

Autoregressive Language Models are Secretly Energy-Based Models: Insights into the Lookahead Capabilities of Next-Token Prediction

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Abstract

Autoregressive models (ARMs) currently constitute the dominant paradigm for large language models (LLMs). Energy-based models (EBMs) represent another class of models, which have historically been less prevalent in LLM development, yet naturally characterize the optimal policy in post-training alignment. In this paper, we provide a unified view of these two model classes. Taking the chain rule of probability as a starting point, we establish an explicit bijection between ARMs and EBMs in function space, which we show to correspond to a special case of the soft Bellman equation in maximum entropy reinforcement learning. Building upon this bijection, we derive the equivalence between supervised learning of ARMs and EBMs. Furthermore, we analyze the distillation of EBMs into ARMs by providing theoretical error bounds. Our results provide insights into the ability of ARMs to plan ahead, despite being based on the next-token prediction paradigm.

1. Introduction

Autoregressive models (ARMs), which are based on the next-token prediction paradigm, currently constitute the dominant approach for large language models (LLMs). Their primary advantages lie in their highly parallelizable training and the ability to perform exact ancestral sampling. Energy-based models (EBMs) represent another class of models, which inherently have the ability to look ahead, since they define sequence-level distributions. However, they have historically been less prevalent, since they require computing an intractable partition function over the set of all possible sequences. Consequently, they are significantly more challenging to train and sample from, often necessitating Markov-chain Monte-Carlo (MCMC) methods.

Following pre-training, LLMs typically undergo a post-training alignment phase. This process is frequently framed as maximum entropy (MaxEnt) reinforcement learning (RL),

a.k.a. entropy-regularized RL, where we seek a probability distribution (or policy) that maximizes a trade-off between the expected reward and a Kullback-Leibler (KL) regularization term. Crucially, if we maximize over the set of all possible probability distributions, the analytical solution to this objective is exactly an EBM. Therefore, finding an ARM that maximizes this objective is equivalent to distilling an EBM into an ARM.

This perspective raises a fundamental question: To what extent can ARMs approximate EBMs? From a probabilistic graphical model standpoint, ARMs are Bayesian networks (directed graphical models), whereas EBMs are Markov random fields (undirected graphical models). However, ARMs rely on the chain rule of probability, which can, in principle, decompose any probability distribution. It naturally follows that ARMs should be convertible into EBMs, and vice-versa. Building upon these intuitions, we derive several results that provide insights into the approximation power of ARMs w.r.t. EBMs, and consequently their ability to plan ahead, despite being based on the next-token prediction paradigm.

Contributions.

- We provide a unified view of ARMs and EBMs, exhibiting clear structural analogies between these two model classes.
- In function space (a.k.a. tabular setting in RL), we establish an exact bijection between ARMs and EBMs (Proposition 1). While our starting point is the chain rule of probability, our bijection can be viewed as an instance of the soft Bellman equation in MaxEnt RL. Our result demonstrates that in our setting the soft Bellman equation naturally emerges as a direct consequence of the chain rule of probability.
- Building upon this bijection, we derive the equivalence between supervised learning of ARMs and EBMs (Proposition 2). Furthermore, we derive error bounds for distilling EBMs into ARMs (Proposition 3), a process identical to MaxEnt RL. Our results, validated through numerical experiments, provide some theoretical justification for the next-token prediction paradigm and for teacher forcing.

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sequences of size t in the vocabulary by \mathcal{V}^t . We consider two special tokens that are excluded from \mathcal{V} : a BOS (beginning of sequence) token that encodes the beginning of a prompt and a EOS (end of sequence) token that encodes the end of a response. We then denote the set of prompts of maximal size U (BOS included) by $\mathcal{X} = \{\text{BOS}\} \times \cup_{t=1}^{U-1} \mathcal{V}^t$, and the set of responses of maximal size T (EOS included) by $\mathcal{Y} = \cup_{t=1}^{T-1} \mathcal{V}^t \times \{\text{EOS}\}$. A response $\mathbf{y} = (y_1, \dots, y_T) \in \mathcal{Y}$ always ends with EOS: $y_T = \text{EOS}$. We denote the length of \mathbf{y} (including EOS) by $|\mathbf{y}|$. We denote $\mathbf{y}_{<t} := (y_1, \dots, y_{t-1})$ for $t > 1$ and we set $\mathbf{y}_{<1} := \emptyset$. We denote the vocabulary augmented with the EOS token as $\mathcal{A} := \mathcal{V} \cup \{\text{EOS}\}$. We use \oplus to indicate concatenation. We denote random variables by capital letters, e.g., Y . Given the finite set \mathcal{Y} , we define the space of probability distributions *with full support* over \mathcal{Y} as $\mathcal{P}(\mathcal{Y})$ and the set of functions $f: \mathcal{Y} \rightarrow \mathbb{R}$ as $\mathcal{F}(\mathcal{Y})$. Given a function $f \in \mathcal{F}(\mathcal{Y})$, we define $\text{softargmax}(f) \in \mathcal{P}(\mathcal{Y})$ by $\text{softargmax}(f)(\mathbf{y}) := \frac{\exp f(\mathbf{y})}{\sum_{\mathbf{y}' \in \mathcal{Y}} \exp f(\mathbf{y}')}$.

2. A unified perspective on EBMs and ARMs

2.1. Energy-based models (EBMs)

Model definition. EBMs (Ackley et al., 1985; LeCun et al., 2007) use a function $R: \mathcal{X} \times \mathcal{Y} \rightarrow \mathbb{R}$, measuring the “affinity” between an input $\mathbf{x} \in \mathcal{X}$ (a prompt) and an output $\mathbf{y} \in \mathcal{Y}$ (a complete response). We use the convention that higher value means higher affinity, therefore R can be interpreted as a negative energy. EBMs are defined as

$$p_R^{\text{EBM}}(\mathbf{y}|\mathbf{x}) := \frac{\exp(R(\mathbf{x}, \mathbf{y}))}{\sum_{\mathbf{y}' \in \mathcal{Y}} \exp(R(\mathbf{x}, \mathbf{y}'))}, \quad (1)$$

or more concisely, $p_R^{\text{EBM}}(\cdot|\mathbf{x}) = \text{softargmax}(R(\mathbf{x}, \cdot))$. We use the letter R on purpose, as it will coincide with the notion of reward function in RL. The reward could be a learned model or a given function, such as a verifier.

The associated sequence-level log-partition function is

$$A_R^{\text{EBM}}(\mathbf{x}) := \underset{\mathbf{y} \in \mathcal{Y}}{\text{LSE}} R(\mathbf{x}, \mathbf{y}) := \log \sum_{\mathbf{y} \in \mathcal{Y}} \exp(R(\mathbf{x}, \mathbf{y})).$$

We then have $p_R^{\text{EBM}}(\mathbf{y}|\mathbf{x}) = \exp(R(\mathbf{x}, \mathbf{y}) - A_R^{\text{EBM}}(\mathbf{x}))$.

Unfortunately, the log-partition costs $O(V^T)$ to compute exactly. This makes both learning EBMs and making inference with EBMs very challenging.

EBMs as undirected graphical models. We can view EBMs as specifying a sequence-level Gibbs (Boltzmann) distribution parameterized by a function R . From a probabilistic graphical model perspective, EBMs are (conditional) Markov random fields, that is, undirected graphical models.

Validity of the distribution. Since all sequences $\mathbf{y} \in \mathcal{Y}$ have a maximal size T , and therefore \mathcal{Y} is finite, the denom-

inator in (1) is well-defined. Exponentiation and renormalization ensure that it is a valid probability distribution.

Learning R from data using Transformers. To learn R from data, we must use a model that can cope with variable-length sequences \mathbf{x} and \mathbf{y} . This can be achieved using a Transformer (Vaswani et al., 2017). Because R is sequence-level, the Transformer can be non-causal (bidirectional). A Transformer embeds an input sequence $\mathbf{s} = \mathbf{x} \oplus \mathbf{y}$ of size M into a latent space \mathbb{R}^D , processing it through multiple attention, feedforward and normalization layers, yielding M output vectors $(\mathbf{h}_1, \dots, \mathbf{h}_M)$, where $\mathbf{h}_i \in \mathbb{R}^D$. When using a non-causal Transformer, each $\mathbf{h}_i \in \mathbb{R}^D$ depends on the entire sequence \mathbf{s} . To obtain a scalar-valued $R(\mathbf{x}, \mathbf{y})$, one can for example use an affine layer on top of a single representation $\bar{\mathbf{h}}$ of the sequence. The latter can be the average of all \mathbf{h}_i , or simply the first vector \mathbf{h}_1 , which mirrors the CLS token in BERT encoders (Devlin et al., 2019).

Learning R from (\mathbf{x}, \mathbf{y}) pairs is challenging due to the intractable normalization constant, and has attracted a large body of work (Song & Kingma, 2021; Sander et al., 2025). To work around this difficulty, R is popularly learned from pairwise preferences $(\mathbf{x}, \mathbf{y}^+, \mathbf{y}^-)$, where \mathbf{y}^+ is preferred over \mathbf{y}^- given \mathbf{x} (Ziegler et al., 2019; Stiennon et al., 2020; Ouyang et al., 2022) or from scored pairs $(\mathbf{x}, \mathbf{y}, s)$, where s is the affinity score (binary or real valued) between \mathbf{x} and \mathbf{y} , that $R(\mathbf{x}, \mathbf{y})$ should approximate (Cobbe et al., 2021).

Sampling. Given R , drawing i.i.d. sequence samples

$$Y \sim p_R^{\text{EBM}}(\cdot|\mathbf{x})$$

typically requires Markov-chain Monte-Carlo (MCMC) methods, such as Gibbs sampling. However, such samplers are typically inherently sequential and difficult to parallelize. Moreover, since they are never run to convergence in practice, they do not generate truly i.i.d. samples.

Optimal solution of MaxEnt RL as an EBM. It is well-known that an EBM can be seen as the solution of

$$p_R^{\text{EBM}} = \underset{p \in \mathcal{P}(\mathcal{Y}|\mathcal{X})}{\text{argmax}} \mathbb{E}_X \mathbb{E}_{Y \sim p(\cdot|X)} R(X, Y) + H(p(\cdot|X)),$$

where $H(\cdot)$ is the entropy of a distribution. More generally, RL-based post-training of LLMs is commonly formulated as the KL-regularized problem (Ziegler et al., 2019; Stiennon et al., 2020; Ouyang et al., 2022)

$$\underset{p \in \mathcal{P}(\mathcal{Y}|\mathcal{X})}{\text{argmax}} \mathbb{E}_X \mathbb{E}_{Y \sim p(\cdot|X)} R(X, Y) - \text{KL}(p(\cdot|X), p_{\text{ref}}(\cdot|X)), \quad (2)$$

where $p_{\text{ref}} \in \mathcal{P}(\mathcal{Y}|\mathcal{X})$ is a reference “anchor” distribution. The optimal solution p^* is then

$$p^*(\mathbf{y}|\mathbf{x}) = \frac{p_{\text{ref}}(\mathbf{y}|\mathbf{x}) \exp(R(\mathbf{x}, \mathbf{y}))}{\sum_{\mathbf{y}' \in \mathcal{Y}} p_{\text{ref}}(\mathbf{y}'|\mathbf{x}) \exp(R(\mathbf{x}, \mathbf{y}'))}.$$

Using (1), we can write p^* more concisely as $p^* = p_{R+R_{\text{ref}}}^{\text{EBM}}$, where $R_{\text{ref}}(\mathbf{x}, \mathbf{y}) := \log p_{\text{ref}}(\mathbf{y}|\mathbf{x})$. Therefore, the optimal solution of the KL-regularized RL objective (2) is exactly an EBM, with the reward function $R + R_{\text{ref}}$. Recently, several papers have replaced the KL divergence in the regularization term by other f -divergences (Go et al., 2023; Wang et al., 2024; Roulet et al., 2025; Sander et al., 2025).

2.2. Autoregressive models (ARMs)

Model definition. Let us define the set of contexts $\mathcal{S} := \{\text{BOS}\} \times \cup_{t=1}^{U+T-2} \mathcal{V}^t$. We can think of \mathcal{S} as the set of partial (incomplete) sequences, including the initial prompt. Recall that we denoted $\mathcal{A} := \mathcal{V} \cup \{\text{EOS}\}$ the augmented vocabulary used to encode finished responses. Given a pair (\mathbf{x}, \mathbf{y}) , where $\mathbf{y} = (y_1, \dots, y_T)$, it will be convenient to define the context (state) at time t by

$$\mathbf{s}_t := \mathbf{x} \oplus \mathbf{y}_{<t} \in \mathcal{S}(\mathbf{x}),$$

where $\mathcal{S}(\mathbf{x}) \subseteq \mathcal{S}$ is the set of partial sequences prolonging the prompt \mathbf{x} . We assume that we have at our disposal a function $q: \mathcal{S} \times \mathcal{A}$, for scoring the “affinity” between a context (state) $\mathbf{s}_t \in \mathcal{S}$ and a next token $y_t \in \mathcal{A}$ (potentially EOS). We can think of q as a local scoring function, while R used by EBMs is a global scoring function. ARMs use the chain rule of probability to define the probability of a sequence \mathbf{y} given \mathbf{x} as

$$p_q^{\text{ARM}}(\mathbf{y}|\mathbf{x}) := \prod_{t=1}^{|\mathbf{y}|} \pi_q(y_t | \underbrace{\mathbf{x} \oplus \mathbf{y}_{<t}}_{\mathbf{s}_t}),$$

where

$$\pi_q(y_t | \mathbf{s}_t) := \frac{\exp(q(\mathbf{s}_t, y_t))}{\sum_{j \in \mathcal{A}} \exp(q(\mathbf{s}_t, j))}.$$

The latter can be rewritten more concisely as $\pi_q(\cdot | \mathbf{s}_t) = \text{softmax}(q(\mathbf{s}_t, \cdot))$. The associated log-partition is

$$V_q(\mathbf{s}_t) := \text{LSE } q(\mathbf{s}_t, j) := \log \sum_{j \in \mathcal{A}} \exp(q(\mathbf{s}_t, j)).$$

We then have $\pi_q(y_t | \mathbf{s}_t) = \exp(q(\mathbf{s}_t, y_t) - V_q(\mathbf{s}_t))$.

ARMs as directed graphical models. From a probabilistic graphical model perspective, ARMs are Bayesian networks, that is, directed graphical models. More specifically, we can view ARMs as specifying a time-inhomogeneous infinite-order Markov chain (assuming unlimited context window size) with discrete states Y_t .

Validity of the distribution. For $p_q^{\text{ARM}}(\cdot | \mathbf{x})$ to define a valid probability distribution over all possible sequences of size at most T , we need to enforce that sequences cannot be of size more than T . This can be achieved by fixing

$$q(\mathbf{s}_T, y_T) := \begin{cases} 0 & \text{if } y_T = \text{EOS} \\ -\infty & \text{if } y_T \neq \text{EOS} \end{cases}. \quad (3)$$

This ensures that $\pi_q(\text{EOS} | \mathbf{s}_T) = 1$, which in turn ensures that the ARM defines a valid probability distribution over all possible sequences of size at most T . See Appendix A.1 for more details and a proof.

Analogy with EBMs. We now rewrite the equations in order to build an analogy with EBMs. We define the “log-partition” **along** the sequence (path) \mathbf{y} given \mathbf{x} as

$$A_q^{\text{ARM}}(\mathbf{x}, \mathbf{y}) := \sum_{t=1}^{|\mathbf{y}|} V_q(\mathbf{x} \oplus \mathbf{y}_{<t}) = \sum_{t=1}^{|\mathbf{y}|} \text{LSE } q(\mathbf{x} \oplus \mathbf{y}_{<t}, y'_t).$$

Mirroring the EBM notation, we then have

$$p_q^{\text{ARM}}(\mathbf{y} | \mathbf{x}) = \exp(Q_q(\mathbf{x}, \mathbf{y}) - A_q^{\text{ARM}}(\mathbf{x}, \mathbf{y})),$$

where

$$Q_q(\mathbf{x}, \mathbf{y}) := \sum_{t=1}^{|\mathbf{y}|} q(\mathbf{x} \oplus \mathbf{y}_{<t}, y_t).$$

Sampling. To draw an i.i.d. sequence $Y \sim p_q^{\text{ARM}}(\cdot | \mathbf{x})$, we can use autoregressive (a.k.a. ancestral) sampling,

$$Y_t \sim \pi_q(\cdot | S_t),$$

where $S_1 := \mathbf{x}$ and $S_t := \mathbf{x} \oplus Y_{<t}$ for $t > 1$. The sampling is repeated until an EOS token is emitted.

Learning q from data using Transformers. To learn q from data, we must use a model that can score a next token y_t using only the past context \mathbf{s}_t , which has variable length. This can be achieved using a causal Transformer \mathcal{T} , which uses an attention mask to ensure that each token can only attend to previous tokens. The causal Transformer outputs a vector of logits $\mathbf{h}_t = \mathcal{T}(\mathbf{s}_t) \in \mathbb{R}^{|\mathcal{A}|}$. Intuitively, $\mathcal{T}(\mathbf{s}_t)[y_t]$ can be interpreted as the score of token $y_t \in \mathcal{A}$ given the context \mathbf{s}_t . We can therefore define $q(\mathbf{s}_t, y_t) := \mathcal{T}(\mathbf{s}_t)[y_t]$.

MaxEnt RL as distilling an EBM into an ARM. We saw that the optimal solution of the regularized RL problem (2) is exactly an EBM. This creates a paradox: if we know the optimal solution, why cannot we use the EBM directly at inference time and why do we even need RL-based training? Unfortunately, as we discussed, sampling from an EBM in combinatorially-large spaces is typically intractable, often requiring Markov-chain Monte-Carlo (MCMC) methods. Therefore, (2) is often reformulated as

$$\underset{q \in \mathcal{F}(\mathcal{S} \times \mathcal{A})}{\text{argmax}} \mathbb{E}_X \mathbb{E}_Y R(X, Y) - \text{KL}(p_q^{\text{ARM}}(\cdot | X), \rho(\cdot | X)),$$

where Y above is distributed according to $p_q^{\text{ARM}}(\cdot | X)$.

Intuitively, instead of performing maximization in the space $\mathcal{P}(\mathcal{Y} | \mathcal{X})$ of all possible distributions, we perform maximization in the space of ARMs parameterized by a function

$q \in \mathcal{F}(\mathcal{S} \times \mathcal{A})$. Thus, we can see RL-based language model post-training as approximating the EBM $p_{R+R_\rho}^{\text{EBM}}(\cdot | \mathbf{x})$ with the ARM $p_q^{\text{ARM}}(\cdot | \mathbf{x})$, or put differently, as distilling this EBM into this ARM.

3. From the chain rule to Bellman equations

3.1. Bijection between distributions

The chain rule of probability factorizes a joint probability distribution into a product of conditional probabilities. In this section, we show how it can be used to derive a procedure for converting any sequence distribution $p \in \mathcal{P}(\mathcal{Y}|\mathcal{X})$ to a next-token distribution $\pi \in \mathcal{P}(\mathcal{A}|\mathcal{S})$, and vice-versa.

From sequence to next-token distributions. For any $\mathbf{x} \in \mathcal{X}$ and any $\mathbf{y} \in \mathcal{Y}$ such that $|\mathbf{y}| = \tau$, with $1 \leq \tau \leq T$, the procedure works by successively marginalizing and conditioning in backward order. First, starting from $p(\mathbf{y}_{\leq \tau} | \mathbf{x}) := p(\mathbf{y} | \mathbf{x})$, we define from $t = \tau - 1$ to $t = 1$,

$$p(\mathbf{y}_{\leq t} | \mathbf{x}) := \sum_{y_{t+1} \in \mathcal{A}} p(\mathbf{y}_{\leq t}, y_{t+1} | \mathbf{x}).$$

Second, we define from $t = \tau$ to $t = 2$

$$\pi(y_t | \mathbf{x}, \mathbf{y}_{<t}) := \frac{p(\mathbf{y}_{\leq t} | \mathbf{x})}{p(\mathbf{y}_{\leq t-1} | \mathbf{x})},$$

ending with $\pi(y_1 | \mathbf{x}) := p(y_1 | \mathbf{x})$.

From next-token to sequence distributions. Conversely, from any next-token distribution $\pi \in \mathcal{P}(\mathcal{A}|\mathcal{S})$, we can reconstruct a sequence distribution $p \in \mathcal{P}(\mathcal{Y}|\mathcal{X})$ by

$$p(\mathbf{y} | \mathbf{x}) = \prod_{t=1}^{|\mathbf{y}|} \pi(y_t | \mathbf{x}, \mathbf{y}_{<t}). \quad (4)$$

Indeed, by substituting the definition of π , we observe that the product forms a telescoping sequence that exactly recovers the joint distribution: $\prod_{t=1}^{|\mathbf{y}|} \pi(y_t | \mathbf{x}, \mathbf{y}_{<t}) = \frac{p(\mathbf{y}_{\leq 1} | \mathbf{x})}{1} \times \frac{p(\mathbf{y}_{\leq 2} | \mathbf{x})}{p(\mathbf{y}_{\leq 1} | \mathbf{x})} \times \cdots \times \frac{p(\mathbf{y}_{\leq \tau} | \mathbf{x})}{p(\mathbf{y}_{\leq \tau-1} | \mathbf{x})} = p(\mathbf{y} | \mathbf{x})$.

The chain rule of probability as a bijection. Since there is a unique correspondence between p and π , the procedure defines a bijection between $\mathcal{P}(\mathcal{Y}|\mathcal{X})$ and $\mathcal{P}(\mathcal{A}|\mathcal{S})$.

3.2. Bijection between EBMs and ARMs

We now instantiate the bijection for EBMs and ARMs, which can be seen as using sequence and next-token Gibbs (Boltzmann) distributions, respectively. In this section, we assume without loss of generality that R decomposes as

$$R_r(\mathbf{x}, \mathbf{y}) := \sum_{t=1}^{|\mathbf{y}|} r(\underbrace{\mathbf{x} \oplus \mathbf{y}_{<t}}_{\mathbf{s}_t}, y_t), \quad (5)$$

where $r: \mathcal{S} \times \mathcal{A} \rightarrow \mathbb{R}$ is the immediate (next-token) reward. Indeed, if R does not naturally decompose as above, from any $R: \mathcal{X} \times \mathcal{Y} \rightarrow \mathbb{R}$, we can always define

$$r(\mathbf{s}_t, y_t) := \begin{cases} 0 & \text{if } y_t \neq \text{EOS} \\ R(\mathbf{x}, \mathbf{y}) & \text{if } y_t = \text{EOS} \end{cases}. \quad (6)$$

We now show how to transform $r: \mathcal{S} \times \mathcal{A} \rightarrow \mathbb{R}$ used by an EBM into $q: \mathcal{S} \times \mathcal{A} \rightarrow \mathbb{R}$ used by an ARM, and vice-versa.

From EBM to ARM. Suppose $r: \mathcal{S} \times \mathcal{A} \rightarrow \mathbb{R}$ is given. We define the mapping $q = \mathcal{M}(r)$ as

$$q(\mathbf{s}_t, y_t) := \begin{cases} r(\mathbf{s}_t, y_t) & \text{if } y_t = \text{EOS} \\ r(\mathbf{s}_t, y_t) + V_q(\mathbf{s}_t \oplus y_t) & \text{if } y_t \neq \text{EOS} \end{cases}, \quad (7)$$

where $\mathbf{s}_t \in \mathcal{S}$ and $y_t \in \mathcal{A}$. For all τ and all $\mathbf{y} = (y_1, \dots, y_\tau)$, defining the contexts $\mathbf{s}_1 := \mathbf{x}$, ..., $\mathbf{s}_\tau := \mathbf{x} \oplus \mathbf{y}_{<\tau}$ we obtain by unrolling (7) backwards,

$$\begin{aligned} q(\mathbf{s}_\tau, y_\tau) &= r(\mathbf{s}_\tau, y_\tau) \\ &\vdots \\ q(\mathbf{s}_t, y_t) &= r(\mathbf{s}_t, y_t) + V_q(\mathbf{s}_t \oplus y_t) \\ &\vdots \\ q(\mathbf{s}_1, y_1) &= r(\mathbf{s}_1, y_1) + V_q(\mathbf{s}_1 \oplus y_1). \end{aligned}$$

Because $V_q(\mathbf{s}_t \oplus y_t) = \underset{y_{t+1} \in \mathcal{A}}{\text{LSE}} q(\mathbf{s}_t \oplus y_t, y_{t+1})$, we can see that $q(\mathbf{s}_t, \cdot)$ depends on $q(\mathbf{s}_{t+1}, \cdot)$ and therefore computing q from r must be done sequentially for all possible states.

From ARM to EBM. Suppose $q: \mathcal{S} \times \mathcal{A} \rightarrow \mathbb{R}$ is now given. We define the inverse mapping $r = \mathcal{M}^{-1}(q)$ as

$$r(\mathbf{s}_t, y_t) := \begin{cases} q(\mathbf{s}_t, y_t) & \text{if } y_t = \text{EOS} \\ q(\mathbf{s}_t, y_t) - V_q(\mathbf{s}_t \oplus y_t) & \text{if } y_t \neq \text{EOS} \end{cases}. \quad (8)$$

Applying (8), we obtain

$$\begin{aligned} r(\mathbf{s}_1, y_1) &= q(\mathbf{s}_1, y_1) - V_q(\mathbf{s}_1 \oplus y_1) \\ &\vdots \\ r(\mathbf{s}_t, y_t) &= q(\mathbf{s}_t, y_t) - V_q(\mathbf{s}_t \oplus y_t) \\ &\vdots \\ r(\mathbf{s}_\tau, y_\tau) &= q(\mathbf{s}_\tau, y_\tau). \end{aligned}$$

Computing r from q can be done in parallel.

Bijection. Having defined the mapping \mathcal{M} and its inverse \mathcal{M}^{-1} , we can now formally state our bijection.

Proposition 1 (Bijection between EBMs and ARMs).
If $q = \mathcal{M}(r)$ or equivalently $r = \mathcal{M}^{-1}(q)$, then, for all $\mathbf{x} \in \mathcal{X}$ and $\mathbf{y} \in \mathcal{Y}$, we have

$$\begin{aligned} p_{R_r}^{\text{EBM}}(\mathbf{y}|\mathbf{x}) &= p_q^{\text{ARM}}(\mathbf{y}|\mathbf{x}) \\ A_{R_r}^{\text{EBM}}(\mathbf{x}) &= V_q(\mathbf{x}). \end{aligned}$$

A proof is given in Appendix B.2. This shows that an EBM can be transformed into an ARM if r is “corrected” by adding the log-partition V_q of the next states. In MaxEnt RL terminology (see Section 3.3 for more details), V_q is known as the soft value function and $V_q(s_t)$ captures the future (soft) value of being in state s_t . Accordingly, since an ARM has the capacity to learn an EBM, which is a globally normalized distribution, an ARM inherently has the ability to look ahead, provided that we can learn q appropriately.

Computational cost. The cost of converting an EBM into an ARM is $O(V^T)$, exponential in the sequence length. This is due to the fact that the log-sum-exp on time t depends on $q(s_{t+1}, \cdot)$, which creates a recursive dependency. The cost of converting an ARM to an EBM, however, is $O(VT)$, linear in the sequence length. Again, the log-sum-exp on time t depends on $q(s_{t+1}, \cdot)$. The crucial difference is that, this time, q is given, not recursively defined. This makes it possible to compute $r(s_t, y_t)$ for all $t \in [T]$, in parallel.

3.3. Maximum-entropy RL perspective

Autoregressive models as MDPs. Let \mathcal{S} be the set of states and \mathcal{A} be the set of actions. ARMs can be seen as a special case of Markov decision processes (MDPs) where

- states are contexts: $s_t := \mathbf{x} \oplus \mathbf{y}_{<t} \in \mathcal{S}$;
- actions are tokens: $y_t \in \mathcal{A}$;
- next states append the last token: $s_{t+1} := s_t \oplus y_t$;
- horizon is finite and there is no decay factor ($\gamma = 1$);
- r is the immediate reward function.

From this perspective, an ARM is a particular instance of a MDP, where the transition kernel $\mu(\cdot|s_t, y_t)$ is deterministic with $\mu(s_t \oplus y_t|s_t, y_t) = 1$. These particularly simple state transition dynamics imply that each state is never visited more than once. This perspective should not be confused with the (combinatorial) contextual bandit perspective, where \mathbf{x} corresponds to the single state, \mathbf{y} corresponds to an action and R is the sequence-level reward function.

Soft Bellman equation. In MaxEnt RL, we seek the policy

$$\pi^* = \underset{\pi \in \mathcal{P}(\mathcal{A}|\mathcal{S})}{\operatorname{argmax}} \mathbb{E} \sum_{t=1}^{\infty} \gamma^t (r(S_t, A_t) - \log \pi(A_t|S_t)). \quad (9)$$

The expectation is over trajectories of state-action pairs

starting from $S_1 \sim p_{\mathcal{X}}$ and following

$$\begin{aligned} A_t &\sim \pi(\cdot|S_t) \\ S_{t+1} &\sim \mu(\cdot|S_t, A_t). \end{aligned}$$

It is well-known in this literature (see Section 6 for a detailed review) that an optimal solution is

$$\pi^*(a|\mathbf{s}) = \exp(q^*(\mathbf{s}, a) - V_{q^*}(\mathbf{s}))$$

where q^* is a solution of the fixed point equation

$$q(\mathbf{s}, a) = r(\mathbf{s}, a) + \gamma \mathbb{E}_{S \sim \mu(\cdot|\mathbf{s}, a)} V_q(S). \quad (10)$$

Existence and uniqueness of the fixed point. In the general RL setting (infinite horizon, cyclic MDPs), the existence and uniqueness of the fixed point q^* rely on the Banach fixed point theorem. The standard condition is simply $\gamma < 1$, which guarantees that the soft Bellman operator $(\mathcal{B}_r q)(\mathbf{s}, a) := r(\mathbf{s}, a) + \gamma \mathbb{E}_{S \sim \mu(\cdot|\mathbf{s}, a)} V_q(S)$ is a contractive mapping. Typically, q^* does not enjoy an explicit formula and finding q^* requires some form of fixed point iterations. In contrast, in our setting (finite horizon, acyclic MDP), $q^* = \mathcal{M}(r)$ is the explicit formula of the fixed point solution, which guarantees both existence and uniqueness (invertibility). Moreover, we constructed the bijection through the chain rule of probability, unraveling a deep connection with the soft Bellman equation in our particular setting.

3.4. Entropy-regularized DP on a DAG perspective

We can also view our bijection as regularized dynamic programming (DP) on a directed acyclic graph (DAG). In this perspective, we define a DAG where

- there is one start (root) node corresponding to $s_1 = \mathbf{x}$;
- there is one end node;
- intermediate nodes are contexts $s_t := \mathbf{x} \oplus \mathbf{y}_{<t}$;
- edge weights indicate the value $r(s_t, y_t)$ of appending y_t to context s_t (higher is better);
- nodes such that $s_t := \mathbf{x} \oplus (y_1, \dots, \text{EOS})$ have a single out-going edge of weight 0, connected to the end node.

Computing $\max_{\mathbf{y} \in \mathcal{Y}} \sum_{t=1}^{|\mathbf{y}|} r(\mathbf{x} \oplus \mathbf{y}_{<t}, y_t)$ then amounts to finding the path in the DAG of maximum value and computing the log-partition $A_{R_r}^{\text{EBM}}(\mathbf{x}) = \text{LSE}_{\mathbf{y} \in \mathcal{Y}} \sum_{t=1}^{|\mathbf{y}|} r(\mathbf{x} \oplus \mathbf{y}_{<t}, y_t)$ amounts to finding the path of soft maximum value.

Top-down vs. bottom-up DP. To compute the soft-maximum $A_{R_r}^{\text{EBM}}(\mathbf{x}) = V_q(\mathbf{x})$ for $q = \mathcal{M}(r)$ by DP, two approaches are possible. In *top-down* DP, we start from $V_q(\mathbf{x})$, the quantity we wish to compute, and recurse. This corresponds to traversing the DAG forward in time. In

bottom-up DP (tabulation), we start from the base cases and make our way up to $V_q(\mathbf{x})$. This corresponds to traversing the DAG backward in time. As shown in (Mensch & Blondel, 2018), the associativity of the log-sum-exp and of the distributivity of $+$ over the log-sum-exp guarantee the optimality of dynamic programming. Indeed, we have (fixing $|\mathbf{y}| = T$ to simplify the notation)

$$\begin{aligned} A_{R_r}^{\text{EBM}}(\mathbf{x}) &= \text{LSE}_{\mathbf{y} \in \mathcal{Y}} \sum_{t=1}^T r(\mathbf{x} \oplus \mathbf{y}_{<t}, y_t) \\ &= \text{LSE}_{y_1 \in \mathcal{V}} \dots \text{LSE}_{y_T \in \mathcal{V}} \sum_{t=1}^T r(\mathbf{x} \oplus \mathbf{y}_{<t}, y_t) \\ &= \text{LSE}_{y_1 \in \mathcal{V}} \left[r(\mathbf{x}, y_1) + \text{LSE}_{y_2 \in \mathcal{V}} \left[r(\mathbf{x} \oplus y_1, y_2) + \dots \right. \right. \\ &\quad \left. \left. + \text{LSE}_{y_T \in \mathcal{V}} r(\mathbf{x} \oplus \mathbf{y}_{<T}, y_T) \right] \right]. \end{aligned}$$

It is well-known that the gradient of the log-partition exactly coincides with marginal probabilities (Wainwright et al., 2008). In Appendix A.11, we show that the gradient w.r.t. r of $A_{R_r}^{\text{EBM}}(\mathbf{x}) = V_q(\mathbf{x})$ for $q = \mathcal{M}(r)$ indeed exactly coincides with the marginal probabilities of response prefixes.

4. Theoretical analysis

4.1. Learning EBMs and ARMs from input-output pairs

In this section, building upon our bijection in Section 3.2, we state equivalence results between learning EBMs and learning ARMs from (\mathbf{x}, \mathbf{y}) pairs.

Negative log-likelihood of EBMs. The negative log-likelihood of \mathbf{y} given \mathbf{x} according to p_R^{EBM} is

$$\ell_R^{\text{EBM}}(\mathbf{x}, \mathbf{y}) := -\log p_R^{\text{EBM}}(\mathbf{y}|\mathbf{x}) = A_R^{\text{EBM}}(\mathbf{x}) - R(\mathbf{x}, \mathbf{y}).$$

The loss is convex in R and satisfies the property

$$\ell_R^{\text{EBM}}(\mathbf{x}, \mathbf{y}) = 0 \iff p_R^{\text{EBM}}(\mathbf{y}|\mathbf{x}) = 1.$$

Negative log-likelihood of ARMs. The negative log-likelihood of \mathbf{y} given \mathbf{x} according to p_q^{ARM} is

$$\begin{aligned} \ell_q^{\text{ARM}}(\mathbf{x}, \mathbf{y}) &:= -\log p_q^{\text{ARM}}(\mathbf{y}|\mathbf{x}) \\ &= A^{\text{ARM}}(\mathbf{x}, \mathbf{y}) - Q_q(\mathbf{x}, \mathbf{y}). \end{aligned}$$

The loss is convex in q and satisfies the property

$$\ell_q^{\text{ARM}}(\mathbf{x}, \mathbf{y}) = 0 \iff p_q^{\text{ARM}}(\mathbf{y}|\mathbf{x}) = 1.$$

Unlike A^{EBM} , A^{ARM} is a function of \mathbf{x} and \mathbf{y} , not just \mathbf{x} . Therefore, contrary to EBMs, the negative log-likelihood of an ARM is using the ground-truth sequence \mathbf{y} as a path. This is known as **teacher forcing**. Despite what the name may suggest, this behavior arises naturally as a consequence of using negative log-likelihood on ARMs.

Equivalence of minima. Let us define the expected risks

$$\mathcal{L}^{\text{ARM}}(q) := \mathbb{E}_{(\mathbf{X}, \mathbf{Y}) \sim \rho} [\ell_q^{\text{ARM}}(\mathbf{X}, \mathbf{Y})] \quad (11)$$

$$\mathcal{L}^{\text{EBM}}(R) := \mathbb{E}_{(\mathbf{X}, \mathbf{Y}) \sim \rho} [\ell_R^{\text{EBM}}(\mathbf{X}, \mathbf{Y})]. \quad (12)$$

We then have the following equivalence, which is a straightforward consequence of our bijection in Section 3.2.

Proposition 2 (Equivalence of minima). *For any joint distribution ρ over $\mathcal{X} \times \mathcal{Y}$, we have*

$$\begin{aligned} \min_{q \in \mathcal{F}(\mathcal{S} \times \mathcal{A})} \mathcal{L}^{\text{ARM}}(q) &= \min_{r \in \mathcal{F}(\mathcal{S} \times \mathcal{A})} \mathcal{L}^{\text{EBM}}(R_r) \\ &= \min_{R \in \mathcal{F}(\mathcal{X} \times \mathcal{Y})} \mathcal{L}^{\text{EBM}}(R) \end{aligned}$$

and, with $q^* = \mathcal{M}(r^*)$, we have

$$\begin{aligned} q^* \in \operatorname{argmin}_{q \in \mathcal{F}(\mathcal{S} \times \mathcal{A})} \mathcal{L}^{\text{ARM}}(q) &\iff r^* \in \operatorname{argmin}_{r \in \mathcal{F}(\mathcal{S} \times \mathcal{A})} \mathcal{L}^{\text{EBM}}(R_r) \\ &\implies R_{r^*} \in \operatorname{argmin}_{R \in \mathcal{F}(\mathcal{X} \times \mathcal{Y})} \mathcal{L}^{\text{EBM}}(R). \end{aligned}$$

See Appendix B.3 for a proof. Proposition 2 shows that, when the goal is to fit a model to observed input-output pairs (\mathbf{x}, \mathbf{y}) by negative log-likelihood minimization, EBMs and ARMs are equivalently powerful, provided that we perform minimization in function space, which means that the functions are able to fit the data perfectly.

Optimality of teacher forcing. Learning the reward R from data corresponds to an **inverse RL** setting (Ziebart et al., 2008). From a duality perspective (Sander et al., 2025), the optimal primal variable R^* is linked to the optimal dual variable p^* through, for all $\mathbf{x} \in \mathcal{X}$,

$$p^*(\cdot | \mathbf{x}) = \operatorname{softargmax}(R^*(\mathbf{x}, \cdot)) = p_{R^*}^{\text{EBM}}(\cdot | \mathbf{x}).$$

Unfortunately, recovering p^* from R^* is difficult, due to the intractable normalization constant. However, given q^* (the optimal solution via teacher forcing), p^* can be constructed from π_{q^*} using the chain rule of probability in (4),

$$p^*(\mathbf{y}|\mathbf{x}) = \prod_{t=1}^{|\mathbf{y}|} \pi_{q^*}(y_t | \mathbf{x}, \mathbf{y}_{<t}). \quad (13)$$

This demonstrates that teacher forcing is optimal when optimizing in function space. We emphasize that the mapping \mathcal{M} is completely implicit in this case (we do not need to explicitly compute it).

4.2. Distilling EBMs into ARMs

We saw in Section 2 that KL-regularized RL can be seen as distilling EBMs into ARMs. This motivates the need for approximation guarantees of EBMs by ARMs.

Function space. Stated differently, Proposition 1 shows that the exact mapping $q = \mathcal{M}(r)$ satisfies for all $\mathbf{x} \in \mathcal{X}$

$$\text{KL}(p_{R_r}^{\text{EBM}}(\cdot|\mathbf{x}), p_q^{\text{ARM}}(\cdot|\mathbf{x})) = 0.$$

Such a result holds in function space. This is the so-called tabular setting in RL, where the functions $q: \mathcal{S} \times \mathcal{A} \rightarrow \mathbb{R}$ and $r: \mathcal{S} \times \mathcal{A} \rightarrow \mathbb{R}$ are represented as (gigantic) arrays, exploiting the fact that the space of contexts (states) \mathcal{S} and the space of next tokens \mathcal{A} are finite.

Function approximation setting. In practice, q and r are implemented using parameterized functions. In this setting, there may no longer be an exact mapping between EBMs and ARMs, but we can bound their KL divergence.

Proposition 3 (KL bound). *For all $r: \mathcal{S} \times \mathcal{A} \rightarrow \mathbb{R}$, $q: \mathcal{S} \times \mathcal{A} \rightarrow \mathbb{R}$ and $\mathbf{x} \in \mathcal{X}$, we have*

$$\text{KL}(p_{R_r}^{\text{EBM}}(\cdot|\mathbf{x}), p_q^{\text{ARM}}(\cdot|\mathbf{x})) \leq 2T \max_{\substack{s \in \mathcal{S}(\mathbf{x}) \\ y \in \mathcal{A}}} |q^*(s, y) - q(s, y)|,$$

where $q^* := \mathcal{M}(r)$.

A proof is given in Appendix B.4.

Approximation using a Transformer. For a fixed EBM parameterized by R_r , let $q^* = \mathcal{M}(r)$. We now show that q^* can be approximated by a causal Transformer model by leveraging a powerful approximation result of causal mappings by causal Transformers (Furuya et al., 2025, Theorem 2). More precisely, for all $\varepsilon > 0$, there exists a causal Transformer $\mathcal{T}: \mathcal{S} \rightarrow \mathbb{R}^{|\mathcal{A}|}$ such that, for all $\mathbf{x} \in \mathcal{X}$,

$$\max_{s \in \mathcal{S}(\mathbf{x}), y \in \mathcal{A}} |q^*(s, y) - \mathcal{T}(s)[y]| \leq \varepsilon.$$

Together with Proposition 3, this gives for all $\mathbf{x} \in \mathcal{X}$,

$$\text{KL}(p_{R_r}^{\text{EBM}}(\cdot|\mathbf{x}), p_{\mathcal{T}(\cdot)}^{\text{ARM}}(\cdot|\mathbf{x})) \leq 2T\varepsilon.$$

However, this result requires the embedding dimension of \mathcal{T} to scale with the vocabulary size $|\mathcal{V}|$ (Furuya et al., 2025).

5. Numerical validation

In this section, we validate our theory using synthetic tiny language models. We focus on small vocabulary V and small maximum length T , enabling exact computation of the EBM’s log-partition, without resorting to approximate algorithms. We minimize the expected risks in (11) and (12), using a non-causal Transformer for the EBM and a causal Transformer for the ARM. The minimum risk is defined as $\mathcal{L}^* := -\mathbb{E}_{(X, Y) \sim \rho} \log \rho(X, Y)$. All experimental details are included in Appendix C.

In Figure 1 (left), we plot the optimality gap $\mathcal{L} - \mathcal{L}^*$ of both the EBM and the ARM as a function of optimization steps.

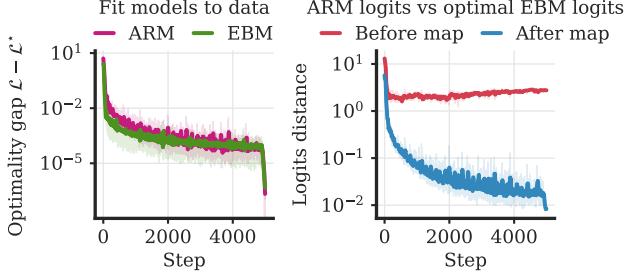


Figure 1. Empirical validation of Proposition 2. **Left:** Minimizing the expected risk of an ARM and an EBM parameterized by causal and non-causal Transformers, respectively. **Right:** L_∞ distance between the logits of the trained ARM and the logits of the **optimal** EBM, before and after applying the mapping \mathcal{M} .

Our results confirm that the EBM and ARM converge to the same minima, as predicted by Proposition 2. Perhaps more surprisingly, our results also show that the loss curves of both models are very close, during the entire training course. These findings are confirmed across several model sizes, and sequence-length / vocabulary ratios (Appendix C).

In Figure 1 (right), we show the L_∞ distance between the logits of the trained ARM and the logits of the optimal EBM, before and after applying the mapping \mathcal{M} . Our results therefore confirm that the mapping \mathcal{M} can be used to explicitly convert the logits of the EBM and ARM. However, we emphasize that explicit logit conversion is not needed, since we can also factorize the EBM distribution using (13).

6. Related work

Maximum-entropy RL. Maximum entropy was used for inverse RL, where the goal is to recover the reward function from offline trajectories (Ziebart et al., 2008). In the forward setting, a precursor is dynamic policy programming (Azar et al., 2012). Many papers subsequently formally established the equivalence between policy-based methods, that seek to solve (9) w.r.t. π , and value-based methods, that seek to satisfy (10) w.r.t. q (O’Donoghue et al., 2017; Haarnoja et al., 2017; Nachum et al., 2017; Schulman et al., 2017). The equivalence was revisited in continuous action space using convex duality (Richemond & Maginnis, 2017). Entropy-regularized RL was further studied (Neu et al., 2017) and extended to other strongly-convex regularizers (Geist et al., 2019). Several papers proposed one-step and multi-step consistency loss functions based on applying the squared loss to the optimality condition (10) (Nachum et al., 2017; Schulman et al., 2017; Clavier et al., 2025). Several papers proposed soft actor-critic algorithms (O’Donoghue et al., 2017; Haarnoja et al., 2017; 2018) or joint learning of the policy and value function (Richemond et al., 2024).

RL as probabilistic inference. Maxent RL can be viewed from a probabilistic inference perspective, using undirected graphical models (Toussaint et al., 2009; Ziebart, 2010), defining EBMs (a.k.a. conditional random fields), or directed graphical models, mirroring hidden Markov models (Attias, 2003; Levine, 2018). Notably, this connection has been leveraged to solve inference problems using MCTS and learned soft value functions (Buesing et al., 2020). Conversely, probabilistic inference tools can be leveraged for maxent RL (Korbak et al., 2022), such as twisted sequential Monte Carlo (Zhao et al., 2024). The equivalence between optimal estimation (Kalman filtering) and optimal control (for linear-quadratic systems) is known as Kalman duality (Todorov, 2008). We revisit the probabilistic inference perspective in our setting and notation in Appendix A.9.

Energy-based models. The standard approach for learning an EBM from (\mathbf{x}, \mathbf{y}) pairs by stochastic gradient descent requires sampling from the EBM (Song & Kingma, 2021), which usually involves MCMC algorithms such as Langevin when \mathcal{Y} is continuous or Gibbs sampling when \mathcal{Y} is discrete. Since that approach learns the negative energy R (the reward in inverse RL; see Section 4.1), and not a generative model π , MCMC is needed for generating samples from the EBM parameterized by the learned R . A min-min formulation was proposed to jointly learn R and the log-partition A (Sander et al., 2025). While this bypasses the need for MCMC at train time, it still requires it for sampling from the EBM. We emphasize however that if we do not need to sample but just to predict the mode of the EBM (the most likely output \mathbf{y} given \mathbf{x}), then we only need to maximize R , which does not involve the log-partition and is tractable for some sets \mathcal{Y} . On the other hand, min-max formulations can be used to jointly learn a discriminator (reward) R and a generator (policy) π from (\mathbf{x}, \mathbf{y}) pairs (Ho & Ermon, 2016). Such approach does not require MCMC if the generator easily generates samples by design, as is the case with ARMs.

GFlowNets. GFlowNets (Bengio et al., 2021; 2023) can be used to learn discrete samplers for amortized probabilistic inference. Flow consistency equations play the same role as soft Bellman equations, enabling the design of consistency loss functions (Malkin et al., 2022). In fact, recent work has established that GFlowNets can be cast as MaxEnt RL, even in the general DAG setting (Tiapkin et al., 2024).

Limitations of teacher forcing. Recent work argued that the next-token prediction objective (teacher forcing) is structurally “myopic” and fails to backpropagate future value information effectively, leading to a failure in planning (Bachmann & Nagarajan, 2024). In contrast, Proposition 2 shows that the global minimum of the teacher forcing objective (in function space) is an EBM, which inherently performs lookahead via the partition function V_q . Our work therefore

suggests that the limitation of teacher forcing is not in the objective itself but in the difficulty of reaching its minimum, due to optimization or approximation error. This aligns with prior work showing that planning failures stem from overfitting to spurious correlations under weak supervision, rather than inherent structural incapacity (Frydenlund, 2024).

7. Conclusion

Significance of this work. EBMs and ARMs are usually thought as two very distinct classes of models. EBMs are globally consistent but are difficult to train and sample from, while ARMs are easy to train and sample from but are only backward looking. Our paper shows that EBMs and ARMs are in fact intimately related. Our first contribution is to establish a bijective mapping \mathcal{M} between EBMs and ARMs in function space. While this mapping is a special case of soft Bellman equation in general MDPs (Section 3.3) and of entropy-regularized dynamic programming in a DAG (Section 3.4), we arrive at it from a very different angle, that of the chain rule of probability (Section 3.1 and Section 3.2). When learning from (\mathbf{x}, \mathbf{y}) pairs, Proposition 2 shows that, in function space, EBMs and ARMs are equivalently powerful, establishing the optimality of teacher forcing in this case. When distilling an EBM teacher into an ARM student, Proposition 3 shows that the KL between the EBM and the ARM is bounded by the L_∞ norm of the bijective mapping \mathcal{M} . Our results, validated through numerical experiments, provide some justification for the next-token prediction paradigm and for teacher forcing.

Limitations. When learning from (\mathbf{x}, \mathbf{y}) pairs, Proposition 2 establishes that ARMs and EBMs are equally powerful when optimizing for R and q in function space. However, in practice, R can be a non-causal Transformer while q must be causal. In addition, Proposition 1 establishes that, in order for ARMs and EBMs to be equivalent, q must take the form $q(\mathbf{s}, \mathbf{y}) = r(\mathbf{s}, \mathbf{y}) + V_q(\mathbf{s} \oplus \mathbf{y})$, where V_q represents the (soft) optimal value of all future continuations. The function q is therefore burdened with a dual task: it must model the immediate local score r , and it must learn to implicitly compute a potentially complex future-looking value function V_q (marginalizing over all possible futures) using only a backward-looking architecture. Proposition 2 does not account for optimization or approximation error. Formally comparing the complexity of learning R versus that of learning q is a promising future direction. Another important direction is to study the impact of latent variables (thinking traces) in enhancing the expressivity of ARMs.

Bridging communities. This paper builds bridges between ARMs, EBMs and Maxent RL. We hope that our paper contributes to shedding additional light on how many works and perspectives relate to each other.

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A. Supplementary materials

Table of contents:

- Handling variable-length sequences
 - In ARMs (Section A.1).
 - In EBMs (Section A.2).
- Chain rule
 - Chain rule of entropy (Section A.3).
 - Chain rule of KL (Section A.4).
- Bijection
 - Bijection with a reference measure (Section A.5).
 - Chain rule of probability perspective (Section A.6).
 - Variational perspective (Section A.7).
 - Adversarial and variational inference perspectives (Section A.8).
 - Probabilistic inference perspective (Section A.9).
- Gradients
 - Gradient maps (Section A.10).
 - Backpropagation (Section A.11).

A.1. Handling variable-length sequences in ARMs

For completeness, we review here the crucial role of EOS to induce a valid probability distribution over variable-length sequences of finite size. For more details, we refer the reader to Cotterell et al. (2023, Section 2.5). See also Eisenstein (2019, Chapter 6) for a simple introduction to language models.

Probability of finished vs. unfinished responses. Let us define the set of possible sequences up to size T in a vocabulary \mathcal{V} as $\mathcal{V}^{\leq T} := \cup_{t=1}^T \mathcal{V}^t$. We use $X \in \mathcal{X}$ to denote the random variable of a prompt and $Y \in \mathcal{V}^{\leq T}$ to denote the random variable of a **finished** response of size at most T . We then define the probability that a sequence $\mathbf{y} = (y_1, \dots, y_\tau)$ is a finished response given \mathbf{x} as

$$\mathbb{P}(Y = \mathbf{y}|X = \mathbf{x}) := \mathbb{P}(Y_1 = y_1, \dots, Y_\tau = y_\tau, \text{len}(Y) = \tau|X = \mathbf{x}).$$

It is the probability that the first τ tokens in Y are y_1, \dots, y_τ **and** that the sentence is of length $0 \leq \tau \leq T$.

This probability should not be confused with the **marginal probability** of an **unfinished response**,

$$\mathbb{P}(Y_{\leq \tau} = \mathbf{y}|X = \mathbf{x}) := \mathbb{P}(Y_1 = y_1, \dots, Y_\tau = y_\tau|X = \mathbf{x}).$$

It is the probability that the first τ tokens in Y are y_1, \dots, y_τ , while Y is of potentially larger length. Formally, the event $\{Y_1 = y_1, \dots, Y_\tau = y_\tau, \text{len}(Y) = \tau'\}$ for $\tau' > \tau$ is not a singleton, while the event $\{Y_1 = y_1, \dots, Y_\tau = y_\tau, \text{len}(Y) = \tau\}$ does reduce to the singleton $\{Y = \mathbf{y}\}$. Said differently, $\{Y_{\leq \tau} = \mathbf{y}\} \neq \{Y = \mathbf{y}\}$.

Explicit length handling. A natural way to describe finished responses of variable length would be to define a random variable $L \in \mathbb{N}$ encoding the length and to define the distribution over fixed size sequences $Y_{1:l}|L = l$ for $l \in \mathbb{N}$. Unfortunately, in an autoregressive setting, this breaks the information flow: we do not foresee the final length before starting to output tokens. Instead, autoregressive models can condition the length on the past tokens, i.e., they can decompose the probability $\mathbb{P}(Y = \mathbf{y}|X = \mathbf{x})$ as

$$\begin{aligned} \mathbb{P}(Y = \mathbf{y}|X = \mathbf{x}) &= \mathbb{P}(Y_1 = y_1, \dots, Y_\tau = y_\tau|X = \mathbf{x})\mathbb{P}(\text{len}(Y) = \tau|X = \mathbf{x}, Y_1 = y_1, \dots, Y_\tau = y_\tau) \\ &= \mathbb{P}(Y_1 = y_1|S_1 = \mathbf{s}_1) \dots \mathbb{P}(Y_\tau = y_\tau|S_\tau = \mathbf{s}_\tau)\mathbb{P}(\text{len}(Y) = \tau|S_\tau = \mathbf{s}_\tau), \end{aligned}$$

where we used the contexts (states) $\mathbf{s}_t := \mathbf{x} \oplus \mathbf{y}_{<t}$ and $\mathbf{s}_1 = \mathbf{x}$, and similarly for S_t and S_1 .

Implicit length handling using EOS. This decomposition suggests a simple way to encode the length in an autoregressive model: adding a new possible output token, called `EOS`, such that for any $t \geq 0$,

$$\mathbb{P}(Y_t = \text{EOS} | S_t = \mathbf{s}_t) = \mathbb{P}(\text{len}(Y) = t | S_t = \mathbf{s}_t).$$

Using this approach, finished responses should now always include `EOS` as the last token, and the length of a sequence now includes `EOS`. More formally, instead of defining $Y \in \mathcal{V}^{\leq T}$, we now define $Y \in \mathcal{Y}$, where $\mathcal{Y} = \bigcup_{t=1}^T (\mathcal{V}^t \times \{\text{EOS}\})$. It should be noted that `EOS` is just a convenient way to encode the length and does not change the cardinality of the set of possible sequences, since

$$|\mathcal{V}^t \times \{\text{EOS}\}| = |\mathcal{V}^t| = V^t.$$

The advantage of the `EOS` approach is that we can support seamlessly both the probability of finished responses (by appending `EOS` as last token) and the marginal probability of unfinished responses (by **not** appending `EOS` as last token). Indeed, assuming $y_\tau \neq \text{EOS}$, we have

$$\mathbb{P}(Y_{\leq \tau} = \mathbf{y} | X = \mathbf{x}) = \mathbb{P}(Y_1 = y_1 | S_1 = \mathbf{s}_1) \dots \mathbb{P}(Y_\tau = y_\tau | S_\tau = \mathbf{s}_\tau).$$

The function q used to define π_q takes a (context, next-token) pair and returns a scalar-valued score. Strictly speaking, the context tokens are in the vocabulary \mathcal{V} while the next token is in the augmented vocabulary $\mathcal{A} := \mathcal{V} \cup \{\text{EOS}\}$. Therefore, $q: \mathcal{S} \times \mathcal{A} \rightarrow \mathbb{R}$, where $\mathcal{S} := \bigcup_{t=1}^T \mathcal{X} \times \mathcal{V}^{t-1}$.

Validity of the probability distribution over sequences. We formally give below a sufficient condition which guarantees that an ARM defines a valid probability distribution over finished responses.

Proposition 4 (Validity of the distribution defined by an ARM). *Let $\mathcal{Y} := \bigcup_{\tau=1}^T \mathcal{V}^{\tau-1} \times \{\text{EOS}\}$ be the set of valid finished responses of length at most T . If $\pi_q(\text{EOS} | \mathbf{s}_T) = 1$ for all $\mathbf{s}_T \in \mathcal{X} \times \mathcal{V}^{T-1}$, then for all $\mathbf{x} \in \mathcal{X}$*

$$\sum_{\mathbf{y} \in \mathcal{Y}} p_q^{\text{ARM}}(\mathbf{y} | \mathbf{x}) = 1.$$

That is, the ARM defines a valid probability distribution over finished responses of length at most T .

A proof is given in Appendix B.5.

To enforce the condition $\pi_q(\text{EOS} | \mathbf{s}_T) = 1$, we can define q as in (3).

A.2. Handling variable-length sequences in EBMs

Probability of finished vs. unfinished responses. Defining a probability over finished responses is more straightforward with EBMs, as we can directly parameterize $\mathbb{P}(Y = \mathbf{y} | X = \mathbf{x})$ for all possible $\mathbf{y} \in \mathcal{Y}$. The negative energy R of the EBM is, up to a constant factor, the log-probability of singletons events $\{Y = \mathbf{y}\}$ given $X = \mathbf{x}$,

$$R(\mathbf{x}, \mathbf{y}) = \log \mathbb{P}(Y = \mathbf{y} | X = \mathbf{x}) + \text{const}(\mathbf{x}).$$

Marginal probabilities $\mathbb{P}(Y_{\leq \tau} = \mathbf{y} | X = \mathbf{x})$ can be computed from $\mathbb{P}(Y = \mathbf{y} | X = \mathbf{x})$ by appropriate marginalization and similarly for the probability of response length.

Validity of the probability distribution over sequences. An EBM defines a valid probability over finished responses of length up to T by virtue of its normalization,

$$p_R^{\text{EBM}}(\mathbf{y} | \mathbf{x}) = \frac{\exp R(\mathbf{x}, \mathbf{y})}{\sum_{\mathbf{y}' \in \mathcal{Y}} \exp R(\mathbf{x}, \mathbf{y}')},$$

The denominator is well defined since \mathcal{Y} is finite.

A.3. Chain rule of entropy

In this section, we show how the entropy of p (the sequence distribution) can be computed in terms of the entropy of π (the next-token distribution), using the law of total expectation (tower rule). This allows one to construct an unbiased estimator of the entropy of p by sampling trajectories.

Stochastic state transition dynamics.

Suppose $p(\tau|s_1) := \prod_{t=1}^T \pi(a_t|s_t)\mu(s_{t+1}|s_t, a_t)$ where $\tau = (a_1, s_2, \dots, s_T, a_T, s_{T+1})$. For all s_1 , we then have

$$\begin{aligned} H(p(\cdot|s_1)) &= -\mathbb{E}_{\tau \sim p(\cdot|s_1)} [\log p(\tau|s_1)] \\ &= -\mathbb{E}_{\tau \sim p(\cdot|s_1)} \left[\sum_{t=1}^T \log \pi(A_t|S_t) + \log \mu(S_{t+1}|S_t, A_t) \right] \\ &= -\sum_{t=1}^T \mathbb{E}_{S_t \sim p_t(\cdot|s_1)} [E_{A_t \sim \pi(\cdot|S_t)} [\log \pi(A_t|S_t) + \mathbb{E}_{S_{t+1} \sim \mu(\cdot|S_t, A_t)} [\log \mu(S_{t+1}|S_t, A_t)]]] \\ &= \sum_{t=1}^T \mathbb{E}_{S_t \sim p_t(\cdot|s_1)} [H(\pi(\cdot|S_t))] + \mathbb{E}_{S_t \sim p_t(\cdot|s_1), A_t \sim \pi(\cdot|S_t)} [H(\mu(\cdot|S_t, A_t))] \end{aligned}$$

where $p_t(S_t|s_1)$ is the marginal probability of being in state S_t at time t over all possible trajectories starting from s_1 .

Deterministic state transition dynamics.

Suppose $p(y|x) := \prod_{t=1}^T \pi(y_t|x, y_{<t})$. For all x , we now have

$$\begin{aligned} H(p(\cdot|x)) &= -\mathbb{E}_{Y \sim p(\cdot|x)} [\log p(Y|x)] \\ &= -\mathbb{E}_{Y \sim p(\cdot|x)} \left[\sum_{t=1}^T \log \pi(Y_t|x, Y_{<t}) \right] \\ &= -\sum_{t=1}^T \mathbb{E}_{Y_{<t} \stackrel{\text{AR}}{\sim} \pi(\cdot|x)} [\mathbb{E}_{Y_t \sim \pi(\cdot|x, Y_{<t})} [\log \pi(Y_t|x, Y_{<t})]] \\ &= \sum_{t=1}^T \mathbb{E}_{Y_{<t} \stackrel{\text{AR}}{\sim} \pi(\cdot|x)} [H(\pi(\cdot|x, Y_{<t}))] \\ &= \sum_{t=1}^T H(Y_t|x, Y_{<t}) \end{aligned}$$

where we use $\stackrel{\text{AR}}{\sim}$ to indicate that $Y_{<t}$ is obtained autoregressively.

Taking the expectation over x , we obtain the conditional entropy

$$\mathbb{E}_X [H(p(\cdot|X))] = H(Y|X) = \sum_{t=1}^T H(Y_t|X, Y_{<t}).$$

A.4. Chain rule of Kullback-Leibler divergence

In this section, we show a similar result for the Kullback-Leibler divergence as for the entropy. This allows one to construct an unbiased estimator of the KL divergence by sampling trajectories.

Stochastic state transition dynamics.

Suppose $p(\tau|s_1) := \prod_{t=1}^T \pi(a_t|s_t)\mu(s_{t+1}|s_t, a_t)$ and $p_0(\tau|s_1) := \prod_{t=1}^T \pi_0(a_t|s_t)\mu(s_{t+1}|s_t, a_t)$ where $\tau =$

$(a_1, \mathbf{s}_2, \dots, \mathbf{s}_T, a_T, \mathbf{s}_{T+1})$. For all \mathbf{s}_1 , we have

$$\begin{aligned} \text{KL}(p(\cdot|\mathbf{s}_1), p_0(\cdot|\mathbf{s}_1)) &= \mathbb{E}_{\tau \sim p(\cdot|\mathbf{s}_1)} \left[\log \frac{p(\tau|\mathbf{s}_1)}{p_0(\tau|\mathbf{s}_1)} \right] \\ &= \mathbb{E}_{\tau \sim p(\cdot|\mathbf{s}_1)} \left[\sum_{t=1}^T \log \frac{\pi(A_t|S_t)\mu(S_{t+1}|S_t, A_t)}{\pi_0(A_t|S_t)\mu(S_{t+1}|S_t, A_t)} \right] \\ &= \sum_{t=1}^T \mathbb{E}_{S_t \sim p_t(\cdot|\mathbf{s}_1)} \left[\mathbb{E}_{A_t \sim \pi(\cdot|S_t)} \left[\log \frac{\pi(A_t|S_t)}{\pi_0(A_t|S_t)} \right] \right] \\ &= \sum_{t=1}^T \mathbb{E}_{S_t \sim p_t(\cdot|\mathbf{s}_1)} [\text{KL}(\pi(\cdot|S_t), \pi_0(\cdot|S_t))], \end{aligned}$$

where $p_t(S_t|\mathbf{s}_1)$ is again the marginal probability of being in state S_t at time t over all possible trajectories starting from \mathbf{s}_1 . We see that the state transition kernel μ cancels out.

Deterministic state transition dynamics.

Similarly, suppose $p(\mathbf{y}|\mathbf{x}) := \prod_{t=1}^T \pi(y_t|\mathbf{x}, \mathbf{y}_{<t})$ and $p_0(\mathbf{y}|\mathbf{x}) := \prod_{t=1}^T \pi_0(y_t|\mathbf{x}, \mathbf{y}_{<t})$. For all \mathbf{x} , we have

$$\begin{aligned} \text{KL}(p(\cdot|\mathbf{x}), p_0(\cdot|\mathbf{x})) &= \mathbb{E}_{Y \sim p(\cdot|\mathbf{x})} \left[\log \frac{p(Y|\mathbf{x})}{p_0(Y|\mathbf{x})} \right] \\ &= \mathbb{E}_{Y \sim p(\cdot|\mathbf{x})} \left[\sum_{t=1}^T \log \frac{\pi(Y_t|\mathbf{x}, Y_{<t})}{\pi_0(Y_t|\mathbf{x}, Y_{<t})} \right] \\ &= \sum_{t=1}^T \mathbb{E}_{Y_{<t} \stackrel{\text{AR}}{\sim} \pi(\cdot|\mathbf{x})} \left[\mathbb{E}_{Y_t \sim \pi(\cdot|\mathbf{x}, Y_{<t})} \left[\log \frac{\pi(Y_t|\mathbf{x}, Y_{<t})}{\pi_0(Y_t|\mathbf{x}, Y_{<t})} \right] \right] \\ &= \sum_{t=1}^T \mathbb{E}_{Y_{<t} \stackrel{\text{AR}}{\sim} \pi(\cdot|\mathbf{x})} [\text{KL}(\pi(\cdot|\mathbf{x}, Y_{<t}), \pi_0(\cdot|\mathbf{x}, Y_{<t}))] \\ &:= \sum_{t=1}^T \text{KL}(\pi(Y_t|\mathbf{x}, Y_{<t}), \pi_0(Y_t|\mathbf{x}, Y_{<t})) \end{aligned}$$

where we again use $\stackrel{\text{AR}}{\sim}$ to indicate that $Y_{<t}$ is obtained autoregressively.

Taking the expectation over \mathbf{x} , we obtain the conditional Kullback-Leibler divergence

$$\mathbb{E}_X [\text{KL}(p(\cdot|X), p_0(\cdot|X))] = \text{KL}(p(Y|X), p_0(Y|X)) = \sum_{t=1}^T \text{KL}(\pi(Y_t|X, Y_{<t}), \pi_0(Y_t|X, Y_{<t})).$$

Estimators based on Rao–Blackwellization are studied in (Amini et al., 2025).

A.5. Bijection with a reference measure

Suppose we have a reference distribution

$$p_{\text{ref}}(\mathbf{y}|\mathbf{x}) := \prod_{t=1}^{|\mathbf{y}|} \pi_{\text{ref}}(y_t|\mathbf{x} \oplus \mathbf{y}_{<t}).$$

We then have

$$R_{\text{ref}}(\mathbf{x}, \mathbf{y}) = \log p_{\text{ref}}(\mathbf{y}|\mathbf{x}) = \sum_{t=1}^{|\mathbf{y}|} \log \pi_{\text{ref}}(y_t|\mathbf{x} \oplus \mathbf{y}_{<t}) = \sum_{t=1}^{|\mathbf{y}|} q_{\text{ref}}(\mathbf{x} \oplus \mathbf{y}_{<t}, y_t),$$

where $q_{\text{ref}}(\mathbf{s}, y) := \log \pi_{\text{ref}}(y|\mathbf{s})$. Suppose further that

$$R(\mathbf{x}, \mathbf{y}) := \sum_{t=1}^{|y|} r(\mathbf{x} \oplus \mathbf{y}_{<t}, y_t).$$

Using the bijection for the total energy $R' := R + R_{\text{ref}}$, we obtain the total logits q' ,

$$q'(\mathbf{s}_t, y_t) := \begin{cases} r(\mathbf{s}_t, y_t) + q_{\text{ref}}(\mathbf{s}_t, y_t) & \text{if } y_t = \text{EOS} \\ r(\mathbf{s}_t, y_t) + q_{\text{ref}}(\mathbf{s}_t, y_t) + V_{q'}(\mathbf{s}_t \oplus y_t) & \text{if } y_t \neq \text{EOS} \end{cases}.$$

We now define the residual logits q such that $q' := q + q_{\text{ref}}$, which implies

$$\pi_{q'}(y_t|\mathbf{s}_t) \propto \pi_{\text{ref}}(y_t|\mathbf{s}_t) \exp(q(\mathbf{s}_t, y_t)).$$

Substituting $q' = q + q_{\text{ref}}$ into the recursion above, the term q_{ref} cancels out on both sides. The mapping between r and q is therefore

$$q(\mathbf{s}_t, y_t) := \begin{cases} r(\mathbf{s}_t, y_t) & \text{if } y_t = \text{EOS} \\ r(\mathbf{s}_t, y_t) + V_{q+q_{\text{ref}}}(\mathbf{s}_t \oplus y_t) & \text{if } y_t \neq \text{EOS} \end{cases},$$

where

$$V_{q+q_{\text{ref}}}(\mathbf{s}_t) = \log \mathbb{E}_{Y_t \sim \pi_{\text{ref}}(\cdot|\mathbf{s}_t)} [\exp(q(\mathbf{s}_t, Y_t))],$$

which is the log-sum-exp modulated by the reference measure.

A.6. Chain rule of probability perspective on the bijection

In this section, we revisit Proposition 1 from a chain rule of probability perspective, by using the algorithm outlined in Section 3.1. We use a fixed length T for simplicity of the exposition. We have

$$\begin{aligned} p(\mathbf{y}|\mathbf{x}) &= \frac{\exp(r(\mathbf{s}_1, y_1) + \dots + r(\mathbf{s}_T, y_T))}{Z(\mathbf{x})} \\ &= \frac{\exp(r(\mathbf{s}_1, y_1) + \dots + r(\mathbf{s}_{T-1}, y_{T-1})) \exp(r(\mathbf{s}_T, y_T))}{Z(\mathbf{x})} \end{aligned}$$

where $Z(\mathbf{x})$ is the normalization constant.

Marginalizing the last variable, we obtain

$$\begin{aligned} p(\mathbf{y}_{\leq T-1}|\mathbf{x}) &= \sum_{y_T \in \mathcal{V}} p(\mathbf{y}_{<T}, y_T|\mathbf{x}) \\ &= \frac{1}{Z(\mathbf{x})} \exp(r(\mathbf{s}_1, y_1) + \dots + r(\mathbf{s}_{T-1}, y_{T-1})) \sum_{y_T \in \mathcal{V}} \exp(r(\mathbf{s}_T, y_T)) \\ &= \frac{1}{Z(\mathbf{x})} \exp(r(\mathbf{s}_1, y_1) + \dots + r(\mathbf{s}_{T-1}, y_{T-1})) \exp(V_r(\mathbf{s}_T)). \end{aligned}$$

By conditioning, we obtain

$$\begin{aligned} \pi(y_T|\mathbf{x}, \mathbf{y}_{<T}) &= \frac{p(\mathbf{y}_{\leq T}|\mathbf{x})}{p(\mathbf{y}_{\leq T-1}|\mathbf{x})} \\ &= \exp(r(\mathbf{s}_T, y_T) - V_r(\mathbf{s}_T)) \\ &= \exp(q(\mathbf{s}_T, y_T) - V_q(\mathbf{s}_T)) \end{aligned}$$

where we have used that $p(\mathbf{y}|\mathbf{x}) = p(\mathbf{y}_{\leq T}|\mathbf{x})$ and where we defined $q(\mathbf{s}_T, y_T) := r(\mathbf{s}_T, y_T)$.

Marginalizing once again, we obtain

$$\begin{aligned} p(\mathbf{y}_{\leq T-2} | \mathbf{x}) &= \sum_{y_{T-1} \in \mathcal{V}} p(\mathbf{y}_{< T-1}, y_{T-1} | \mathbf{x}) \\ &= \frac{1}{Z(\mathbf{x})} \exp(r(\mathbf{s}_1, y_1) + \dots + r(\mathbf{s}_{T-2}, y_{T-2})) \sum_{y_{T-1} \in \mathcal{V}} \exp(r(\mathbf{s}_{T-1}, y_{T-1}) + V_q(\mathbf{s}_{T-1} \oplus y_{T-1})) \\ &= \frac{1}{Z(\mathbf{x})} \exp(r(\mathbf{s}_1, y_1) + \dots + r(\mathbf{s}_{T-2}, y_{T-2})) \exp(V_q(\mathbf{s}_{T-1})), \end{aligned}$$

where we defined $q(\mathbf{s}_{T-1}, y_{T-1}) := r(\mathbf{s}_{T-1}, y_{T-1}) + V_q(\underbrace{\mathbf{s}_{T-1} \oplus y_{T-1}}_{\mathbf{s}_T})$.

By conditioning once again, we obtain

$$\begin{aligned} \pi(y_{T-1} | \mathbf{x}, \mathbf{y}_{< T-1}) &= \frac{p(\mathbf{y}_{\leq T-1} | \mathbf{x})}{p(\mathbf{y}_{\leq T-2} | \mathbf{x})} \\ &= \exp(q(\mathbf{s}_{T-1}, y_{T-1}) - V_q(\mathbf{s}_{T-1})). \end{aligned}$$

Repeating the process until $t = 1$, we recover the mapping \mathcal{M}

$$\begin{aligned} q(\mathbf{s}_T, y_T) &:= r(\mathbf{s}_T, y_T) \\ q(\mathbf{s}_{T-1}, y_{T-1}) &:= r(\mathbf{s}_{T-1}, y_{T-1}) + V_q(\mathbf{s}_T) \\ &\vdots \\ q(\mathbf{s}_1, y_1) &:= r(\mathbf{s}_1, y_1) + V_q(\mathbf{s}_2). \end{aligned}$$

A.7. Variational perspective on the bijection

In this section, we revisit Proposition 1 from a variational perspective. We use a fixed length T for simplicity of the exposition. We notice that

$$\begin{aligned} A_{R_r}^{\text{EBM}}(\mathbf{x}) &= \max_{p \in \mathcal{P}(\mathcal{Y} | \mathbf{x})} \mathbb{E}_{Y \sim p(\cdot | \mathbf{x})} [R_r(\mathbf{x}, Y) - \log p(Y | \mathbf{x})] \\ &= \max_{\pi \in \mathcal{P}(\mathcal{V} | \mathcal{S}(\mathbf{x}))} \mathbb{E}_{Y_1 \sim \pi(\cdot | \mathbf{x})} [r(\mathbf{x}, Y_1) - \log \pi(Y_1 | \mathbf{x}) + \dots + \mathbb{E}_{Y_T \sim \pi(\cdot | \mathbf{x} \oplus Y_{< T})} [r(\mathbf{x} \oplus Y_{< T}, Y_T) - \log \pi(Y_T | \mathbf{x} \oplus Y_{< T})]] \\ &= \max_{\pi_1 \in \mathcal{P}(\mathcal{V} | \mathcal{S}_1(\mathbf{x}))} \mathbb{E}_{Y_1 \sim \pi_1(\cdot | \mathbf{x})} [r(\mathbf{x}, Y_1) - \log \pi_1(Y_1 | \mathbf{x}) + \dots + \mathbb{E}_{Y_T \sim \pi_T(\cdot | \mathbf{x} \oplus Y_{< T})} [r(\mathbf{x} \oplus Y_{< T}, Y_T) - \log \pi_T(Y_T | \mathbf{x} \oplus Y_{< T})]] \\ &\quad \vdots \\ &= \max_{\pi_T \in \mathcal{P}(\mathcal{V} | \mathcal{S}_{T-1}(\mathbf{x}))} \mathbb{E}_{Y_1 \sim \pi_1(\cdot | \mathbf{x})} \left[r(\mathbf{x}, Y_1) - \log \pi_1(Y_1 | \mathbf{x}) + \dots + \max_{\pi_T \in \mathcal{P}(\mathcal{V} | \mathcal{S}_{T-1}(\mathbf{x}))} \mathbb{E}_{Y_T \sim \pi_T(\cdot | \mathbf{x} \oplus Y_{< T})} [r(\mathbf{x} \oplus Y_{< T}, Y_T) - \log \pi_T(Y_T | \mathbf{x} \oplus Y_{< T})] \right]. \end{aligned}$$

Solving the nested maxima from right to left, it can indeed be checked that $A_{R_r}^{\text{EBM}}(\mathbf{x}) = V_q(\mathbf{x})$ for all $\mathbf{x} \in \mathcal{X}$ with $q = \mathcal{M}(r)$.

A.8. Adversarial and variational inference perspectives

We have for all $R \in \mathcal{F}(\mathcal{X} \times \mathcal{Y})$, $\mathbf{x} \in \mathcal{X}$ and $\mathbf{y} \in \mathcal{Y}$,

$$\begin{aligned} A_R^{\text{EBM}}(\mathbf{x}) &= \max_{p \in \mathcal{P}(\mathcal{Y} | \mathbf{x})} \mathbb{E}_{Y \sim p(\cdot | \mathbf{x})} [R(\mathbf{x}, Y) - \log p(Y | \mathbf{x})] \\ &\geq \mathbb{E}_{Y \sim p(\cdot | \mathbf{x})} [R(\mathbf{x}, Y) - \log p(Y | \mathbf{x})] \quad \forall p \in \mathcal{P}(\mathcal{Y} | \mathbf{x}). \end{aligned}$$

In the second line, equality holds when $p = p_R^{\text{EBM}}$.

From a convex duality perspective, R is the primal variable and p is the dual variable.

In particular, we have for all $R \in \mathcal{F}(\mathcal{X} \times \mathcal{Y})$, $q \in \mathcal{F}(\mathcal{S} \times \mathcal{A})$ and $\mathbf{x} \in \mathcal{X}$,

$$A_R^{\text{EBM}}(\mathbf{x}) \geq \mathbb{E}_{Y \sim p_q^{\text{ARM}}(\cdot | \mathbf{x})}[R(\mathbf{x}, Y) - \log p_q^{\text{ARM}}(Y | \mathbf{x})] \quad \forall q \in \mathcal{F}(\mathcal{S} \times \mathcal{A}).$$

From Proposition 1, equality holds when $q = \mathcal{M}(r)$ and $R = R_r$.

We can use this perspective to derive a min-max formulation

$$\min_{R \in \mathcal{F}(\mathcal{X} \times \mathcal{Y})} \mathbb{E}_{(X, Y)} [\ell_R^{\text{EBM}}(X, Y)] = \min_{R \in \mathcal{F}(\mathcal{X} \times \mathcal{Y})} \max_{q \in \mathcal{F}(\mathcal{S} \times \mathcal{A})} \mathbb{E}_X \left[\mathbb{E}_{Y' \sim p_q^{\text{ARM}}(\cdot | X)} [R(X, Y') - \log p_q^{\text{ARM}}(Y' | X)] \right] - \mathbb{E}_{(X, Y)} [R(X, Y)].$$

From a GAN or actor-critic perspective, p_q^{ARM} is a generator (actor) and R is a discriminator (critic).

From a variational inference perspective, $A_R^{\text{EBM}}(\mathbf{x})$ is the log-evidence and $(q, R) \mapsto \mathbb{E}_{Y \sim p_q^{\text{ARM}}}[R(\mathbf{x}, Y) - \log p_q^{\text{ARM}}(Y | \mathbf{x})]$ is known as the evidence lower-bound (ELBO). While it is a direct consequence of convex duality, the ELBO can also be derived using Jensen's inequality or using the non-negativity of the KL. The distribution p_q^{ARM} is the proposal distribution (easy to sample from) and the distribution p_R^{EBM} is the target distribution (difficult to sample from).

A.9. Probabilistic inference perspective

In this section, we revisit the bijection from a probabilistic inference perspective. Our exposition differs from (Levine, 2018) and may therefore bring a complementary view. Throughout the section, we define the shorthand notation $s_1 := \mathbf{x}$ and $s_t := \mathbf{x} \oplus \mathbf{y}_{<t}$ for $t > 1$.

The conditional probability of \mathbf{y} given \mathbf{x} according to an EBM is

$$p(\mathbf{y} | \mathbf{x}) = \frac{1}{Z(\mathbf{x})} \prod_{t=1}^T \psi(s_t, y_t),$$

where we defined the potential $\psi(s_t, y_t) := \exp(r(s_t, y_t))$.

The partition function is defined as

$$Z(\mathbf{x}) := \sum_{\mathbf{y} \in \mathcal{Y}} \prod_{t=1}^T \psi(s_t, y_t).$$

Using the distributivity of multiplication over addition, we can expand $Z(\mathbf{x})$ as

$$Z(\mathbf{x}) = \sum_{y_1 \in \mathcal{A}} \psi(s_1, y_1) \sum_{y_2 \in \mathcal{A}} \psi(s_2, y_2) \cdots \sum_{y_T \in \mathcal{A}} \psi(s_T, y_T).$$

Forward and backward variables. Let us define the forward variables as

$$\begin{aligned} \alpha_1(s_1) &:= 1 \\ \alpha_t(s_t) &:= \psi(s_1, y_1) \dots \psi(s_{t-1}, y_{t-1}) \quad \forall t > 1 \\ &= \alpha_{t-1}(s_{t-1}) \psi(s_{t-1}, y_{t-1}). \end{aligned} \tag{14}$$

They capture the accumulated value of a single specific path from the root to the current state s_t (the past).

Likewise, let us define the backward variables as

$$\begin{aligned} \beta_t(s_t) &:= \sum_{y_t \in \mathcal{A}} \psi(s_t, y_t) \cdots \sum_{y_T \in \mathcal{A}} \psi(s_T, y_T) \quad \forall t \leq T \\ &= \sum_{y_t \in \mathcal{A}} \psi(s_t, y_t) \beta_{t+1}(s_t \oplus y_t) \\ \beta_{T+1}(\cdot) &:= 1. \end{aligned} \tag{15}$$

They capture the future value of being in state s_t .

We then have for all $t \in [T]$

$$Z(\mathbf{x}) = \sum_{\mathbf{s}_t \in \mathcal{S}_t(\mathbf{x})} \alpha_t(\mathbf{s}_t) \beta_t(\mathbf{s}_t),$$

where $\mathcal{S}_t(\mathbf{x})$ is the set of all responses \mathbf{y} of length $t - 1$ starting from $\mathbf{s}_1 = \mathbf{x}$ (i.e., nodes at depth $t - 1$ in the tree).

In particular:

- At the root ($t = 1$), the sum collapses to a single term, $Z(\mathbf{x}) = \alpha_1(\mathbf{x}) \beta_1(\mathbf{x}) = \beta_1(\mathbf{x})$.
- At the last step ($t = T$), the sum becomes $Z(\mathbf{x}) = \sum_{\mathbf{s}_T \in \mathcal{S}_T(\mathbf{x})} \alpha_T(\mathbf{s}_T) \beta_T(\mathbf{s}_T)$.

Relationship with the bijection. We can recover the relationship between EBMs and ARMs when examining the recursive definition of β_t . Dividing (15) by $\beta_t(\mathbf{s}_t)$ on both sides, we obtain

$$\sum_{y_t \in \mathcal{A}} \frac{\psi(\mathbf{s}_t, y_t) \beta_{t+1}(\mathbf{s}_t \oplus y_t)}{\beta_t(\mathbf{s}_t)} = 1.$$

Since the terms in the sum are positive and sum to 1, they define a valid probability distribution over the next token y_t . This distribution is exactly π_q . To see why, recall that

$$\pi_q(y_t | \mathbf{s}_t) = \exp(q(\mathbf{s}_t, y_t) - V_q(\mathbf{s}_t)).$$

By identifying the terms, we find that

$$\begin{aligned} V_q(\mathbf{s}_t) &= \log \beta_t(\mathbf{s}_t) \\ q(\mathbf{s}_t, y_t) &= \log \psi(\mathbf{s}_t, y_t) + \log \beta_{t+1}(\mathbf{s}_t \oplus y_t) \\ &= r(\mathbf{s}_t, y_t) + V_q(\mathbf{s}_t \oplus y_t). \end{aligned}$$

We thus recover exactly the mapping $q = \mathcal{M}(r)$ presented in (7).

Furthermore, we can express the joint probability of a sequence \mathbf{y} using the forward and backward variables. Substituting the expression for the policy derived above into the chain rule, we obtain

$$\begin{aligned} p_q^{\text{ARM}}(\mathbf{y} | \mathbf{x}) &= \prod_{t=1}^T \frac{\psi(\mathbf{s}_t, y_t) \beta_{t+1}(\mathbf{s}_{t+1})}{\beta_t(\mathbf{s}_t)} \\ &= \left(\prod_{t=1}^T \psi(\mathbf{s}_t, y_t) \right) \underbrace{\prod_{t=1}^T \frac{\beta_{t+1}(\mathbf{s}_{t+1})}{\beta_t(\mathbf{s}_t)}}_{\text{telescoping product}} \\ &= \left(\prod_{t=1}^T \psi(\mathbf{s}_t, y_t) \right) \frac{\beta_{T+1}(\mathbf{s}_{T+1})}{\beta_1(\mathbf{s}_1)}. \end{aligned}$$

Using the boundary conditions $\beta_{T+1}(\mathbf{s}_{T+1}) = 1$ and $\beta_1(\mathbf{s}_1) = Z(\mathbf{x})$, we recover exactly the definition of the EBM

$$\begin{aligned} p_q^{\text{ARM}}(\mathbf{y} | \mathbf{x}) &= \frac{1}{Z(\mathbf{x})} \prod_{t=1}^T \psi(\mathbf{s}_t, y_t) \\ &= p_{R_r}^{\text{EBM}}(\mathbf{y} | \mathbf{x}). \end{aligned}$$

Irrelevance of forward variables for sampling. While the forward variable $\alpha_t(\mathbf{s}_t)$ is essential for computing the edge marginals $\mu_q(\mathbf{s}, y)$, it is notably absent from the autoregressive generation process. The optimal policy $\pi_q(y_t | \mathbf{s}_t)$ represents the conditional probability of choosing y_t given the current context \mathbf{s}_t . Using the forward-backward decomposition of the joint probability, we have

$$\pi_q(y_t | \mathbf{s}_t) = \frac{\mathbb{P}(\text{path through } \mathbf{s}_t \oplus y_t)}{\mathbb{P}(\text{path through } \mathbf{s}_t)} = \frac{\alpha_{t+1}(\mathbf{s}_t \oplus y_t) \beta_{t+1}(\mathbf{s}_t \oplus y_t)}{\alpha_t(\mathbf{s}_t) \beta_t(\mathbf{s}_t)}.$$

Substituting the recursive definition $\alpha_{t+1}(\mathbf{s}_t \oplus y_t) = \alpha_t(\mathbf{s}_t)\psi(\mathbf{s}_t, y_t)$, we observe that the forward variable cancels out

$$\pi_q(y_t | \mathbf{s}_t) = \frac{[\alpha_t(\mathbf{s}_t)\psi(\mathbf{s}_t, y_t)]\beta_{t+1}(\mathbf{s}_t \oplus y_t)}{\alpha_t(\mathbf{s}_t)\beta_t(\mathbf{s}_t)} = \frac{\psi(\mathbf{s}_t, y_t)\beta_{t+1}(\mathbf{s}_t \oplus y_t)}{\beta_t(\mathbf{s}_t)}.$$

Intuitively, since the decision at time t is conditioned on the fixed history \mathbf{s}_t , the accumulated reward of that history (α_t) is a constant scaling factor that applies equally to all possible next actions, and thus does not affect the relative probabilities. The policy depends exclusively on the immediate reward ψ and the future value β .

Difference with HMMs and CRFs. It is instructive to contrast this formulation with standard hidden Markov models (HMMs) or linear-chain conditional random fields (CRFs). In those models, the transition graph forms a **lattice** or **trellis** where multiple distinct paths merge into the same state due to the Markov property. Consequently, the standard forward variable $\alpha_t(\mathbf{s}_t)$ represents a marginal quantity obtained by **summing** over all incoming paths. If we use a context size of 1 (as in bigram HMMs), the cost of the forward-backward algorithm is $O(TV^2)$.

In contrast, we define the state of an ARM as the unique context $\mathbf{s}_t := \mathbf{x} \oplus \mathbf{y}_{<t}$. The underlying topology is therefore a **prefix tree** (or trie), where every node has exactly one parent (except the end node, which can have several parents). As a result, there is a unique path from $\mathbf{s}_1 = \mathbf{x}$ to \mathbf{s}_t and the summation over paths typically found in the forward recursion collapses to a single product term: there is no summation in (14). The cost of dynamic programming (the algorithm is backward only) is however $O(V^T)$.

Strictly speaking, if the ARM has a fixed context window W and the sequence length T exceeds W , the model becomes an order- W Markov chain and the graph becomes a De Bruijn lattice. However, in most modern LLM settings, the context window is sufficiently large ($W \gg T$) that the non-merging tree topology is the relevant abstraction. If we use a context size of W (as in n -gram HMMs), the cost of forward-backward is $O(TV^{W+1})$.

A.10. Gradient maps

Energy-based models. The gradient of the log-partition w.r.t. R , known as the link function, is defined for all $\mathbf{x} \in \mathcal{X}$ as

$$\nabla_R A_R^{\text{EBM}}(\mathbf{x}) = g \in \mathcal{F}(\mathcal{X} \times \mathcal{Y})$$

where

$$g(\mathbf{x}', \mathbf{y}) := \begin{cases} p_R^{\text{EBM}}(\mathbf{y} | \mathbf{x}) & \text{if } \mathbf{x}' = \mathbf{x} \\ 0 & \text{otherwise} \end{cases}.$$

Autoregressive models. By analogy, the gradient w.r.t. q of the “log-partition” **along** the sequence \mathbf{y} given \mathbf{x} is

$$\nabla_q A_q^{\text{ARM}}(\mathbf{x}, \mathbf{y}) = g \in \mathcal{F}(\mathcal{S} \times \mathcal{A}),$$

where

$$g(\mathbf{s}'_t, \cdot) := \begin{cases} \pi_q(\cdot | \mathbf{s}_t) & \text{if } \mathbf{s}'_t = \mathbf{s}_t \\ 0 & \text{otherwise} \end{cases}$$

and where $\mathbf{s}_t := \mathbf{x} \oplus \mathbf{y}_{<t}$. Critically, this gradient map depends on the specific sequence \mathbf{y} , and the states \mathbf{s}_t it induces. This highlights a fundamental geometric difference: EBMs are defined by global normalization, while ARMs are defined by local normalization **along** a path.

A.11. Backpropagation

In this section, we derive backpropagation through $V_q(\mathbf{x})$ following Mensch & Blondel (2018).

Bottom-up approach. Defining $V_q(\mathbf{s}_{T+1}) := 0$, we run the forward pass (value computation) from $t = T$ to $t = 1$,

$$V_q(\mathbf{s}_t) = \underset{y_t \in \mathcal{A}}{\text{LSE}} r(\mathbf{s}_t, y_t) + V_q(\mathbf{s}_t \oplus y_t).$$

where q is defined from r as in (7). That is, after the forward pass is complete, we obtain $q = \mathcal{M}(r)$. Note that in Mensch & Blondel (2018), the topological order is from $t = 1$ to $t = T$ because the numbering of nodes is opposite to our notation.

From the identity above, the local gradients are

$$\frac{\partial V_q(\mathbf{s}_t)}{\partial V_q(\mathbf{s}_t \oplus y_t)} = \frac{\partial V_q(\mathbf{s}_t)}{\partial r(\mathbf{s}_t, y_t)} = \pi_q(y_t | \mathbf{s}_t).$$

Our goal is to compute the gradient of $V_q(\mathbf{s}_1) = V_q(\mathbf{x})$ w.r.t. the reward r (edge),

$$\nabla_r V_q(\mathbf{s}_1) = G_q \in \mathcal{F}(\mathcal{S} \times \mathcal{A})$$

where

$$G_q(\mathbf{s}_t, y_t) := \frac{\partial V_q(\mathbf{s}_1)}{\partial r(\mathbf{s}_t, y_t)}.$$

For convenience, we also define the accumulated gradient at state (node) \mathbf{s}_t ,

$$\delta(\mathbf{s}_t) := \frac{\partial V_q(\mathbf{s}_1)}{\partial V_q(\mathbf{s}_t)}.$$

Since $r(\mathbf{s}_t, y_t)$ influences only $V_q(\mathbf{s}_t)$, we have

$$G_q(\mathbf{s}_t, y_t) = \frac{\partial V_q(\mathbf{s}_1)}{\partial r(\mathbf{s}_t, y_t)} = \frac{\partial V_q(\mathbf{s}_1)}{\partial V_q(\mathbf{s}_t)} \frac{\partial V_q(\mathbf{s}_t)}{\partial r(\mathbf{s}_t, y_t)} = \delta(\mathbf{s}_t) \pi_q(y_t | \mathbf{s}_t).$$

Similarly, thanks to the prefix tree structure of ARMs, there is only one path from \mathbf{s}_t to $\mathbf{s}_{t+1} = \mathbf{s}_t \oplus y_t$. As a result, $V_q(\mathbf{s}_t \oplus y_t)$ influences only $V_q(\mathbf{s}_t)$ and we have

$$\delta(\mathbf{s}_{t+1}) = \frac{\partial V_q(\mathbf{s}_1)}{\partial V_q(\mathbf{s}_{t+1})} = \frac{\partial V_q(\mathbf{s}_1)}{\partial V_q(\mathbf{s}_t)} \frac{\partial V_q(\mathbf{s}_t)}{\partial V_q(\mathbf{s}_{t+1})} = \delta(\mathbf{s}_t) \pi_q(y_t | \mathbf{s}_t).$$

Therefore, we have

$$G_q(\mathbf{s}_t, y_t) = \delta(\mathbf{s}_t) \pi_q(y_t | \mathbf{s}_t) = \delta(\mathbf{s}_{t+1}).$$

Defining $\delta(\mathbf{s}_1) := 1$, we can compute the backward pass from $t = 1$ to T ,

$$G_q(\mathbf{s}_t, y_t) = \delta(\mathbf{s}_t) \pi_q(y_t | \mathbf{s}_t) = \prod_{k=1}^t \pi_q(y_k | \mathbf{s}_k) = p_q^{\text{ARM}}(\mathbf{y}_{\leq t} | \mathbf{x}).$$

This confirms that the gradient of the log-partition function $V_q(\mathbf{s}_1)$ with respect to the local reward $r(\mathbf{s}_t, y_t)$ for $q = \mathcal{M}(r)$ is exactly the marginal probability of the prefix $\mathbf{y}_{\leq t}$ given \mathbf{x} .

Connection with forward and backward variables. Using the forward and backward variables from Section A.9, the gradient can be equivalently written as

$$\begin{aligned} G_q(\mathbf{s}_t, y_t) &= \frac{\partial V_q(\mathbf{s}_1)}{\partial r(\mathbf{s}_t, y_t)} \\ &= \delta(\mathbf{s}_t) \pi_q(y_t | \mathbf{s}_t) \\ &= \left(\frac{\alpha_t(\mathbf{s}_t) \beta_t(\mathbf{s}_t)}{\beta_1(\mathbf{s}_1)} \right) \left(\frac{\psi(\mathbf{s}_t, y_t) \beta_{t+1}(\mathbf{s}_{t+1})}{\beta_t(\mathbf{s}_t)} \right) \\ &= \frac{\alpha_{t+1}(\mathbf{s}_{t+1}) \beta_{t+1}(\mathbf{s}_{t+1})}{Z(\mathbf{x})}, \end{aligned}$$

where we used $\alpha_{t+1}(\mathbf{s}_{t+1}) = \alpha_t(\mathbf{s}_t) \psi(\mathbf{s}_t, y_t)$ and $\beta_1(\mathbf{s}_1) = Z(\mathbf{x})$.

B. Proofs

B.1. Lemmas

Lemma 1 (Stability of softargmax w.r.t. Kullback-Leibler divergence). *For all $f: [k] \rightarrow \mathbb{R}$ and $g: [k] \rightarrow \mathbb{R}$, we have*

$$\text{KL}(\text{softargmax}(f), \text{softargmax}(g)) \leq 2\|f - g\|_\infty$$

where $\|h\|_\infty := \max_{j \in [k]} |h(j)|$.

Proof. Let us define $p_f := \text{softargmax}(f)$ and $p_g := \text{softargmax}(g)$. We have

$$\begin{aligned} \text{KL}(p_f, p_g) &= \sum_{i \in [k]} p_f(i) \log \frac{p_f(i)}{p_g(i)} \\ &= \sum_{i \in [k]} p_f(i)((f(i) - \log Z_f) - (g(i) - \log Z_g)) \\ &= \mathbb{E}_{i \sim p_f}[f(i) - g(i)] - (\log Z_f - \log Z_g) \end{aligned}$$

where $Z_f := \sum_{j \in [k]} \exp(f(j))$ and $Z_g := \sum_{j \in [k]} \exp(g(j))$.

Let us define $\varepsilon := \|f - g\|_\infty$.

Using $f(j) - g(j) \leq \varepsilon$ for all $j \in [k]$, we obtain

$$\begin{aligned} Z_f &= \sum_{j \in [k]} \exp(f(j)) \\ &= \sum_{j \in [k]} \exp(g(j) + (f(j) - g(j))) \\ &\leq \sum_{j \in [k]} \exp(g(j) + \varepsilon) \\ &= \exp(\varepsilon) \sum_{j \in [k]} \exp(g(j)) \\ &= \exp(\varepsilon) Z_g \end{aligned}$$

and therefore

$$\log Z_f \leq \log Z_g + \varepsilon.$$

Applying the same reasoning with $g(j) - f(j) \leq \varepsilon$ for all $j \in [k]$, we obtain

$$\log Z_g \leq \log Z_f + \varepsilon.$$

Therefore, we obtain the tight bound

$$|\log Z_f - \log Z_g| \leq \varepsilon.$$

We also have

$$\mathbb{E}_{i \sim p_f}[f(i) - g(i)] \leq \mathbb{E}_{i \sim p_f}[\varepsilon] = \varepsilon.$$

Overall, we therefore obtain

$$\text{KL}(p_f, p_g) \leq 2\varepsilon = 2\|f - g\|_\infty.$$

□

B.2. Proof of bijection (Proposition 1)

Mapping from ARM to EBM. Given a context $x \in \mathcal{X}$, the probability according to an ARM of a response $y = (y_1, \dots, y_\tau) \in \mathcal{Y}$, with $y_\tau = \text{EOS}$, decomposes as

$$p_q^{\text{ARM}}(y|x) = \pi_q(y_1|\mathbf{s}_1)\pi_q(y_2|\mathbf{s}_2)\dots\pi_q(y_\tau|\mathbf{s}_\tau).$$

In the above, we defined the intermediate contexts as

$$\mathbf{s}_t := \begin{cases} \mathbf{x} & \text{if } t = 1 \\ \mathbf{x} \oplus \mathbf{y}_{<t} & \text{if } t > 1 \end{cases},$$

the conditional probabilities π_q as

$$\begin{aligned} \pi_q(y_1|\mathbf{s}_1) &:= \exp(q(\mathbf{s}_1, y_1) - V_q(\mathbf{s}_1)) \\ \pi_q(y_2|\mathbf{s}_2) &:= \exp(q(\mathbf{s}_2, y_2) - V_q(\mathbf{s}_2)) \\ &\vdots \\ \pi_q(\text{EOS}|\mathbf{s}_\tau) &:= \exp(q(\mathbf{s}_\tau, \text{EOS}) - V_q(\mathbf{s}_\tau)) \end{aligned}$$

and the (local) log-partitions as

$$V_q(\mathbf{s}_t) := \log \sum_{y_t \in \mathcal{A}} \exp q(\mathbf{s}_t, y_t).$$

We then get

$$\begin{aligned} p_q^{\text{ARM}}(\mathbf{y}|\mathbf{x}) &= \exp(q(\mathbf{s}_1, y_1) + q(\mathbf{s}_2, y_2) + \cdots + q(\mathbf{s}_\tau, \text{EOS}) - V_q(\mathbf{s}_1) - V_q(\mathbf{s}_2) - \cdots - V_q(\mathbf{s}_\tau)) \\ &= \exp(r(\mathbf{s}_1, y_1) + r(\mathbf{s}_2, y_2) + \cdots + r(\mathbf{s}_\tau, \text{EOS}) - V_q(\mathbf{s}_1)) \\ &= p_{R_r}^{\text{EBM}}(\mathbf{y}|\mathbf{x}), \end{aligned}$$

where R_r is defined in (5) and where we defined

$$\begin{aligned} r(\mathbf{s}_1, y_1) &:= q(\mathbf{s}_1, y_1) - V_q(\mathbf{s}_2) \\ &\vdots \\ r(\mathbf{s}_{\tau-1}, y_{\tau-1}) &:= q(\mathbf{s}_{\tau-1}, y_{\tau-1}) - V_q(\mathbf{s}_\tau) \\ r(\mathbf{s}_\tau, \text{EOS}) &:= q(\mathbf{s}_\tau, \text{EOS}). \end{aligned}$$

The value $V_q(\mathbf{s}_1) = V_q(\mathbf{x})$ is a valid log-partition function for $p_{R_r}^{\text{EBM}}$, provided that p_q^{ARM} is a valid distribution. The latter is ensured if $\pi_q(\text{EOS}|\mathbf{s}_T) = 1$. This can be achieved by fixing

$$q(\mathbf{s}_T, y_T) := \begin{cases} 0 & \text{if } y_T = \text{EOS} \\ -\infty & \text{if } y_T \neq \text{EOS} \end{cases}$$

for any $\mathbf{s}_T \in \mathcal{S}_T$, where $\mathcal{S}_T := \mathcal{X} \times (\mathcal{A} \setminus \{\text{EOS}\})^{T-1}$.

The mapping above is valid for any τ and any y_1, \dots, y_τ (with $y_\tau = \text{EOS}$ in all cases) so it can be summarized simply as

$$r(\mathbf{s}, y) := \begin{cases} q(\mathbf{s}, y) & \text{if } y = \text{EOS} \\ q(\mathbf{s}, y) - V_q(\mathbf{s} \oplus y) & \text{if } y \neq \text{EOS} \end{cases},$$

for $\mathbf{s} \in \mathcal{S}$ and $y \in \mathcal{A}$. This is the mapping $r = \mathcal{M}^{-1}(q)$.

Mapping from EBM to ARM. The reverse mapping is obtained by back-substitution

$$\begin{aligned} q(\mathbf{s}_\tau, \text{EOS}) &:= r(\mathbf{s}_\tau, \text{EOS}) \\ q(\mathbf{s}_{\tau-1}, y_{\tau-1}) &:= r(\mathbf{s}_{\tau-1}, y_{\tau-1}) + V_q(\mathbf{s}_T) \\ &\vdots \\ q(\mathbf{s}_1, y_1) &:= r(\mathbf{s}_1, y_1) + V_q(\mathbf{s}_2). \end{aligned}$$

This is the mapping $q = \mathcal{M}(r)$.

B.3. Proof of same minima (Proposition 2)

Because we can always define r from R using (6), we have

$$\min_{r \in \mathcal{F}(\mathcal{S} \times \mathcal{A})} \mathbb{E}_{(X,Y) \sim \rho} [\ell_{R_r}^{\text{EBM}}(X, Y)] = \min_{R \in \mathcal{F}(\mathcal{X} \times \mathcal{Y})} \mathbb{E}_{(X,Y) \sim \rho} [\ell_R^{\text{EBM}}(Y|X)].$$

Because the mapping \mathcal{M} is bijective (and therefore surjective), we have

$$\begin{aligned} \min_{r \in \mathcal{F}(\mathcal{S} \times \mathcal{A})} \mathbb{E}_{(X,Y) \sim \rho} [\ell_{R_r}^{\text{EBM}}(X, Y)] &= \min_{r \in \mathcal{F}(\mathcal{S} \times \mathcal{A})} \mathbb{E}_{(X,Y) \sim \rho} [-\log p_{R_r}^{\text{EBM}}(Y|X)] \\ &= \min_{r \in \mathcal{F}(\mathcal{S} \times \mathcal{A})} \mathbb{E}_{(X,Y) \sim \rho} [-\log p_{\mathcal{M}(r)}^{\text{ARM}}(Y|X)] \\ &= \min_{q \in \mathcal{F}(\mathcal{S} \times \mathcal{A})} \mathbb{E}_{(X,Y) \sim \rho} [-\log p_q^{\text{ARM}}(Y|X)] \\ &= \min_{q \in \mathcal{F}(\mathcal{S} \times \mathcal{A})} \mathbb{E}_{(X,Y) \sim \rho} [\ell_q^{\text{ARM}}(X, Y)]. \end{aligned}$$

B.4. Proof of KL bound (Proposition 3)

From Lemma 1, for all $s_t \in \mathcal{S}$, we have

$$\text{KL}(\pi_{q^*}(\cdot|s_t), \pi_q(\cdot|s_t)) \leq 2\|q^*(s_t, \cdot) - q(s_t, \cdot)\|_\infty.$$

This bounds the token-level distribution error.

We then have, for all $x \in \mathcal{X}$,

$$\begin{aligned} \text{KL}(p_{q^*}^{\text{ARM}}(\cdot|x), p_q^{\text{ARM}}(\cdot|x)) &= \sum_{t=1}^T \mathbb{E}_{S_t} \text{KL}(\pi_{q^*}(\cdot|S_t), \pi_q(\cdot|S_t)) \\ &\leq 2 \sum_{t=1}^T \mathbb{E}_{S_t} \|q^*(S_t, \cdot) - q(S_t, \cdot)\|_\infty \\ &\leq 2T \max_{s \in \mathcal{S}(x)} \|q^*(s, \cdot) - q(s, \cdot)\|_\infty, \end{aligned}$$

where S_t above is defined by $S_t := x \oplus Y_{<t}$, where $Y_{<t} \stackrel{\text{AR}}{\sim} \pi_{q^*}(\cdot|x)$. See also Appendix A.4 for more details.

This bounds the sequence-level distribution error.

Finally, using Proposition 1, we obtain

$$\begin{aligned} \text{KL}(p_{R_r}^{\text{EBM}}(\cdot|x), p_q^{\text{ARM}}(\cdot|x)) &= \text{KL}(p_{\mathcal{M}(r)}^{\text{ARM}}(\cdot|x), p_q^{\text{ARM}}(\cdot|x)) \\ &\leq 2T \max_{s \in \mathcal{S}} \|\mathcal{M}(r)(s, \cdot) - q(s, \cdot)\|_\infty. \end{aligned}$$

B.5. Proof that an ARM defines a valid probability distribution (Proposition 4)

By definition of \mathcal{Y} , we have

$$\sum_{y \in \mathcal{Y}} p_q^{\text{ARM}}(y|x) = \sum_{t=1}^T \sum_{y_{<t} \in \mathcal{V}^{t-1}} p_q^{\text{ARM}}(y_{<t} \oplus \text{EOS}|x) = \sum_{t=1}^T l_t$$

where

$$l_t := \sum_{y_{<t} \in \mathcal{V}^{t-1}} p_q^{\text{ARM}}(y_{<t} \oplus \text{EOS}|x),$$

can be interpreted as the probability that a response has length t . We can decompose l_t for any $1 \leq t \leq T$ as follows

$$\begin{aligned} l_t &= \sum_{\mathbf{y}_{<t} \in \mathcal{V}^{t-1}} \left[\prod_{k=1}^{t-1} \pi_q(y_k | \mathbf{s}_k) \right] \pi_q(\text{EOS} | \mathbf{s}_t) \\ &\stackrel{(i)}{=} \sum_{\mathbf{y}_{<t} \in \mathcal{V}^{t-1}} \left[\prod_{k=1}^{t-1} \pi_q(y_k | \mathbf{s}_k) \right] \left(1 - \sum_{y_t \in \mathcal{V}} \pi_q(y_t | \mathbf{s}_t) \right) \\ &= M_t - M_{t+1}, \end{aligned}$$

where $M_1 := 1$ and for $t > 1$,

$$M_t := \sum_{\mathbf{y}_{<t} \in \mathcal{V}^{t-1}} \prod_{k=1}^{t-1} \pi_q(y_k | \mathbf{s}_k) = \sum_{\mathbf{y}_{<t} \in \mathcal{V}^{t-1}} p_q^{\text{ARM}}(\mathbf{y}_{<t} | \mathbf{x})$$

can be interpreted as the probability mass of sequences that have *not* terminated strictly before step t . In the derivations above, the equality in (i) stems from the definition of the conditional probabilities through a softargmax. Namely, since $\pi_q(\cdot | \mathbf{s}_t) = \text{softargmax}(q(\mathbf{s}_t, \cdot))$, we have that

$$\begin{aligned} \sum_{y_t \in \mathcal{V} \cup \{\text{EOS}\}} \pi_q(y_t | \mathbf{s}_t) &= \sum_{y_t \in \mathcal{V} \cup \{\text{EOS}\}} \text{softargmax}(q(\mathbf{s}_t, y_t)) = 1 \\ \implies \sum_{y_t \in \mathcal{V}} \pi_q(y_t | \mathbf{s}_t) &= 1 - \pi_q(\text{EOS} | \mathbf{s}_t). \end{aligned}$$

We then obtain by telescoping the M_t terms,

$$\sum_{t=1}^T l_t = M_1 - M_{T+1} = 1 - M_{T+1}.$$

By assumption, $\pi_q(\text{EOS} | \mathbf{s}_T) = 1$, which implies $\pi_q(y_T | \mathbf{s}_T) = 0$ for any $y_T \in \mathcal{V}$. Consequently, no mass can continue beyond T , therefore $M_{T+1} = 0$ and we have shown the claim.

C. Details on numerical illustrations

C.1. Setup

Architecture. Both EBMs and ARMs use as a backbone a pre-layer norm Transformer with a scaled dot-product multihead attention, a positional embedder and a ReLU activation. We introduce the following notation:

- Size of the vocabulary: V ,
- Length of the sequences: T ,
- Number of blocks: N ,
- Embedding dimension: D ,
- Number of heads in the attention layer: H ,
- Hidden dimension in the MLP: F .

The backbone Transformer is summarized below in abbreviated Flax code (Heek et al., 2024). It takes a sequence $\mathbf{x}_{\text{TxD}} \in \mathbb{R}^{V^T}$ and outputs a representation $\mathbf{x}_{\text{TxD}} \in (\mathbb{R}^V)^T$.

```
class TransformerBlock(H, D, F):
    def __call__(x_TxD, mask):
        y_TxD = LayerNorm()(x_TxD)
        y_TxD = MultiHeadAttention(H, D)(y_TxD, mask)
        x_TxD = y_TxD + x_TxD

        y_TxD = LayerNorm()(x_TxD)
        y_TxF = Linear(F)(y_TxD)
```

```

y_TxF = relu(y_TxF)
y_TxD = Linear(D)(y_TxF)
x_TxD = y_TxD + x_TxD
return x_TxD

class Transformer(V, T, N, H, D, F):
    def __call__(x_T, mask):
        x_TxD = Embedder(V, D)(x_T)
        y_TxD = Embedder(T, D)([0, ..., L])
        x_TxD = x_TxD + y_TxD
        for i in range(N):
            TransformerBlock(H, D, F)(x_TxD, mask)
        return x_TxD
    
```

For the ARM, the autoregressive dependency pattern is encoded through a `mask` applied to the attention matrix. The EBM does not use any mask. The ARM projects the embedded tokens into a space of size V to define one logit per token. The EBM takes the average representation of the sequence along the sequence indexes and applies a final layer on the D dimensional representation of the whole sequence to get a single score.

```

class AutoRegressiveModel((V, T, N, H, D, F):
    def __call__(x_T):
        mask = make_causal_mask(x)
        x_TxD = Transformer(V, T, N, H, D, F)(x_TxD, mask)
        x_TxV = Linear(V)(x_TxD)
        return x_TxV

class EnergyBasedModel(V, T, N, H, D, F):
    def __call__(x_T):
        x_TxD = Transformer(V, T, N, H, D, F)(x_TxD, None)
        x_D = mean(x_TxD, axis=0)
        x = Linear(1)(x_D)
        return x
    
```

All sequences start with a BOS index. The BOS index is part of the embedder vocabulary but not part of the head (last linear transformation) of the ARM, since sentences can only end and not start again.

Objective function. We compute the exact expected risk (11) and (12) by summing over all possible sequences and parameterizing the data distribution with a probability mass function ρ of our choice. For simplicity, we use a fixed length T . Concretely, using the EBM as an example, we compute the logits $R(\mathbf{x}, \mathbf{y})$ for all possible sequences (\mathbf{x}, \mathbf{y}) of length T and then compute the loss using

$$\mathcal{L}^{\text{EBM}}(R) = \sum_{(\mathbf{x}, \mathbf{y}) \in \mathcal{V}^T} \rho(\mathbf{x}, \mathbf{y}) \ell_R^{\text{EBM}}(\mathbf{x}, \mathbf{y}).$$

For the data distribution ρ , we tried two settings.

1. A Zipfian distribution over the set of all V^T sequences. This gives a distribution over all possible sequences with a large tail.
2. A normal-softmax distribution, i.e., $\rho = \text{softmax}(z/t)$ for $z \sim \mathcal{N}(0, 1)$ a random normal vector, and $t > 0$ a temperature parameter. For small t , this gives a vector of probability close to a one-hot vector among all possible sequences.

We briefly mentioned in the main text that $\mathcal{L}^* = -\mathbb{E}_{(\mathbf{X}, \mathbf{Y}) \sim \rho} \log \rho(\mathbf{x}, \mathbf{y})$ was the minimum of $\mathcal{L}^{\text{EBM}}(R)$. To verify this, it suffices to observe that

$$\mathcal{L}^{\text{EBM}}(R) - \mathcal{L}^* = \text{KL}(\rho, \text{softmax}(R)) \geq 0.$$

Optimization. We use the Adam optimizer (Kingma & Ba, 2014) with a trapezoidal schedule (warm-up of 100 steps, constant learning rate η , decay of 100 steps) with a learning rate η searched in $[3 \cdot 10^{-3}, 1 \cdot 10^{-3}, 10^{-4}]$. We observed that the best learning rate (measured in terms of minimal area under the training curve) for EBMs matched the best learning rate for ARMs. Therefore, in the plots below, we simply choose the best learning rate for the EBM and use the same for the ARM.

C.2. Configurations.

We consider the following sequence spaces.

1. $V = 8, T = 4$, leading to 4 096 sequences.
2. $V = 4, T = 8$, leading to 65 536 sequences.

For these sequence spaces, we consider the following architectures

1. 2-layer Transformer with $N = 2, H = 2, D = 16, V = 16$. For $V = 8, T = 4$ or $V = 4, T = 8$, leading to 3 633 parameters.
2. 3-layer Transformer with $N = 3, H = 4, D = 64, F = 64$. For $V = 8, T = 4$ or $V = 4, T = 8$, leading to 76 609 parameters.

The 2-layer Transformer is under-parameterized for $V = 8, T = 4$ and $V = 4, T = 8$, while the 3-layer Transformer is over-parameterized in those cases.

C.3. Metrics illustrated

To illustrate Proposition 2, we plot the losses along the training of these Transformers. Namely, in the left panel of Figures 1, 2 and 3, we plot

$$\mathcal{L}^{\text{EBM}}(R_{w_k}) - \mathcal{L}^*, \quad \text{and} \quad \mathcal{L}^{\text{ARM}}(q_{w_k}) - \mathcal{L}^*,$$

where w_k^{ARM} and w_k^{EBM} are the weights of, respectively, the ARM and EBM, at iteration k of the training.

To illustrate our bijection result, after having optimized the EBM, we save the corresponding logits $R^*(\mathbf{x}, \mathbf{y})$, and we then compare the logits $q_k(\mathbf{x}, \mathbf{y})$ of the ARM at iteration k of its training, against the optimal EBM logits. We perform two comparisons.

The first one consists in simply summing the logits of the ARM along the sequence to get a scalar $\bar{q}_k(\mathbf{x}, \mathbf{y}) = \sum_{t=1}^T q_k(s_t, y_t)$ with $s_0 = \mathbf{x} = \text{BOS}$ in our case, and s_t, y_t defined as in the main text. This comparison amounts to think of the logits of the ARM as a score in itself like in the definition of the EBM model. We then center the scores of both the ARM and the EBM model (i.e., subtract the mean score among all possible sequences), and measure the maximal absolute difference between them. Formally, we plot

$$\|c(\bar{q}_k) - c(R^*)\|_\infty,$$

where $c(z) = z - \langle z, \mathbf{1} \rangle \mathbf{1}$. In Figures 1, 2 and 3, we call this measurement of the logits distance ‘‘Before mapping’’.

The second comparison consists in computing $q^* = \mathcal{M}(r^*)$ for

$$r^*(s_t, y_t) = \begin{cases} 0 & \text{if } y_t \neq \text{EOS} \\ R^*(\mathbf{x}, \mathbf{y}) & \text{if } y_t = \text{EOS} \end{cases}.$$

This amounts to computing the ARM logits corresponding to the optimal EBM model via the mapping \mathcal{M} used in Proposition 1. We then center along the last axis the logits of the ARM at iteration k and the logits of the EBM mapped in AR form. Finally, we plot their maximal absolute elementwise distance, i.e., we plot

$$\|c_{-1}(q_k) - c_{-1}(\mathcal{M}(r^*))\|_\infty,$$

where c_{-1} denotes centering along the last axis. In Figures 1, 2 and 3, we call this measurement the logits distance ‘‘After mapping’’.

In both cases, the centering is necessary to take care of the fact that, up to a constant factor, logits may define the same probability distribution through the softargmax operator (Blondel & Roulet, 2024, Remark 4.2). Centering lets us discover, whether, up to some constant factor, the logits of the ARM converge to the logits predetermined by the EBM after an appropriate mapping.

C.4. Convergence and logits distance comparisons

Figure 1 illustrates the metrics explained above in the case $V = 8, T = 4$, for the 2-layer Transformer presented above.

We present some additional results here.

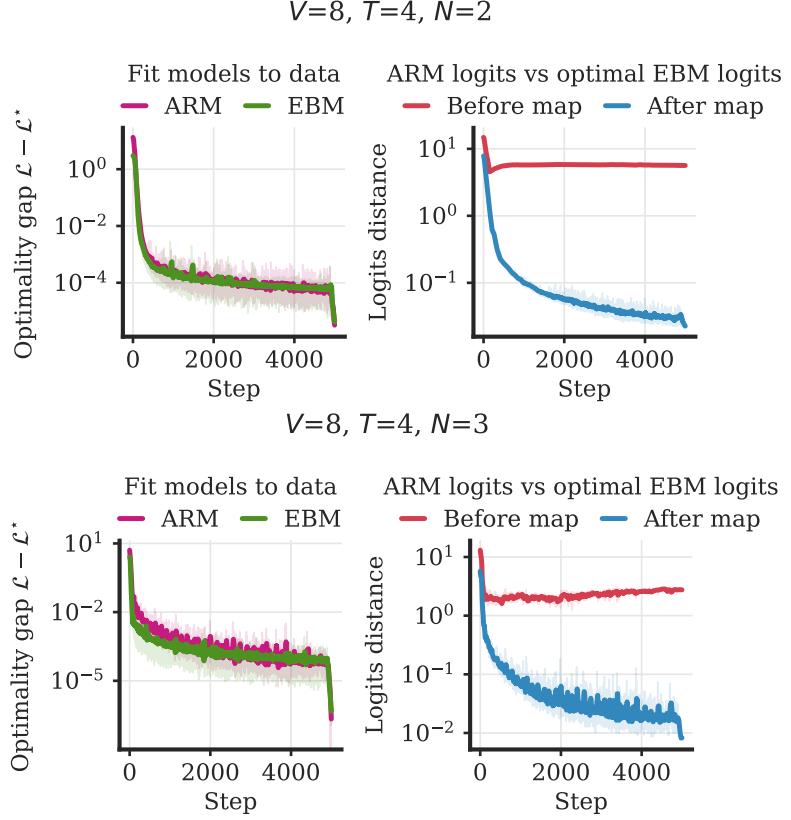


Figure 2. Loss convergence and logits distances for different Transformer sizes.

- In Figure 2, we vary the size of the Transformer and observe the same conclusions as in the main text.
- In Figure 3, we also try the case $T > V$, namely, $T = 8, V = 4$: same conclusions apply as in the main text.

The convergence in logits is challenged when using a different data distribution as explained in the next paragraph.

C.5. Bounding KL divergence by logits distance

In Figure 4, we compare KL divergence and distance between logits in infinity norm. Namely, as in the previous experiments, we compute the optimal logits for the EBM and then compare the logits of the ARM with the logits of the EBM mapped into ARM form. We use either the maximal absolute distance between logits, or we compare the KL distance between the probability distributions that the EBM and ARM define. We consider several setups ($V > T, T < V, N = 2$ or 3) with different definitions of the target distribution ρ .

Proposition 3 stated that the KL should be upper bounded by the maximal absolute distance between logits. This is empirically confirmed in Figure 4.

Note that when we define the target distribution as a softargmax of a normal vector (bottom panels in Figure 4), only the KL converges to 0, not the distance in infinity norm. In this case, the target distribution is extremely peaked towards a single sequence. So even if the distributions match after mapping the logits to the same vertex in the simplex of all sequences, the logits themselves may be far from each other. Another way to see that, is that the inverse mapping of the softargmax is not Lipschitz continuous around a vertex of the simplex.

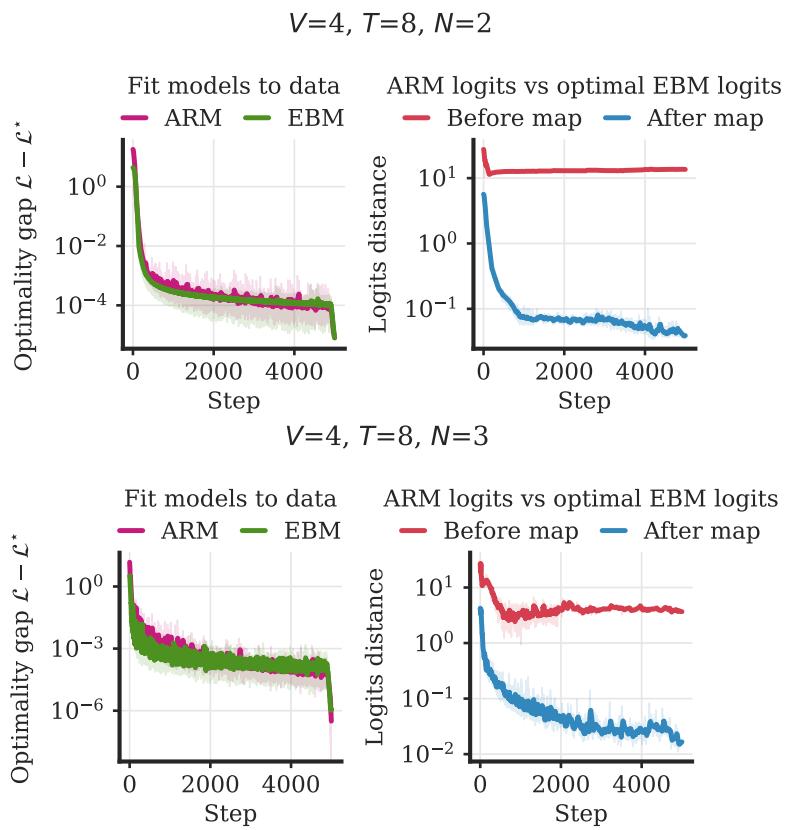


Figure 3. Loss convergence and logits distances for different Transformer sizes in the case $T > V$.

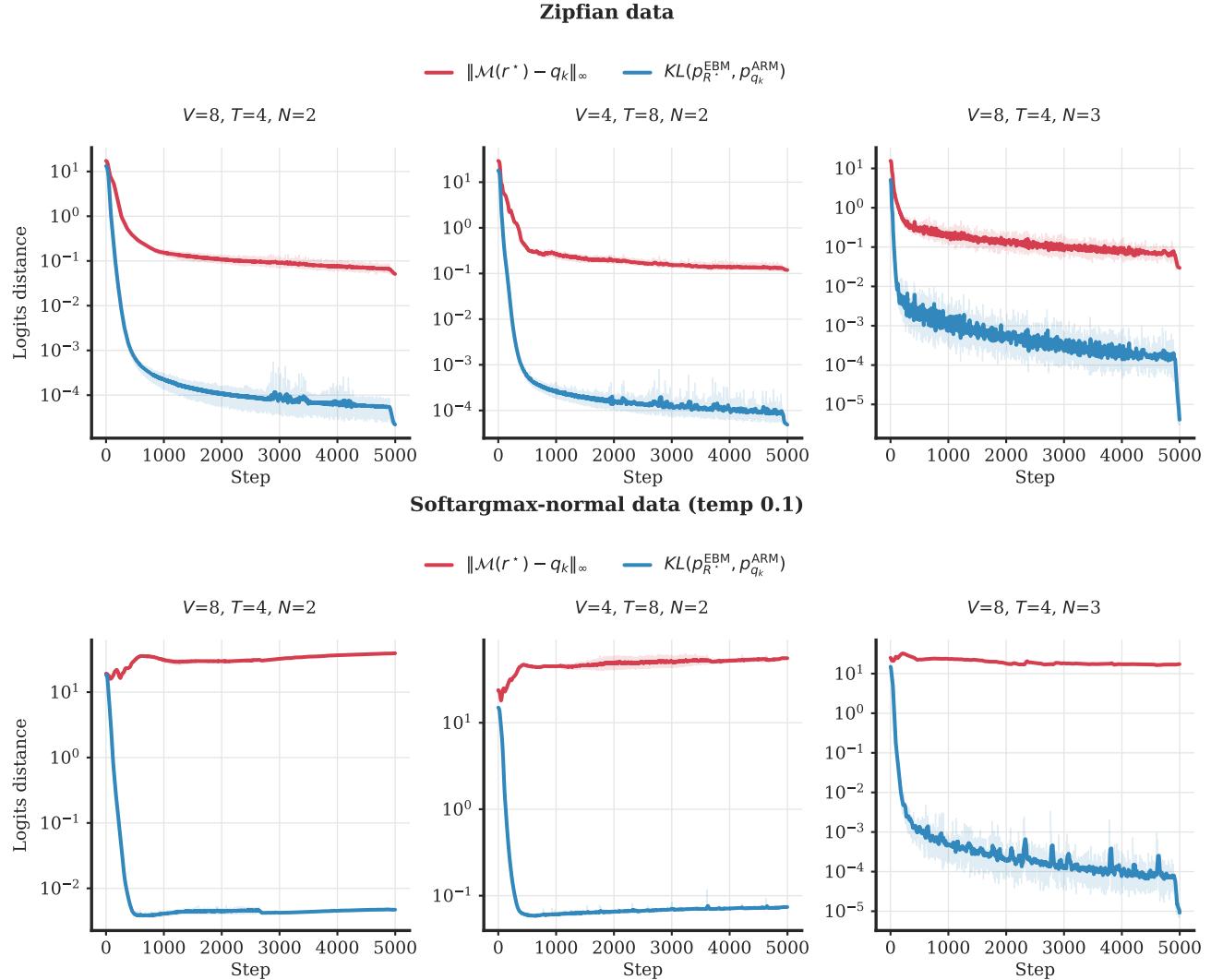


Figure 4. Comparing KL divergence and logits distance in infinity norm.