the Markov chain, selecting the states that most decrease energy often improves performance over selecting states uniformly. In [Table 4,](#page-7-2) we find that selecting states using ∆ energy (fixed-length) outperforms both naive thinning methods by several points. However, ∆ energy (variable-length) underperforms significantly. This may be due to the comparatively short sequence length, or because of the artificial constraint to have sequences shorter than ten iterations.

⁵ <https://huggingface.co/rrivera1849/LUAR-CRUD>

 $6W$ e use the all-mpnet-base-v2 checkpoint within the sentence transformers library.

432 433	Model	Training \uparrow	Extrapolation \uparrow	Fluency	Iterations
434	First/Best	$0.925 \scriptstyle{\pm 0.005}$	$0.734_{\pm 0.008}$	0.132% \pm 0.015	
435	Thinning (fixed-length)	$0.883_{\pm 0.006}$	$0.642_{\pm 0.007}$	0.466% $_{\pm 0.014}$	$\overline{4}$
	Thinning (variable-length)	$0.854_{\pm 0.003}$	0.591 ± 0.012	$0.539\%_{\pm0.010}$	3.997
	Δ Energy (fixed-length)	$0.910_{\pm 0.005}$	$0.692_{\pm 0.016}$	$0.362\% \scriptstyle \pm 0.032$	4
437 438	Δ Energy (variable-length)	$0.881_{\pm0.004}$	$0.677_{\pm 0.006}$	$0.396\% \scriptstyle \pm 0.028$	5.855

439 440 441 442 Table 5: Applying various training episode creation strategies to the sentiment task. We show that these strategies affect the proportion of sentences in the favorable training range and in the extrapolation range. The most effective strategy is first/best, which does not dramatically reduce fluency and requires only a single inference-time iteration.

Model	EER ↑		SBERT \uparrow Iterations.
First/Best	0.132	0.923	
Thinning (fixed-length)	0.209	0.810	
Thinning (variable-length)	0.202	0.809	12.75
Δ Energy (fixed-length)	0.192	0.840	
Δ Energy (variable-length)	0.221	0.839	12.75

Table 6: Anonymization results with our proposed episode strategies. ∆ energy strategies tend to have higher SBERT scores than thinning strategies, with little to no tradeoff on EER.

455 456 457 458 459 460 461 462 463 464 465 466 467 This weakness is not found in the results for sentiment [\(Table 5\)](#page-8-0) or anonymization [\(Table 6\)](#page-8-1), where variable-length Δ energy performs comparatively to fixed-length Δ energy. In sentiment, it's clear that Δ energy methods of selecting training episodes have advantages over thinning; while they achieve similar results in the training range, thinning performs worse in the extrapolation range, and fluency worsens considerably more when using thinning. This pattern is echoed in our interpolation task of anonymization: ∆ energy methods and thinning methods both achieve similar EER, consistent with our observation that both function similarly in the training range. However, Δ energy methods preserve more semantic features of the text compared to uniform thinning, similarly to the fluency results in sentiment. This may indicate that thinning methods tend to change more elements of the text that are irrelevant to the target score, while choosing states that significantly lower energy allows the model to learn which features to transform. Overall, these results suggest that in cases when the model cannot learn a transformation in a single step—our "first/best" variant—choosing states using their change in energy is likely to result in the best outcome.

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6 RELATED WORK

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472 473 474 475 476 477 478 479 480 481 482 483 484 485 Controllable generation Autoregressive decoding is a favored strategy in controllable text generation. Prior to the advent of foundational LLMs, a discriminator model was often used to guide decoding [\(Dathathri et al., 2020;](#page-10-5) [Yang & Klein, 2021\)](#page-16-5). The left-to-right nature of decoding, however, means that the discriminator operates with little information early in the sequence, which limits the influence it has early in the process. Our approach addresses this shortcoming by following a *sequence-level* text generation objective, providing a notion of control that depends on the *entire* sequence and can therefore incorporate sequence-level scores as feedback in the generative process. Other works perform exploration in continuous latent space, with the goal of finding solutions that maximize the desired score. To that end, variational autoencoders have been used in several domains for controllable generation [\(Sevgen et al., 2023;](#page-15-7) [Wang et al., 2019\)](#page-16-6). Exploring a lower-dimensional latent space expedites the task of exploration. However, this assumes a well-defined latent space, and VAEs are challenged by the fact that output samples have higher variance than input sequences [\(Bredell et al., 2023\)](#page-10-6). Apart from VAEs, [Chan et al.](#page-10-4) [\(2021\)](#page-10-4) perturb representations of a sequence in a learned latent space to generate sequences that score well on sequence-level metrics. In general, however, these approaches must reconcile the differences between a continuous latent space and a discrete text space. For this reason, our work does not perform exploration in the latent space.

486 487 488 489 490 491 492 493 494 495 496 497 498 499 Editing models Incremental edits offer models multiple chances to explore the sequence space, increasing the likelihood that they find more optimal solutions. These edits may consist of tokenlevel changes [\(Reid & Neubig, 2022;](#page-15-8) [Malmi et al., 2019;](#page-13-9) [Kasner & Dušek, 2021;](#page-13-10) [Zhang et al.,](#page-16-7) [2020\)](#page-16-7), alterations to short subsequences [\(Schick et al., 2022\)](#page-15-9), or even rewrites of the entire sequence [\(Agrawal & Carpuat, 2022;](#page-10-7) [Shu et al., 2023\)](#page-15-10). A challenge for constructing models with the capability to edit their outputs is the need for paired data for training. Many editing models are trained on sequences of edits from Wikipedia pages [\(Schick et al., 2022;](#page-15-9) [Malmi et al., 2019;](#page-13-9) [Reid & Neubig,](#page-15-8) [2022\)](#page-15-8), as it is an easily accessible repository of edited text. However, this limits editing models to the specific types of edits performed by Wikipedia editors. [Shu et al.](#page-15-10) [\(2023\)](#page-15-10) create an instruction-tuning dataset with diverse "silver" instructions, removing the dependency on making only Wikipedia-style edits. Nonetheless, this limits the tasks that the model can perform to natural language rewriting tasks. To avoid this limitation, [Zhang et al.](#page-16-7) [\(2020\)](#page-16-7) use an MCTS approach that requires no task-specific training data, instead guiding the edits with a variety of hard and soft constraints. Our approach has the same advantages and also offers a means to drastically speed up inference by learning q_{θ} .

500 501 502 503 504 505 506 507 508 509 510 511 512 513 Reinforcement Learning Sequence-level energy scores bear conceptual similarities to rewards, suggesting that reinforcement learning (RL) is a natural fit to maximize a sequence-level score during generation. Indeed, reinforcement learning has previously been applied to molecular generation [\(Olivecrona et al., 2017;](#page-14-1) [Simm et al., 2020;](#page-15-11) [Zhou et al., 2019\)](#page-16-8), anonymization [\(Mosallanezhad](#page-14-2) [et al., 2019\)](#page-14-2), and sentiment-controlled generation [\(Ziegler et al., 2019;](#page-16-9) [Khalifa et al., 2021\)](#page-13-11). RL is effective at learning a policy to maximize its reward; however, the formulation of the reward function can greatly impact the success of the policy, as policies may overfit to a proxy reward function rather than satisfying the underlying objective[\(Gao et al., 2023\)](#page-12-9). This indicates the necessity of picking a reward function that approximates the true objective well. [Khalifa et al.](#page-13-11) [\(2021\)](#page-13-11) approximate a learned EBM distribution with an autoregressive policy, demonstrating success on tasks such as sentiment control and keyword inclusion. Most methods of approximating an EBM's distribution are sample-inefficient, and even in cases with theoretically guaranteed convergence such as the Metropolis-Hastings algorithm, it can be impossible to determine whether convergence has actually occurred. Learning an autoregressive policy bypasses many of the issues with sampling from an EBM, while taking advantage of the flexibility and ability to capture complex structures that the EBM provides.

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7 CONCLUSION

518 519 520 521 522 523 524 525 526 527 528 Can pre-trained language models be leveraged to learn a sample-efficient extrapolation model? Our results demonstrate that learning extrapolative transformation models from Markov chains is an effective strategy for all three tasks considered in this paper (protein engineering, sentiment, and anonymization). We outperform baseline methods in dramatically fewer steps than MCMC. We find that our trained model improves performance over MCMC in protein engineering, where we optimize for a single metric; the only notion of fluency in this task is whether the generated protein can successfully be evaluated by FoldX, allowing us to greedily optimize for protein stability with no penalty. In cases where we optimize for two metrics, we approximate the performance of MCMC for both metrics in several orders of magnitude fewer iterations. Some variations of training episode creation, as discused in [Appendix B](#page-17-0) and [Appendix C,](#page-18-1) do not conclusively benefit or harm the model. Examining strategies for constructing training episode in [§5,](#page-7-3) we find that using information from changes in energy increases the fine-tuned model's performance.

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530 531 532 533 534 535 536 537 538 539 Limitations & future work Our experiments include three distinct problems to demonstrate the generality of the proposed approach. However, for specific tasks, further detailed experimentation and comparisons would be required to make more specific claims. For example, for protein engineering, future work should evaluate our approach in a wider range of benchmark conditions [\(Notin et al.,](#page-14-3) [2024\)](#page-14-3). In addition, while we are optimistic that further experiments for different tasks such as molecule design [\(Gao et al., 2022\)](#page-12-1) would further support our conclusions, we cannot rule out the possibility of obtaining surprising results that would require adjusting some aspects of our conclusions. Finally, our experiments employ a limited number of masked language models, and we cannot rule out that different pre-training strategies (e.g., de-noising methods) could impact our results. Future work should experiment with a wider range of pre-training strategies in the context of our proposed extrapolative generation approach.

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918 A RELATED WORKS: ADDENDUM

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Monte Carlo Tree Search (MCTS) is a search algorithm which optimizes a long term score by determining the optimal sequence of intermediate steps. Unlike autoregressive decoding, MCTS does not require most of the sequence to be generated before it can effectively control generation. To that end, MCTS has been effectively used to generate sequences with optimized sequence level scores [\(Lutz et al., 2023;](#page-13-12) [Chaffin et al., 2022\)](#page-10-8). MCTS attempts to find optimal solutions rather than exploring a probability distribution; however, MCTS otherwise shares some drawbacks with MCMC methods, including computational inefficiency and not having the capability to learn from previous samples.

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B MARKOV ASSUMPTION

932 933 934 935 936 We train q_θ with and without the Markov assumption. There are theoretical benefits to each: in the case where models see all previous edits, they may perform future edits on sections that have not been edited yet, potentially avoiding repeated edits to the same section. This may also be a disadvantage, however; there may be situations where revising previously edited segments is beneficial, in which case basing current edits only on the previous step may confer an advantage to the model.

937 938 939 940 941 942 943 944 945 946 [Table 7](#page-17-1) shows that for the protein synthesis task, the Markov assumption always improves score. However, [Table 8](#page-17-2) shows an opposing result, where the Markov assumption often does not help, and universally worsens fluency. We suggest this may be explained by the fact that training with the Markov assumption functionally multiplies the number of sequences in the training dataset by the number of iterations. In our protein engineering task, we limit q_θ to a single epoch of training to try to minimize overfitting. Increasing the size of the dataset also increases the number of training steps and thus backwards passes through the model. Because it is challenging to assess overfittting and underfitting in the protein task without a validation dataset, we cannot conclusively determine whether the Markov assumption aids in extrapolation. In our main-text experiments, we do not generate with a Markov model.

Model	Assumption	-1	-2.5^{\wedge}	-51	-6↑	-71
	Non-Markov	0.961	0.915	0.715	0.580	0.422
Thinning (fixed-length)	Markov	0.984	0.956	0.810	0.686	0.528
Thinning (variable-length)	Non-Markov	0.972	0.929	0.714	0.570	0.420
	Markov	0.981	0.940	0.778	0.663	0.537
	Non-Markov	0.972	0.938	0.748	0.616	0.464
Δ Energy(fixed-length)	Markov	0.985	0.959	0.794	0.658	0.493
Δ Energy(variable-length)	Non-Markov	0.964	0.883	0.424	0.252	0.133
	Markov	0.971	0.890	0.524	0.373	0.244

Table 7: Comparing Markov and non-Markov models on the ACE2 protein engineering task.

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Table 8: Comparing Markov and non-Markov models on the sentiment task.

972 C REWARD CHOICE

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975 976 977 978 979 980 We predicate our method on the assumption that there is an energy function s that can guide the edit sequence. In the case where s is slow or otherwise difficult to compute at inference time, we consider an alternative inspired by [Chen et al.](#page-10-3) [\(2024\)](#page-10-3). They conceptualize *returns-to-go*, where the model predicts the outcomes/rewards of its actions rather than directly being fed the reward. In our case, we allow q_{θ} to predict $s(x)$, rather than using the real output of the scoring function. As an ablation, we also examine the effects of using no reward whatsoever– can q_θ achieve similar success using only the implicit reward derived from the sequence?

981 982 983 984 985 Analyzing the results shown in [Table 9,](#page-18-2) [Table 10,](#page-18-3) and [Table 11,](#page-19-1) we find that it is not uniformly beneficial to use the energy function at each step, and that calculating the real energy is in fact sometimes disadvantageous. This suggests the best strategy is either to use no energy or to predict the energy. Such a strategy also benefits efficiency, as running the proxy function is no longer necessary. In our main-text experiments, we choose to predict the energy.

Table 10: Comparing varying reward types on the sentiment task.

1018 1019 D EXTRAPOLATION EXPERIMENTAL DETAILS

1020 1021 D.1 PROTEIN ENGINEERING

1022 1023 1024 1025 Starting from wildtype ACE2, we iteratively sample for 83 steps, using the trained ddG scorer and Hamming distance as our experts in the product of experts energy function. We use the pre-trained Prot-T5-XL model from [\(Elnaggar et al., 2020\)](#page-12-8) as our proposal distribution, and following the experimental procedure of [Padmakumar et al.](#page-15-2) [\(2023\)](#page-15-2), we restrict the sampler from resampling a constant span of 8 tokens (NTNITEEN) to prevent too much divergence from the wildtype sequence.

Table 11: Comparing varying reward types on the anonymization task.

1042 1043 1044 1045 To train q_θ , we finetune Prot-T5-XL using low rank adaptation (LoRA)[\(Hu et al., 2021\)](#page-13-13). Further details can be found in [Appendix E.](#page-19-2) At inference time, we prompt with the wildtype sequence and sample 10,000 mutants.

1046 1047 1048 1049 1050 1051 1052 One challenge of this task is the lack of separate test/validation splits, as the protein always mutates from the wildtype sequence. We take several measures to attempt to avoid overfitting. Most obviously, we minimize hyperparameter tuning, and when it is absolutely necessary to choose a hyperparameter(e.g. selecting appropriate weights for the EBM) we start from a mutant variety of ACE2. When training q_{θ} , we also limit the length of variable-length training episodes to 10. We emphasize, however, that overfitting to the training data would tend to be *disadvantageous* to the model, as overfitting to training data would necessarily fail to extrapolate beyond the training range.

1053 D.2 SENTIMENT

1054 1055 1056 1057 1058 1059 1060 1061 In our energy function, the first term is the training-time scorer proposed by [Padmakumar et al.](#page-15-2) [\(2023\)](#page-15-2), which incentivizes sentiment control. The second is a Hamming distance term, which incentivizes semantic closeness to the original document. We use this EBM and sample 66,163 sentences $\frac{7}{1}$ $\frac{7}{1}$ $\frac{7}{1}$ using a pretrained T5-3B model [\(Raffel et al., 2023\)](#page-15-3) as our proposal distribution for both conversion to positive sentiment and negative sentiment, giving us a combined training dataset of 132,326 markov chains. We finetune T5-base [\(Raffel et al., 2023\)](#page-15-3) on these chains to train q_θ ; we add a prefix "Make this {positive, negative}: " to cue the direction of edits, rather than training two separate models. Hyperparameters can be found in [Appendix E.](#page-19-2)

1063 1064 1065 1066 1067 1068 We also implement a popular controllable generation method, FUDGE [Yang & Klein](#page-16-5) [\(2021\)](#page-16-5), as for the sentiment control task. To train the forward looking model, we fine-tune RoBERTa [Liu et al.](#page-13-14) [\(2020\)](#page-13-14) on the three classes in our training regime (2, 3, 4 star reviews) for 5000 total steps. Instead of running FUDGE with a decoder only model, we use PEGASUS [Zhang et al.](#page-16-10) [\(2019\)](#page-16-10), a sequence to sequence paraphraser of similar size to the models used in our other approaches. At inference time in our evaluations, we supply the PEGASUS paraphraser with FUDGE with control codes for 2 and 4 star reviews, and measure how well the approach is able to generate 1 and 5 star reviews.

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E HYPERPARAMETERS

1072 1073 1074 1075 1076 1077 1078 1079 [Table 12](#page-20-2) shows the hyperparameters used in our framework. *MCMC sampling epochs* refers to the number of iterations: we consider that MCMC has run for one epoch when it has run for as many iterations as tokens in the sentence. *Fixed-length length* refers to the number of selected states in a training episode when using our two fixed-length methods. ∆ *energy (variable-length) threshold* and *thinning factor(variable-length)* refer to the hyperparameters used to determine sequence length for the variable-length training episodes, as described in [§3.1.](#page-3-1) *LoRA rank* and *learning rate* are the hyperparameters used while training q_{θ} ; as sentiment did not use LoRA, we do not report LoRA rank.

 7 For computational efficiency, we run MCMC only on sentences with length of 64 tokens or fewer.

1080 1081 1082 1083 *Decoding temperature* and *Decoding top k* refer to the hyperparameters used while generating using q_{θ} . Detailed implementation details for sentiment and protein engineering tasks are reported in the main text, and the details of the energy function used during MCMC are reported below; detailed implementation details for anonymization are reported in [Appendix F.](#page-20-0)

	Protein engineering Sentiment Anonymization		
MCMC sampling epochs			40
Fixed-length length			
Δ energy (variable-length) threshold	20%	2%	1%
Thinning factor(variable-length)		100	
LoRA rank	16		16
Learning rate	$2E-4$	1E-4	5E-5
Decoding temperature	1.5	1.1	1.1
Decoding top k		16	50

Table 12: Hyperparameters

1098 1099 Protein engineering energy function In our energy function, we use a weight of 500 on the training scorer term (ddG) and a weight of 10 on the Hamming distance term. In other words:

$$
s(x) = 500 * s_{\text{ddg}}(x) + 10 * s_{\text{hamming}}(x)
$$
 (1)

1102 1103 1104 Sentiment energy function In our energy function, we use a weight of 1E5 on the training scorer term (sentiment) and a weight of 100 on the Hamming distance term. In other words:

$$
s(x) = 1E5 * s_{\text{sentiment}}(x) + 100 * s_{\text{hamming}}(x)
$$
 (2)

1107 1108 F TEXT ANONYMIZATION IMPLEMENTATION

1109 1110 F.1 BASELINE SYSTEMS

1111 1112 GPT3.5 and 4 use the following prompt to anonymize text:

1113 1114 1115 "You are a helpful assistant who follows instructions and is helping anonymize text. Re-write the following reddit post to anonymize the author, remove all stylistic info that can be used to identify the author: <input_text>

1117 1118 1119 1120 Based on optimal validation performance, we ran DIPPER with a lexical diversity of 60, order diversity of 40, and temperature of 0.75 ^{[8](#page-20-3)}. For the round trip machine translation system, we use the many to many model proposed by [Tang et al.](#page-16-11) [\(2020\)](#page-16-11). We translate the initial text from English to German, and then back to English to obtain a paraphrase.

1121 1122 F.2 DATA

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1123 1124 1125 1126 1127 1128 We sample training and evaluation data from the Reddit IUR dataset proposed by [Andrews & Bishop](#page-10-9) [\(2019\)](#page-10-9). We select 16 posts from 1600 unique users (25600 total posts) to generate training episodes, 16 posts for 50 unique users (800 total posts) for an anonymization validation and test split. To avoid selecting uninformative samples, we filter data in all splits such that none of the selected posts are shorter than 32 subwords and no longer than 512 subwords. We use the RoBERTa-base model tokenizer to count subwords [\(Liu et al., 2020\)](#page-13-14).

1129 1130 1131 1132 To generate training episodes, we largely follow the approach proposed by [Khan et al.](#page-13-6) [\(2024\)](#page-13-6), using four experts to parameterize an energy function. OPT-1.3B is used to capture fluency [\(Zhang et al.,](#page-16-7) [2020\)](#page-16-7), hamming distance is used to discourage excessive edits, LUAR is used to measure stylistic

¹¹³³ ⁸We used the released checkpoint here: [https://huggingface.co/kalpeshk2011/](https://huggingface.co/kalpeshk2011/dipper-paraphraser-xxl) [dipper-paraphraser-xxl](https://huggingface.co/kalpeshk2011/dipper-paraphraser-xxl)

1134 1135 1136 similarity [\(Rivera-Soto et al., 2021\)](#page-15-6), and SBERT is used to measure semantic retention 9 9 9 [\(Reimers &](#page-15-12) [Gurevych, 2019\)](#page-15-12). The weights associated with each expert are 10, 1, 1E7, 5E5 respectively. In other words:

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$$
s(x) = 10 * s_{\text{fluency}}(x) + 1 * s_{\text{hamming}}(x) + 1E7 * s_{\text{LUAR}}(x) + 5E5 * s_{\text{SBERT}}(x)
$$
(3)

1140 1141 F.3 q_θ AND INFERENCE

1142 1143 1144 1145 1146 1147 1148 1149 We learn q_{θ} with Llama3.1 using supervised finetuning and the extracted training episodes [\(Dubey](#page-10-10) [et al., 2024\)](#page-10-10). We finetune using LoRA [\(Hu et al., 2021\)](#page-13-13), with a rank of 16 and scaling factor of 32. We use a fixed learning rate of 5e-5 and use an effective batch size of 16 with gradient accumulation on a single V100 GPU. During training, a sequence of states is sampled from a given chain using one of the strategies outlined in [§3.1.](#page-3-1) Each of the states is separated by a special token, and model is trained on the entire sequence. An example of a sample is as follows: & $\text{&$ [SEQ1]...<eos>. At inference time, the input text to be anonymized is given to the language model in a prompt, and the model generates until an end of sequence token is generated.

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- **1151** G EXAMPLE GENERATIONS
- **1153** G.1 SENTIMENT
- **1155** [Table 13](#page-22-0) shows 5 randomly selected positive and negative examples from q_{θ} .
- **1157** G.2 ANONYMIZATION
- **1159** [Table 14](#page-23-0) shows 5 randomly selected examples from q_{θ} .
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1162 H TOY EXAMPLE

1163 1164 1165 We provide a simple example to illustrate how state sequences extracted from Markov chains can successfully extrapolate.

1166 1167 1168 1169 Problem setup Consider the space of binary sequences of fixed length L. Given an initial sequence $x^{(0)}$ of all zeros, the objective is to search for sequences that maximize a scalar score function $s(x) = \exp \sum_{i}^{L} r_i$ where

 $s_i = \begin{cases} ix_i/L & i > L/2 \\ \vdots & \text{otherwise} \end{cases}$ $-i x_i/L$ otherwise

1172 1173 1174 which is maximized by placing 0's in the first $L/2$ positions followed by 1's in the last $L/2$ positions (for even L). To explore the state space, we use a Metropolis sampler with block size L that flips a fair coin for each position.

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1176 1177 1178 1179 1180 1181 1182 1183 1184 1185 1186 1187 Experiment We consider the space of sequences of length $L = 16$, which has a maximum reward of 314.2. Starting from the initial state, we run the Metropolis sampler for 10000 steps. The sampler had an acceptance rate of 43.7% and the highest achieved reward was 244.7. Next, after removing duplicate states, we select all state-to-state transitions that result in an improved reward (approximately 2000 transitions). This data is used to train a Markov policy q_θ parametrized as a two-layer multi-layer perceptron (MLP) with hidden dimensions 16 for the embedding matrix and two 128 dimensional layers with relu activations. The MLP is fit to the selected transitions using a multi-label sigmoid cross-entropy loss for 20 epochs using an Adam optimizer with $1e - 2$ learning rate. Finally, q_θ was iteratively applied starting at x_0 five times to produce a sequences of states $x^{(1)}$, $x^{(2)}, \ldots, x^{(5)}$ where $x^{(t)} = q_{\theta}(x^{(t-1)})$ and predictions from q_{θ} are obtained deterministically by decoding all L positions in parallel. For our learned policy, this achieved the following sequence of rewards: 1, 3.3, 15.6, 314.2, 314.2. Thus, the learned policy successfully extrapolates beyond the

⁹Note the SBERT checkpoint used here is different than the one used in our evaluations.

