

A Mathematical Theory of Attention

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Abstract

Attention is a powerful component of modern neural networks across a wide variety of domains. However, despite its ubiquity in machine learning, there is a gap in our understanding of attention from a theoretical point of view. We propose a framework to fill this gap by building a mathematically equivalent model of attention using measure theory. With this model, we are able to interpret self-attention as a system of self-interacting particles, we shed light on self-attention from a maximum entropy perspective, and we show that attention is actually Lipschitz-continuous (with an appropriate metric) under suitable assumptions. We then apply these insights to the problem of mis-specified input data, and infinitely-deep, weight-sharing self-attention networks, and more general Lipschitz estimates for a specific type of attention studied in concurrent work.

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1 Introduction

Attention (Bahdanau et al., 2014; Vaswani et al., 2017) has recently joined the multi-layer perceptron, convolution, and recurrent neural network cell as a fundamental building block of modern neural networks. Mathematical theories of the multilayer perceptron (Cybenko, 1989; Hornik et al., 1989) and convolution (Mallat, 2016; Cohen et al., 2016) exist, and explain these operations as instances of broader mathematical objects. From these explanations, we gain the support of these theories to further investigate the behaviour of neural networks containing these constituents.

However, despite its meteoric rise within deep learning (or perhaps, because of it), we believe there is a gap in our theoretical understanding of what attention is, and why it works. In particular, attention cannot be considered an instance of any existing building blocks (e.g. linear transformation, convolution), therefore we have mainly intuitive explanations and empirical evidence – see the recent rise of “Bertology” (Tenney et al., 2019; Clark et al., 2019) – to understand its inner workings. Additionally, there is recent evidence that the success of attention is not restricted to the natural language (Veličković et al., 2017; Parmar et al., 2018; Baker et al., 2019) and is a general phenomenon.

Objective and Contributions. Our goal is to study attention in a framework that allows for a systematic and principled exploration of its properties. We approach this goal in three steps: (i) Identify a natural mathematical model with which to study attention; (ii) Leverage this model to establish basic results about the properties of attention; (iii) Apply these insights to deepen our understanding and intuition about attention-based models. We provide a framework, built using measure theory and Markov kernels, as an alternative (but equivalent) modelling paradigm which grants us access to the powerful tools of analysis on the space of measures. One example of these tools at work, to be proven in Section 5, is a proof of the following continuity estimate

$$\|\text{Attention}(q_1, K, V) - \text{Attention}(q_2, K, V)\| \leq \text{constant} \cdot \|q_1 - q_2\|$$

and an upper bound on what “constant” should be.

Specifically, our contributions are:

1. We show that attention can be interpreted as system of interacting particles, and we model the evolution of this system as a nonlinear transformation of probability measures;
2. We show that attention contains the solution to a maximum entropy problem and a minimum entropy projection, and is therefore characterized by these problems;
3. We show that attention is a Lipschitz-continuous operation under suitable assumptions, and give quantitative estimates of the Lipschitz coefficient;
4. We apply these theories to study sub-sampled input data; infinitely-deep, weight-sharing self-attention networks; and relaxing the boundedness assumptions in our Lipschitz estimates to obtain more general results than other concurrent works.

The paper is organized as follows. We first introduce preliminaries in Section 2. In Section 3, we describe attention and the Transformer using measure theory. We then qualitatively study how attention works using Kullback-Leibler projections (Section 4), and in Section 5 we obtain quantitative Lipschitz continuity estimates for self-attention. We apply these results to some concrete problems in Section 6 and review related work in Section 7.

2 Preliminaries

2.1 Attention and Structured Data

The fundamental definition of attention is due to Bahdanau et al. (2014), which we provide below with some additional terminology for the various components that we will study later on.

Definition 1 (Attention, Bahdanau et al. (2014)). Let $\mathcal{Q} \subseteq \mathbb{R}^{d_q}$, $\mathcal{K} \subseteq \mathbb{R}^{d_k}$, $\mathcal{V} \subseteq \mathbb{R}^{d_v}$ the query-space, key-space, and value-space respectively. Let $K = \{k_1, \dots, k_N\} \subset \mathcal{K}$ be a set of keys, $V = \{v_1, \dots, v_N\} \subset \mathcal{V}$ a set of values, and $q \in \mathcal{Q}$ a query. Finally, let $a : \mathcal{Q} \times \mathcal{V} \rightarrow \mathbb{R}$ be a similarity function. Attention is the mapping

$$\text{Attention}(q, K, V) := \sum_{i=1}^N \text{softmax}_i(q, K) \cdot v_i,$$

where $\text{softmax}_i(q, K)$ is a probability distribution over the elements of K defined as

$$\text{softmax}_i(q, K) := \frac{\exp(a(q, k_i))}{\sum_{j=1}^N \exp(a(q, k_j))} = \text{softmax}_j(\{a(q, k_j)\}_j). \quad (1)$$

While $\text{Attention}(\bullet, K, V)$ is defined point-wise for a given query, it is almost always used to process a set of queries $Q = \{q_1, \dots, q_M\} \subset \mathcal{Q}$ in parallel. Thus, we will usually write $\text{Attention}(Q, K, V) := \{\text{Attention}(q_i, K, V)\}_{i=1}^M$. Also, while we must have $|K| = |V| = N$, M does not have to equal N in general. Moreover, when $K = V = Q$, we call the following mapping **self-attention**:

$$Q \mapsto \text{SelfAttention}(Q) := \text{Attention}(Q, Q, Q).$$

In the sequel, we are primarily interested in the phenomenon of self-attention as it *can be composed to arbitrary depth*, making it a key building block of many neural network architectures.

The attention operation is very versatile, and has become a key component of many neural networks that operate on discrete data with some type of structure on the elements, i.e. “structured data”. More precisely, consider a finite collection of elements $X = \{x_1, \dots, x_T\}$ indexed by a finite set $t \in \mathcal{T}$, where each $x_t \in \mathcal{V}$ for some finite *vocabulary* \mathcal{V} . In the representation learning framework of attention, we assume \mathcal{V} has been embedded in \mathbb{R}^d , so we identify each x_t with one of *finitely-many* vectors in \mathbb{R}^d . Hence, we will consider $X \subset E$, where E is some fixed subset of \mathbb{R}^d . We assume that the structure (positional information, adjacency information, etc) is encoded in these vectors.

2.2 Markov Kernels

In the sequel, (E, \mathcal{E}) denotes a subset of \mathbb{R}^d endowed with its Borel σ -algebra, and $\mathcal{P}(E)$ the space of all probability measures on E . We use the following notation for expectations with respect to $\mu \in \mathcal{P}(E)$: for a real-valued measurable function f , we denote $\mu(f) := \int f(x) \mu(dx)$ when it exists. For a vector-valued function $F : E \rightarrow \mathbb{R}^l$ with $F(x) = [F_1(x), \dots, F_l(x)]^T$, we denote $\mu(F) := [\mu(F_1), \dots, \mu(F_l)]^T$ when all the components exist.

Our framework will heavily rely on linear transformations of measures modelled by **Markov kernels**; see e.g. Del Moral (2004).

Definition 2 (Markov kernel). A Markov kernel is an E -indexed family of probability measures $M(x, dy) \in \mathcal{P}(E)$ such that $\forall A \in \mathcal{E}, x \mapsto M(x, A)$ is measurable.

A Markov kernel M defines a linear operator $\mathcal{P}(E) \rightarrow \mathcal{P}(E)$ by $\mu M(dy) := \int \mu(dx) M(x, dy)$. It also defines a linear operator on measurable functions by $M(f)(x) := \int f(y) M(x, dy)$. Markov kernels M, N can be composed by integration, $MN(x, dz) := \int M(x, dy) N(y, dz)$.

3 Modelling Attention

In this section, we model attention (Bahdanau et al., 2014) and the Transformer (Vaswani et al., 2017) in measure-theoretic language. Our construction casts the action of attention and the Transformer on a collection of vectors as a nonlinear Markov transport on $\mathcal{P}(E)$ by reformulating existing linear algebra and point-wise operations in-terms of operators on $\mathcal{P}(E)$.

3.1 Basic Model of Attention

The fundamental parts of Attention from Definition 1 are the softmatch_a operation, the key-value correspondence, and the value-averaging w.r.t. the softmatch distribution. We will treat each of these in turn.

Softmatch and Boltzmann-Gibbs Transformations. At the core of the softmatch function, and indeed attention in general, are the interactions between queries and keys. These interactions are a specific case of a nonlinear measure transformation, the Boltzmann-Gibbs transformation.

Definition 3 (Boltzmann-Gibbs Transformation). *Let $g : E \rightarrow \mathbb{R}_{>0}$ be a bounded measurable function. The **Boltzmann-Gibbs transformation** associated to g is the mapping $\Psi_g : \mathcal{P}(E) \rightarrow \mathcal{P}(E)$ defined as*

$$\Psi_g(\nu)(dx) := \frac{g(x)\nu(dx)}{\nu(g)}.$$

To implement the softmatch_a operation, we will need a function $G : E \times E \rightarrow \mathbb{R}_+^*$ taking the form $G(x, y) = \exp(a(x, y))$, where a is a similarity function as in Definition 1. We call G an **interaction potential**.

Definition 4 (Softmatch Kernel). *For an interaction potential G , we call the **softmatch kernel** the family of Markov kernels $\{\Psi_G(\nu)\}_{\nu \in \mathcal{P}(E)}$ indexed by $\nu \in \mathcal{P}(E)$, where for $A \in \mathcal{E}$*

$$\Psi_G(\nu)(x, A) = \int_A \Psi_{G(x, \bullet)}(\nu)(dy).$$

To see how Ψ_G can be used to model the softmatch operation, we need to introduce some simple but useful constructions from measure theory. Denote by $\mathcal{P}_\delta(E) := \{\delta_x \mid x \in E\}$ the subset of **Dirac measures** in $\mathcal{P}(E)$. There is a natural bijection between E and $\mathcal{P}_\delta(E)$ defined by $x \leftrightarrow \delta_x$ which will be the primary entry point for measure theory in our model of attention. We can associate to any realization of the structured data $X = \{x_1, \dots, x_T\}$ a measure in $\mathcal{P}(E)$ via the **empirical measure mapping**:

$$X \mapsto m(X) := \frac{1}{|\mathcal{T}|} \sum_{t \in \mathcal{T}} \delta_{x_t}.$$

In what follows, we will often use X and $\{\delta_{x_1}, \dots, \delta_{x_T}\}$ interchangeably to represent the individual vectors and $m(X)$ to represent the joint configuration of X . We will see below that $m(X)$ is a very natural object to represent this joint configuration and to model how it behaves with attention.

Hence consider a “query” representation δ_q and “key” representations $K = \{\delta_{k_1}, \dots, \delta_{k_N}\}$ and the empirical measure $m(K)$. The softmatch kernel models the interaction between q and K using the left-action of the Markov kernels $\Psi_G(m(K))$ on the Dirac measure δ_q induced by integration:

$$\delta_q \Psi_G(m(K)) = \int \delta_q(dq') \Psi_{G(q', \bullet)}(m(K)) = \Psi_{G(q, \bullet)}(m(K)) = \sum_{s=1}^N \frac{G(q, k_s)}{\sum_{r=1}^N G(q, k_r)} \delta_{k_s}.$$

Furthermore, given set of queries $Q = \{\delta_{q_1}, \dots, \delta_{q_M}\}$, we can leverage the linearity of integration to model the interaction between the two sets of representations Q and K using the same principle:

$$\begin{aligned} m(Q) \Psi_G(m(K)) &= \frac{1}{M} \sum_{t=1}^M \int \delta_{q_t}(dq) \Psi_{G(q, \bullet)}(m(K)) \\ &= \frac{1}{M} \sum_{t=1}^M \Psi_{G(q_t, \bullet)}(m(K)) = \frac{1}{M} \sum_{t=1}^M \sum_{s=1}^N \frac{G(q_t, k_s)}{\sum_{r=1}^N G(q_t, k_r)} \delta_{k_s}. \end{aligned}$$

This new measure represents the joint configuration of the set of queries Q *after* they have been allowed to interact with the keys K through the potential G and associated Boltzmann-Gibbs transformation. It is a *weighted sum* of particle measures, and will allow us to model the softmatch from Eq. 1.

Key-Value Relationships. To generalize the relationship between keys and values, we now introduce the lookup kernel.

Definition 5 (Lookup Kernel). *Assume that the key and value spaces are measurable spaces $(\mathcal{K}, \mathbb{K})$ and $(\mathcal{V}, \mathbb{V})$ respectively. A lookup kernel is a Markov kernel, $L : \mathcal{Q} \times \mathbb{V} \rightarrow [0, 1]$, also denoted $L(k, dv)$, that maps keys to distributions on values. When the mapping is a deterministic lookup table, we have $L(k, dv) = \sum_{i=1}^N \mathbb{1}_{\{k=k_i\}} \delta_{v_i}(dv)$.*

Averaging and Moment Projections. The final element of our construction is the averaging w.r.t. the set of values being attended over. To define this operation in our framework, we need to introduce the concept of moments encoded in a measure and a family of measures parameterized by a moment vector.

Definition 6 (Moment Encoding). *Let $F : E \rightarrow E' \subset \mathbb{R}^l$ be a measurable map representing an l -dimensional **feature map**. We say that a measure $\mu \in \mathcal{P}(E)$ **encodes a moment vector** $f \in E'$ with respect to F if $\mu(F) = f$.*

This notion is particularly useful when $E = E'$ and $F(x) = x$ in which case $\delta_x(F_j) = x_j$, so the Dirac measure δ_x encodes the moment vector x . This will allow us to translate notions about vector-space representations to notions about measures and vice versa.

Definition 7 (Moment Subspace of $\mathcal{P}(E)$). *Let $F : E \rightarrow E'$ be a fixed measurable map, and suppose we have identified an injective mapping $f \mapsto \nu_f \in \mathcal{P}(E)$ such that ν_f encodes the moment vector f w.r.t. F . Then we denote by $\mathcal{F}_F = \{\nu_f \mid f \in E'\}$ the **moment subspace** of all such distributions, usually omitting the subscript F when there is no chance of confusion.*

Since we are interested in analyzing finite-dimensional representations in the (uncountable) infinite-dimensional space $\mathcal{P}(E)$, a moment subspace identifies a finite-dimensional parametric family of measures, where our representations can easily be recovered. Two particular cases of moment subspaces are used in the sequel: (1) a natural exponential family with l -dimensional sufficient statistics F , and (2) the set $\mathcal{P}_\delta(E) = \{\delta_x \mid x \in E\}$ of Dirac measures, with $E' = E$ and $F(x) = x$. Finally, we define the **moment projection** onto \mathcal{F} , denoted $\Pi_{\mathcal{F}} : \mathcal{P}(E) \rightarrow \mathcal{F}$, as

$$\Pi_{\mathcal{F}}(\mu) := \nu_{\mu(F)}. \quad (2)$$

$\Pi_{\mathcal{F}}(\mu)$ is the unique measure in \mathcal{F} that encodes the moments $f := \mu(F)$.

Now we claim (to be justified in a moment) that the averaging w.r.t. input values is accomplished by the moment projection $\Pi := \Pi_{\mathcal{F}}$ described in Eq. 2, with $\mathcal{F} = \mathcal{P}_\delta(E)$ and $F(x) = x$.

The Attention Kernel. Putting all of these elements together, we obtain our primary model for attention, the attention kernel.

Definition 8 (Attention Kernel). *The attention kernel \mathbf{A} is the composition of the projection Π , the softmax kernel and the lookup kernel, defined for $x \in E$ and $\mu \in \mathcal{P}(E)$ as:*

$$\mathbf{A}_\mu(x, dz) := \Pi[\Psi_{G(x, \bullet)}(\mu)L](dz) = \Pi \left[\int \Psi_{G(x, \bullet)}(\mu)(dy) L(y, \bullet) \right] (dz).$$

This attention kernel is consistent with attention from Definition 1, for suitable choices of G and L .

Proposition 9. *Let $G(x, y) = \exp(a(x, y))$, $L(k, dv) = \sum_{i=1}^N \mathbb{1}_{\{k=k_i\}} \delta_{v_i}(dv)$, and Q, K, V be as in the definition of attention. Then, using the left action of kernels on measures, the mapping:*

$$(Q, K, V) \mapsto \{\delta_{q_1} \mathbf{A}_{m(K)}, \dots, \delta_{q_T} \mathbf{A}_{m(K)}\}$$

implements attention as in Definition 1.

Proof. Using the remarks from earlier, for $q \in \mathcal{Q}$, we have:

$$[\Psi_{G(q, \bullet)}(m(K))L](dv) = \sum_{j=1}^N \int \frac{G(q, k_j)}{\sum_{p=1}^N G(q, k_p)} \delta_{k_j}(dk) L(k, dv) = \sum_{j=1}^N \frac{G(q, k_j)}{\sum_{p=1}^N G(q, k_p)} \delta_{v_j}(dv).$$

Applying Π thus yields: $\mathbf{A}_{m(K)}(q, dv) = \delta_{\sum_{j=1}^N \frac{G(q, k_j)}{\sum_{p=1}^N G(q, k_p)} v_j}(dv)$. Using the (linear) left-action of this kernel on δ_{q_t} , we then obtain:

$$\delta_{q_t} \mathbf{A}_{m(K)}(dv) = \int \delta_{q_t}(dq) \mathbf{A}_{m(K)}(q, dv) = \delta_{\sum_{j=1}^N \frac{G(q_t, k_j)}{\sum_{p=1}^N G(q_t, k_p)} v_j}(dv).$$

Plugging in the definition of G and using the usual bijection $\delta_x \leftrightarrow x$ concludes the proof. \square

Attention as a System of Interacting Particles. Let us step back and understand the attention kernel \mathbf{A} from a higher level. Consider self-attention: we have effectively factorized the original, linear-algebraic self-attention operation into a series of measure transformations:

$$E \xrightarrow{x \mapsto \delta_x} \mathcal{P}_\delta(E) \xrightarrow{\Psi_{GL}} \mathcal{P}(E) \xrightarrow{\Pi} \mathcal{P}_\delta(E) \xrightarrow{\delta_x \mapsto x} E.$$

More importantly, we have a closed-form expression for the evolution of the joint configuration $m(Q)$ of Q , i.e. $m(Q) \mapsto m(Q) \mathbf{A}_{m(Q)}$. Since interaction with the joint configuration is central to the function of attention, having a framework that describes the evolution of $m(Q)$ will be vital to further analysis.

Moreover, as we noted earlier, self-attention can be composed arbitrarily. Indeed, let $Q^0 := Q$ and consider the evolution of a the set of “particles” $Q^h = \{\delta_{q_1^h}, \dots, \delta_{q_M^h}\}$ for $h = 0, 1, 2, \dots, H-1$ whose dynamics are given by

$$q_i^{h+1} \sim \mathbf{A}_{m(Q^h)}^h(q_i^h, \bullet)$$

or equivalently as a measure-valued flow

$$\delta_{q_i^{h+1}} = \delta_{q_i^h} \mathbf{A}_{m(Q^h)}^h.$$

Our framework shows that self-attention networks, including the Transformer architecture (Vaswani et al., 2017) which is now ubiquitous in natural language processing (see below), are actually simulating deterministic interacting particle systems for a finite number of time steps corresponding to the number of layers H . The representations one obtains are the states of the system after H steps of the dynamics. We use the measure-valued flow interpretation rather than the particle interpretation since it allows us to study the analytical properties of \mathbf{A} to derive insights about attention.

Remark 10. Let us also point out a connection with Bayesian statistics: the case when $G(q, \bullet) = p(q|\bullet)$ is a likelihood function, $\nu \mapsto \Psi_{G(q, \bullet)}(\nu)$ is the mapping which takes a prior distribution $\nu(dk)$ over keys and returns a posterior distribution $P(dk|q)$. Moreover, under a Markov assumption that $v|k, q \sim v|k$, $\Psi_{GL}(q, dv)$ models the conditional probability of $v|q$. Moreover, the moment projection operator effectively reduces this to a measure concentrated on a single point, i.e. $\mathbb{E}[V|q]$, which is consistent with the existing interpretation of attention.

Recovering the Traditional Definition. We have introduced a framework for attention-based models that uses measure theory and Markov kernels as the principal building blocks, and we have shown that it is equivalent (i.e. Proposition 9). It is reasonable to wonder if there is a way to recover the traditional linear-algebraic definition of attention from our framework, and the answer is yes.

Before proceeding, recall three basic facts about Markov kernels and measures on *discrete* spaces:

1. probability measures are stochastic vectors,
2. Markov kernels are stochastic matrices, and

3. integration against these kernels is matrix multiplication.

Suppose now that E is the discrete set $E = \{1, \dots, N\}$ and let $Q = \{q_1, \dots, q_N\}$, $K = \{k_1, \dots, k_N\}$, and $V = \{v_1, \dots, v_N\}$ be subsets of \mathbb{R}^d . Then we set $G : Q \times V \rightarrow \mathbb{R}_{\geq 0}$ to be $G(i, j) := \exp \langle Q[i], K[j] \rangle$, $L : K \times 2^V$ is the (discrete) Markov kernel $L(i, dj) = \delta_i(dj)$ and $\Pi : \mathcal{P}(V) \rightarrow \mathbb{R}^d$ is defined by $\Pi(\mu) := \sum_{j=1}^N V[j] \mu_j =: V'[i]$. Then the analog of the attention kernel is the attention map

$$\mathbf{A}_{m(K)}(i) := \Pi[\Psi_{G(i, \bullet)}(m(K))L].$$

Having now defined discrete analogs of the components of attention defined in this section, we can make the following remarks. Firstly, $\delta_{q_i}(dj)$ is the Kronecker delta δ_i^j and $m(K) = \frac{1}{N} \mathbf{1}$ where $\mathbf{1} := [1, \dots, 1]$ (i.e. N times). Secondly, the Boltzmann-Gibbs Markov kernel $\Psi_{G(i, \bullet)}(dj)$ is then equal to the usual softmax definition:

$$\Psi_{G(i, \bullet)}(m(K))(dj) = \text{softmax}(Q[i]K^T).$$

The softmax kernel is the stochastic matrix $\Psi_G(m(K)) = \text{softmax}(QK^T)$. Thirdly, composition of kernels is matrix multiplication, so $\Psi_G(m(K))L = \text{softmax}(QK^T)Id = \text{softmax}(QK^T)$ since L is the $N \times N$ identity matrix Id . Finally, the attention map corresponds to the matrix multiplications

$$\begin{aligned} \delta_{Q[i]} \mathbf{A}_{m(K)} &= \Pi[\Psi_{G(i, \bullet)}(m(K))L] \\ &= \sum_{j=1}^n \Psi_{G(i, \bullet)}(m(K))(dj) V[j] = \sum_{j=1}^n \text{softmax}(Q[i]K^T)[j] V[j] = \text{softmax}(Q[i]K^T) V. \end{aligned}$$

This is the attention definition from [Bahdanau et al. \(2014\)](#) and is used widely throughout the machine learning community.

It is perhaps reassuring that the constructions we have proposed are not so exotic as they might appear at first glance. However, we feel that using measures on the representation space rather than the index space offers significant gains. The reason for this is that distributions on \mathbb{R}^d are much more expressive than distributions on $\{1, \dots, N\}$, and therefore admit more interesting analysis; see for example our analysis of the regularity of attention in Section 5 relies on the 1-Wasserstein distance, which is trivial in the discrete case.

3.2 Extension to the Transformer

We now sketch how to extend the measure-theoretic model of self-attention described in the previous section to the popular Transformer encoder architecture ([Vaswani et al., 2017](#)). It is a straightforward application of the techniques above. We only describe here how our framework can model a single head Transformer¹, and refer the interested reader to Appendix A for the extension to a full multi-headed transformer. We seek to model

$$\text{Transformer}(X) = \text{FFN} \circ \text{SelfAttention}(X), \quad (3)$$

where $X = \{x_1, \dots, x_N\} \subset \mathbb{R}^d$ is the input data, $\text{SelfAttention}(\bullet)$ is the scaled dot-product attention ([Vaswani et al., 2017](#)) and $\text{FFN}(\bullet)$ represents a feedforward neural network. We set $\tilde{a}(x, y) = x^T y / \sqrt{d}$ and let

$$a(x, y) = \tilde{a}((W^Q)^T x, W^K y), \quad L(k_i, dv) = \delta_{W^V v_i}(dv),$$

where W^Q, W^K, W^V are matrices in $\mathbb{R}^{d' \times d}$. These correspond to the various matrix operations performed by the Transformer. We let $f : E \rightarrow E$ be the FFN in 3 and define the FFN kernel as $\mathbf{F}(x, dy) = \delta_{f(x)}(dy)$. Using the attention kernel A from Definition 8, we define $\mathbf{T} := \mathbf{A}\mathbf{F}$, and show in the proposition below that \mathbf{T} implements the self-attention transformer (see Appendix A for the proof).

Proposition 11. *Let $X = \{x_1, \dots, x_N\} \subset \mathbb{R}^d$ be a collection of inputs. The nonlinear Markov transport equation $\delta_{x_i} \mapsto \delta_{x_i} \mathbf{T}_{m(X)}$ implements the self-attention Transformer.*

¹We only consider the encoder part of the transformer, since it uses self-attention. Our framework is fully compatible with the cross-attention from the transformer decoder ([Vaswani et al., 2017](#)).

4 Structural Analysis of Attention

We have proposed a model of attention that encompasses transformers and is amenable to mathematical analysis. We will now exploit the model using tools from analysis on the space $\mathcal{P}(E)$ to study attention in various contexts. We first seek to understand ways in which Ψ_G and Π implement a feature extractor from a collection of inputs $\mathbf{x} = \{x_1, \dots, x_T\}$ (the deterministic lookup-table implementation of the lookup kernel is not relevant to this analysis, WLOG assume it is the identity).

Background. We will work with the Wasserstein metric on $\mathcal{P}(E)$. Let $\mathcal{P}_1(E)$ be the set of probability measures with finite 1st moment. The **1-Wasserstein distance** between $\mu, \nu \in \mathcal{P}_1(E)$ is

$$W_1(\mu, \nu) := \inf_{\pi \in \mathcal{C}(\mu, \nu)} \iint_{E \times E} \|x - y\|_1 \pi(dx, dy)$$

where $\mathcal{C}(\mu, \nu)$ is the set of distributions on $(E \times E, \mathcal{E} \times \mathcal{E})$ with marginals μ, ν on the first and second components, respectively. W_1 is a metric on $\mathcal{P}_1(E)$ which turns the pair $\mathcal{W}_1 := (\mathcal{P}_1(E), W_1)$ into a complete, separable metric space (Villani, 2008, Ch 6) called the **1-Wasserstein space**. We equip \mathcal{W}_1 with the Borel σ -algebra induced by W_1 .

We will also need the generalized entropy functional: let $\nu \in \mathcal{P}(E)$ and define $H_\nu : \mathcal{P}(E) \rightarrow \mathbb{R} \cup \{\infty\}$ by

$$H_\nu(\mu) := \begin{cases} -\text{KL}(\mu \parallel \nu) & \text{if } \mu \ll \nu \\ \infty & \text{otherwise.} \end{cases}$$

where $\text{KL}(\mu \parallel \nu) := \int \log\left(\frac{d\mu}{d\nu}\right) d\nu$ denotes the Kullback-Leibler divergence. This cost functional on $\mathcal{P}(E)$ generalizes the entropy functional to non-uniform base measures.

Definition 12 (Measure Convolution). *Let $\mu, \nu \in \mathcal{P}(\mathbb{R}^d)$ be measures. Then we define the **measure convolution** of μ and ν , denoted $\mu * \nu$, by*

$$(\mu * \nu)(f) := \int f(x + y) \mu(dx) \nu(dy) \quad \forall f \in \mathcal{B}_b(\mathbb{R}^d)$$

where $\mathcal{B}_b(\mathbb{R}^d)$ denotes the space of bounded, measurable functions from \mathbb{R}^d to \mathbb{R} .

4.1 The Boltzmann-Gibbs Transformation Ψ_G

Recall that a collection of inputs $X = \{\delta_{x_1}, \dots, \delta_{x_N}\}$ has joint configuration $m(X)$, and that the attention kernel \mathbf{A} produces new representations $\delta_{x_i} \mathbf{A}_{m(X)}$ and a new joint configuration $m(X) \mathbf{A}_{m(X)}$ by nonlinear Markov transport². These new measures have encoded in them features about the inputs; our goal is to understand this process.

Recall from Section 2.2 that we say a measure $\mu \in \mathcal{P}(E)$ encodes a feature $f \in E'$ w.r.t. a function $F : E \rightarrow E'$ if $\mu(F) = f$. Self-attention has the ability to extract features that depend on the inputs — this was the original motivation for the attention mechanism in Bahdanau et al. (2014). Therefore we replace the function F from above with a bi-measurable map $k : E \times E \rightarrow E'$ so that for any fixed $x \in E$, μ encodes a feature $f(x) \in E'$ w.r.t. $k(x, \bullet)$, i.e. $\mu(k(x, \bullet)) = f(x)$.

Suppose now that $m(X)$ and x are fixed, and that $\Psi_{G(x, \bullet)}(m(X))$ encodes $f(x)$ w.r.t. $k(x, \bullet)$. Then we will show that the measure $\Psi_{G(x, \bullet)}(m(X))$ is actually optimal among *all* measures $\mu_x \ll m(X)$ which encode $f(x)$ w.r.t. $k(x, \bullet)$ in the maximum entropy sense. This property characterizes the Softmatch kernel.

In this section and the next, we make the assumption below, which will hold unless otherwise stated.

²By nonlinear Markov transport, we mean that the mass of a measure μ is transported by a Markov kernel \mathbf{A} which depends on the measure μ , i.e. $\mu \mapsto \mu \mathbf{A}_\mu$

Assumption 1. $E \subset \mathbb{R}^d$ is a compact, convex set³.

Theorem 13. Let $k : E \times E \rightarrow E'$ be a bi-measurable bounded function, $f : E \rightarrow E'$ a measurable function, and $\nu \in \mathcal{W}_1$ be fixed. Define the set

$$\mathcal{Q}(\nu, x) := \{\mu \in \mathcal{W}_1 \mid \mu \ll \nu, \quad \mu(k(x, \bullet)) = f(x)\}, \quad \forall x \in E.$$

Then for each $x \in E$, there exists a unique maximizer μ_x^* to the maximum entropy problem

$$\max_{\mu_x \in \mathcal{Q}(\nu, x)} H_\nu(\mu_x) \quad (4)$$

given by $\mu_x^* = \Psi_{G(x, \bullet)}(\nu)$ with $G(x, y) = \exp \langle \lambda(x), k(x, y) \rangle$ for some $\lambda(x) \in \mathbb{R}^{d'}$. Furthermore, $x \mapsto \mu_x^*$ is measurable, so $(x, dy) \mapsto \mu_x^*(dy)$ is the Markov kernel $(x, dy) \mapsto \Psi_{G(x, \bullet)}(\nu)(dy)$.

Proof Sketch. See Appendix B for the full proof. Existence and uniqueness of μ_x^* are classical results. To ensure that μ_x^* coincides with the Markov kernel $\Psi_{G(x, \bullet)}(\nu)$ we use the additional result that $x \mapsto \mu_x^*$ is measurable which is a technical measurable selection theorem in the appendix. \square

The maxent property is not particularly surprising, given the well-known properties of the softmax and maximum entropy, but it is not *a priori* clear that the dependence of such a measure on x should possess any good properties. We show that the pointwise maximum entropy measure depends measurably on x if k, f are measurable, so the former is indeed the the softmatch kernel⁴.

Remark 14. The minimization problem (4) is an instance of the “information projection” operator (Koller and Friedman, 2009). Below, we see how it relates to the dual notion of moment projection.

4.2 The Moment Projection Π

Without the moment projection Π in the definition of the attention kernel \mathbf{A} , successive applications of \mathbf{A} would result in a measure of arbitrary complexity. On the other hand, we work with finite-dimensional representations, so using the entire space $\mathcal{P}(E)$ is simply too large to be practical. Therefore, we view $\Pi_{\mathcal{F}} : \mathcal{P}(E) \rightarrow \mathcal{F}$ as a crucial element of attention which ensures that the output measure remains on a finite-dimensional subspace of $\mathcal{P}(E)$ while preserving moments.

We study two choices of (\mathcal{F}, F) . The first is when \mathcal{F} is an exponential family on E with sufficient statistics F and base measure λ , $\mathcal{F} := \left\{ \nu_\theta(dx) = e^{\langle \theta, F(x) \rangle - A(\theta)} \lambda(dx) \mid \theta \in \mathbb{R}^{d'} \right\}$ and the second is $\mathcal{F} = \mathcal{P}_\delta(E)$ with $F(x) = x$. Our main result in this section is a connection between the “synthetic” definition of Π with an “analytic” description as a minimization problem.

Proposition 15. Let $E \subseteq \mathbb{R}^d$ and \mathcal{F} be a natural exponential family with sufficient statistics $F : E \rightarrow E' \subseteq \mathbb{R}^{d'}$ and base measure λ supported on E as above. Suppose that, for $\mu \in \mathcal{P}(E)$, $\mu \sim \nu$, $\forall \nu \in \mathcal{F}$. Then $\Pi : \mathcal{P}(E) \rightarrow \mathcal{F}$ satisfies the projection-like equation

$$\Pi(\mu) = \arg \min_{\nu \in \mathcal{F}} \text{KL}(\mu \parallel \nu).$$

See Appendix B for the proof, which is standard. Extending the result to the case of $\mathcal{F} = \mathcal{P}_\delta(E)$ and $F(x) = x$ requires different arguments because $\mu \not\ll \nu$ in general. Intuitively, we can think of $\mathcal{P}_\delta(E)$ as the limit of exponential family $\mathcal{F}_\sigma := \{\mathcal{N}(dx, \sigma) \mid x \in E\}$ as $\sigma \rightarrow 0$. Our approach leverages properties of F and convolution with $\mathcal{N}(dx, \sigma)$ to regularize \mathcal{F} and Π while preserving the encoded moments, then take a limit as $\sigma \rightarrow 0$.

³Convexity is assumed only to guarantee that the moment-projection onto $\mathcal{P}_\delta(E)$ is well-defined.

⁴This is actually a stronger result — to be a Markov kernel, we need $x \mapsto \mu_x^*(A)$ to be measurable for each $A \in \mathcal{E}$, but we have actually shown that $x \mapsto \mu_x^*$ as a mapping from $E \rightarrow \mathcal{P}(E)$ is measurable.

Proposition 16. Let $\mu \in \mathcal{W}_1$, and $F(x) = x$. Setting $\mathcal{F}_n := \{\rho_n * \delta_x \mid \delta_x \in \mathcal{P}_\delta(E)\} (= \{\mathcal{N}(x, \sigma_n I), x \in E\})$, where $\rho_n := \mathcal{N}(0, \sigma_n I)$ with $\sigma_n \rightarrow 0$, then in the 1-Wasserstein topology:

$$\Pi_{\mathcal{F}}(\mu) = \lim_{n \rightarrow \infty} \arg \min_{\nu \in \mathcal{F}_n} \text{KL}(\rho_n * \mu \parallel \nu).$$

Sketch. The idea of the proof is to regularize both μ and \mathcal{F} by convolution with a sequence of Gaussians ρ_n , thereby ensuring that $\rho_n * \mu$ and $\nu \in \mathcal{F}_n$ have the same supports without affecting the encoded moments. Theorem 15 then applies, and we show that the sequence of regularized minimizers tends to $\Pi_{\mathcal{F}}(\mu)$. \square

Remark 17. On a practical note, the choice of \mathcal{F} can greatly affect how efficient Π is to compute. When $\mathcal{F} = \mathcal{P}_\delta(E)$ and $F(x) = x$, then this reduces to linear algebra operations since elements of $\mathcal{P}_\delta(E)$ (and mixtures thereof) have easy closed-form moments. On the other hand, if \mathcal{F} is an arbitrary exponential family, e.g. Gaussians with $F(x) = [x \parallel x^2]$, then a closed form solution to $\mu(F)$ or $\Psi_G(\mu)$ may not exist, so one is reduced to computing the projection and/or the normalizing constant via approximation.

4.3 Interaction Between the Components

We have seen how the transformation Ψ_G extracts a set of features determined by G and encodes them as moments into $\mu = \Psi_G(\nu)$ in a maximum-entropy transformation. The cost to pay for this encoding is an expansion of the degrees of freedom of the measure, i.e. μ no longer lives in the finite-dimensional moment subspace \mathcal{F}_F . On the other hand, the projection Π “squeezes” the measure μ through a bottleneck, reducing the degrees of freedom to those determined by \mathcal{F}_F . This is accomplished via the moment projection, and can be seen as discarding extra information in the system while preserving a set of moments determined by F .

5 Regularity of Attention

In this section, we consider self-attention as a non-linear map from $\mathcal{P}(E)$ to $\mathcal{P}(E)$ through $\mathbf{A} : \mu \rightarrow \mu \mathbf{A}_\mu$, and derive a contraction estimate for this map on the metric space $(\mathcal{P}_1(E), \mathbb{W}_1)$ via an inequality of the form:

$$\sup_{\mu \neq \nu} \mathbb{W}_1(\mu \mathbf{A}_\mu, \nu \mathbf{A}_\nu) \leq \tau(\mathbf{A}) \mathbb{W}_1(\mu, \nu)$$

for some constant $\tau(\mathbf{A})$ to be determined. These estimates naturally lead to sufficient conditions on G, L relative to E which guarantee the stability of self-attention networks. Recall that Assumption 1 is in effect.

Our approach is to estimate contraction coefficients for Ψ_G, L, Π separately and then combine them. We will need the following notions: for a real-valued function f , $\|f\|_{Lip}$ is the Lipschitz semi-norm $\|f\|_{Lip} := \sup_{x \neq y} |f(x) - f(y)|/d(x, y)$. For a function G of two variables, $G : E \times E \rightarrow \mathbb{R}$, we let $\|G\|_{Lip, \infty} := \sup_{x \in E} \|G(\bullet, x)\|_{Lip}$ and $\|G\|_{\infty, Lip} := \sup_{x \in E} \|G(x, \bullet)\|_{Lip}$.

We now prove contraction estimates on the various components of attention. Their proofs can be found in Appendix C, they mainly rely on the Kantorovich dual formulation of \mathbb{W}_1 .

Proposition 18. Suppose $\mu, \nu \in \mathcal{P}_1(E)$ and $G : E \times E \rightarrow \mathbb{R}$, $G(x, y) \geq \epsilon(G) > 0$ is an interaction potential s.t. $\|G\|_{\infty, Lip} < \infty$ and $\|G\|_{Lip, \infty} < \infty$. Then, $\forall x, y \in E$:

$$\begin{aligned} \mathbb{W}_1(\Psi_{G(x, \bullet)}(\mu), \Psi_{G(y, \bullet)}(\mu)) &\leq 2 \frac{\|G\|_{Lip, \infty} \text{diam}(E)}{\epsilon(G)} \cdot d(x, y), \\ \mathbb{W}_1(\Psi_{G(x, \bullet)}(\mu), \Psi_{G(x, \bullet)}(\nu)) &\leq \frac{2\|G\|_{\infty, Lip} \text{diam}(E)}{\epsilon(G)} \cdot \mathbb{W}_1(\mu, \nu). \end{aligned}$$

Proposition 19. Suppose that $F(x) = x$, $\mathcal{F} = \mathcal{P}_\delta(E)$, and $\Pi := \Pi_{\mathcal{F}}$ is the moment projection onto \mathcal{F} . Then, for $\mu, \nu \in \mathcal{P}_1(E)$, $\mathbb{W}_1(\Pi(\mu), \Pi(\nu)) \leq d \cdot \mathbb{W}_1(\mu, \nu)$.

Proposition 20. Suppose $L : E \times \mathcal{E} \rightarrow [0, 1]$ is a lookup kernel implementing a deterministic lookup function $\ell : E \rightarrow E$, (i.e. $L(x, dy) = \delta_{\ell(x)}(dy)$) and suppose that ℓ is K_ℓ -Lipschitz in the 1-norm, then $W_1(\mu L, \gamma L) \leq K_\ell W_1(\mu, \gamma)$.

Combining the propositions allows to bound the Wasserstein contraction coefficient of the attention kernel \mathbf{A} , defined as:

Definition 21 (Wasserstein Contraction Coefficient). Let $\Phi : \mathcal{P}_1(E) \rightarrow \mathcal{P}_1(E)$ be a (possibly nonlinear) mapping. We define the **Wasserstein contraction coefficient** by

$$\tau(\Phi) := \sup_{\mu \neq \nu} \frac{W_1(\Phi(\mu), \Phi(\nu))}{W_1(\mu, \nu)}.$$

Theorem 22. Let $E \subset \mathbb{R}^d$ be compact, $\mathcal{F} = \mathcal{P}_\delta(E)$, and $\Pi := \Pi_{\mathcal{F}}$. Let \mathbf{A} be the attention kernel from definition 8, with $L(x, dy) = \delta_{\ell(x)}(dy)$. Let G be an interaction potential such that $G(x, y) \geq \epsilon(G) > 0$, $\|G\|_{Lip, \infty} < \infty$ and $\|G\|_{\infty, Lip} < \infty$. Then, with $\tau(\mathbf{A})$ the 1-Wasserstein contraction coefficient of \mathbf{A} considered as a mapping on $\mathcal{P}(E)$ through $\mathbf{A} : \mu \rightarrow \mu \mathbf{A}_\mu$, we have:

$$\tau(\mathbf{A}) \leq \tau(\Pi) \tau(\Psi_G) \tau(L)$$

where $\tau(\Pi) = d$, $\tau(\Psi_G) = \frac{2(\|G\|_{Lip, \infty} + \|G\|_{\infty, Lip}) \text{diam}(E)}{\epsilon(G)}$ and $\tau(L) = K_\ell$.

Proof. See Appendix C. □

Corollary 23. Let $K = \{k_1, \dots, k_N\} \subset E \subset \mathbb{R}^d$ and $V = \{v_1, \dots, v_n\} \subset E \subset \mathbb{R}^d$ and the attention function $\text{Attention}(\bullet, K, V)$ be as in the original definition of attention from Bahdanau et al. (2014), Definition 1. Assume that the components of $\text{Attention}(\bullet, K, V)$ satisfy Theorem 22. Then the mapping

$$q \mapsto \text{Attention}(q, K, V)$$

is Lipschitz continuous as a mapping from $\mathbb{R}^d \rightarrow \mathbb{R}^d$ with the Euclidean distance, and moreover

$$\|\text{Attention}(q_1, K, V) - \text{Attention}(q_2, K, V)\|_2 \leq d^{3/2} \cdot \|\ell\|_{Lip} \cdot \frac{2\|G\|_{Lip, \infty} \text{diam}(E)}{\epsilon(G)} \cdot \|q_1 - q_2\|_2$$

Proof. Using proof from Theorem 22 in Appendix C we have

$$\begin{aligned} \|\text{Attention}(q_1, K, V) - \text{Attention}(q_2, K, V)\|_2 &\leq \|\text{Attention}(q_1, K, V) - \text{Attention}(q_2, K, V)\|_1 \\ &= W_1(\delta_{q_1} \mathbf{A}_{m(K)}, \delta_{q_2} \mathbf{A}_{m(K)}) \\ &\leq d \cdot \|\ell\|_{Lip} \cdot \frac{2\|G\|_{Lip, \infty} \text{diam}(E)}{\epsilon(G)} \cdot W_1(\delta_{q_1}, \delta_{q_2}) \\ &= d \cdot \|\ell\|_{Lip} \cdot \frac{2\|G\|_{Lip, \infty} \text{diam}(E)}{\epsilon(G)} \cdot \|q_1 - q_2\|_1 \\ &= d^{3/2} \cdot \|\ell\|_{Lip} \cdot \frac{2\|G\|_{Lip, \infty} \text{diam}(E)}{\epsilon(G)} \cdot \|q_1 - q_2\|_2 \end{aligned}$$

using $\|x\|_2 \leq \|x\|_1 \leq \sqrt{d}\|x\|_2$ for norms on \mathbb{R}^d . □

The reader should note that the dependence of the above estimate on the geometry of V w.r.t. K is contained in the Lipschitz constant $\|\ell\|_{Lip}$.

6 Applications

In this section, we provide insights into existing applications of self-attention that one can gain using the analysis developed above.

6.1 Attention is Continuous in the Input Data

Let $X = \{x_t\}_{t \in \mathcal{T}}$ be a set of structured data. In many cases, such as graphs, there is a neighbourhood structure $\mathcal{N} : \mathcal{T} \rightarrow 2^{\mathcal{T}}$ which effectively determines the statistical dependence of elements of different elements by $P(x_t|X_{-t}) = P(x_t|X_{\mathcal{N}(t)})$. Modelling X amounts to picking a family of distributions Q_θ and a neighbourhood structure $\hat{\mathcal{N}}$ to approximate $P(x_t|X_{-t}) \approx Q_\theta(x_t|X_{\hat{\mathcal{N}}(t)})$. Often, e.g. when X represents a graph or an image, the choice of $\hat{\mathcal{N}}$ is not obvious so a modelling decision needs to be made, sometimes to include only elements inside a ball around t (if \mathcal{T} has a metric structure), or to randomly sample elements from \mathcal{T} .

Our framework provides techniques for understanding how this modelling decision impacts self-attention based models. In particular, the following results characterizes how modelling errors of the form $\hat{\mathcal{N}}(t) \neq \mathcal{N}(t)$ propagate through a self-attention network — the output representations cannot be arbitrarily far from the “true representations”.

Proposition 24. *Suppose $X = \{x_t\}_{t \in \mathcal{T}}$ is a set of structure data and let $t \in \mathcal{T}$. Suppose $\mathcal{N}(t), \hat{\mathcal{N}}(t) \subset \mathcal{T}$ are two neighbourhoods that both contain t . Denote by $X_{\mathcal{N}(t)} := \{x_t\}_{t \in \mathcal{N}(t)}$ and similarly for $X_{\hat{\mathcal{N}}(t)}$. Lastly, assume that the assumptions of Theorem 22 hold. Then*

$$\begin{aligned} & \|\text{Attention}(x_t, X_{\mathcal{N}(t)}, X_{\mathcal{N}(t)}) - \text{Attention}(x_t, X_{\hat{\mathcal{N}}(t)}, X_{\hat{\mathcal{N}}(t)})\| \\ & \leq d \cdot \tau_1(L) \frac{2\|G(x_t, \bullet)\|_{Lip} \text{diam}(E)}{\varepsilon(G)} \cdot W_1(m(X_{\mathcal{N}(t)}), m(X_{\hat{\mathcal{N}}(t)})) \end{aligned}$$

Proof. We can adapt an argument from the proof of Theorem 22. Firstly, for simplicity write $\mu_t := m(X_{\mathcal{N}(t)})$, $\hat{\mu}_t := m(X_{\hat{\mathcal{N}}(t)})$ and note that

$$\|\text{Attention}(x_t, X_{\mathcal{N}(t)}, X_{\mathcal{N}(t)}) - \text{Attention}(x_t, X_{\hat{\mathcal{N}}(t)}, X_{\hat{\mathcal{N}}(t)})\| = W_1(\delta_{x_t} \mathbf{A}_{\mu_t}, \delta_{x_t} \mathbf{A}_{\hat{\mu}_t}).$$

Then

$$\begin{aligned} W_1(\delta_{x_t} \mathbf{A}_{\mu_t}, \delta_{x_t} \mathbf{A}_{\hat{\mu}_t}) &= W_1(\delta_{x_t} \Pi[\Psi_{G(\bullet, \bullet)}(\mu_t)L], \delta_{x_t} \Pi[\Psi_{G(\bullet, \bullet)}(\hat{\mu}_t)L]) \\ &= W_1(\Pi[\Psi_{G(x_t, \bullet)}(\mu_t)L], \Pi[\Psi_{G(x_t, \bullet)}(\hat{\mu}_t)L]) \\ &\leq \tau_1(\Pi) \tau_1(L) W_1(\Psi_{G(x_t, \bullet)}(\mu_t), \Psi_{G(x_t, \bullet)}(\hat{\mu}_t)) \\ &\leq \tau_1(\Pi) \tau_1(L) \frac{2\|G(x_t, \bullet)\|_{Lip} \text{diam}(E)}{\varepsilon(G)} W_1(\mu_t, \hat{\mu}_t) \\ &= d \cdot \tau_1(L) \frac{2\|G(x_t, \bullet)\|_{Lip} \text{diam}(E)}{\varepsilon(G)} W_1(\mu_t, \hat{\mu}_t). \quad \square \end{aligned}$$

Let us make a few remarks on this result. Firstly, it is automatically *permutation invariant*, w.r.t. the input data $X_{\mathcal{N}(t)}$. This property is a consequence of the choice to use measure theory and represent the input data using a measure. In the case that $|\mathcal{N}(t)| = |\hat{\mathcal{N}}(t)| = m$, we can obtain an explicit formula for $W_1(\mu, \hat{\mu})$ (see e.g. [Bobkov and Ledoux \(2014\)](#) Lemma 4.2)

$$W_1(\mu, \hat{\mu}) = \inf_{\sigma \in \Sigma(m)} \frac{1}{m} \sum_{i=1}^m \|x_s - y_{\sigma(s)}\|_1$$

where $x_s \in X_{\mathcal{N}(t)}$, $y_s \in X_{\hat{\mathcal{N}}(t)}$ and $\Sigma(m)$ is the set of permutations on m elements.

6.2 Infinitely Deep Transformers

Using our framework, we can also investigate some properties of infinitely-deep transformers. Indeed, the work by [Dehghani et al. \(2018\)](#) describes the “Universal Transformer” which processes a collection of inputs using self-attention in a recurrently-connected model. This model can be thought of as an infinitely-deep self-attention transformer with weight sharing between the layers, and our quantitative

contraction estimates from Section 5 provide an opportunity to study the Universal Transformer’s behaviour as the number of processing steps (i.e. layers) tends to ∞ . In particular, one can consider the model

$$X^{\ell+1} = \text{Transformer}(X^\ell), \quad X = \{x_1, \dots, x_N\} \subset \mathbb{R}^d$$

where $\text{Transformer}(\bullet)$ is defined in Appendix A. One natural question is: does there exist a limit to this recurrence? This amounts to having a fixed-point for the transformer mapping.

Proposition 25. *Let $\tau(\mathbf{T})$ be the contraction coefficient for the self-attention Transformer. Then if $\tau(\mathbf{T}) < 1$, there exists a unique fixed point to the Universal Transformer recurrence.*

Proof. This is a straightforward application of the Banach fixed point theorem. One can calculate the exact requirements on the constituents of the nonlinear Markov kernel \mathbf{T} in the same way as Theorem 22. \square

Remark 26. *We should note that the result from Proposition 25 is quite strong — the fixed point we describe is the same for all input data X . It is not clear what properties this fixed point might have, and whether they are interesting, but we provide this result as a possible line of future work.*

6.3 Lipschitz Constants for $E = \mathbb{R}^d$

The results of Section 5 depend on the boundedness of the representation space E . While this enables us to provide rather general estimates on the Lipschitz coefficient for attention that are verified by most reasonable choices of G, L , it is reasonable to question how realistic this assumption is, and whether it can be relaxed.

In concurrent work by Kim et al. (2020), the authors investigate Lipschitz constants for self-attention on $X = \{x_1, \dots, x_N\}$ as a mapping from $\mathbb{R}^{d \times N} \rightarrow \mathbb{R}^{d \times N}$ without assuming E is bounded. The authors show that, for the case of $G(x, y) = \exp \langle x, y \rangle$ on the whole of \mathbb{R}^d , attention is not Lipschitz by showing the norm of Jacobian is unbounded (Kim et al. (2020) Theorem 3.1). The authors characterize this failure (adapted to our notation) as being due to the unbounded variance of $m(X)\Psi_G(m(X))$. Moreover, they show that using (a variation of) $G(x, y) = \exp(-\|x - y\|_2^2)$ as an interaction potential leads to a uniform Lipschitz bound (Kim et al. (2020) Theorem 3.2). The authors provide empirical evidence that this potential function does not severely degrade performance.

As further evidence of the strength of our framework, we provide below an analysis of the same basic Gaussian interaction potential $G(x, y) = \exp(-\|x - y\|_2^2)$ as in Kim et al. (2020)⁵ for unbounded $E = \mathbb{R}^d$. We are able to use the same basic tools (1-Wasserstein contractions, estimation techniques from analysis, etc) and a similar approach to Section 5 but exchanging boundedness assumptions on E for exponential decay of $G(x, y)$ and $\|\nabla G(x, y)\|$ as $\|x - y\|_2 \rightarrow \infty$. The proofs can be found in Appendix D.

Proposition 27. *Let $E = \mathbb{R}^d$ and suppose $X = \{x_1, \dots, x_N\}$ and $Y = \{y_1, \dots, y_N\}$. Let $\mu = m(X)$, $\nu = m(Y)$. Then for $x \in \text{supp}(\mu)$ and $y \in \text{supp}(\nu)$, we have*

$$W_1(\Psi_{G(x, \bullet)}(\mu), \Psi_{G(y, \bullet)}(\nu)) \leq \left[\sqrt{d} \sqrt{\ln N + \frac{1}{2e}} \|G\|_{Lip} + \|G\|_\infty + \sqrt{d} + 2 \right] (d(x, y) + W_1(\mu, \nu)).$$

Theorem 28. *Let $E = \mathbb{R}^d$ and suppose $X = \{x_1, \dots, x_N\}$ and $Y = \{y_1, \dots, y_M\}$. Let $G(x, y) = \exp(-\|x - y\|_2^2)$, $L(x, dy) = \delta_{l(x)}(dy)$, and Π be the usual projection onto \mathcal{F}_δ . Then for $\mu = m(X)$ and $\nu = m(Y)$,*

$$W_1(\mu \mathbf{A}_\mu, \nu \mathbf{A}_\nu) \leq 2\tau(\Pi)\tau(L) \left[\sqrt{d} \sqrt{\ln(\min(N, M)) + \frac{1}{2e}} \|G\|_{Lip} + \|G\|_\infty + \sqrt{d} + 2 \right] W_1(\mu, \nu).$$

⁵We chose the un-parameterized potential for simplicity, we see no reason our framework would not extend to the parameterized case as well.

Theorem 28 provides an alternate path to the Lipschitz constant of self-attention compared to methods based on computing Jacobians (Kim et al., 2020). In particular, it applies to sequences of tokens of various lengths and allows to study the effect of perturbing a sequence by e.g. removing a given word, or negating a sentence, which is out of immediate reach for Jacobian-based techniques. Finally, we can recover a bound for sequences of equal lengths:

Corollary 29. *Applying Theorem 28 to the case of $N = M$ gives:*

$$\mathbb{W}_1(\mu \mathbf{A}_\mu, \nu \mathbf{A}_\nu) \leq 2\tau(\Pi)\tau(L) \left[\sqrt{d} \sqrt{\ln N + \frac{1}{2e}} \|G\|_{Lip} + \|G\|_\infty + \sqrt{d} + 2 \right] \mathbb{W}_1(\mu, \nu).$$

Our bound appears to have a better dependence on $N := |X|$ (although perhaps at a worse dependence on d) than in Kim et al. (2020); ours is $\mathcal{O}(\sqrt{\ln N})$ and theirs is at best $\mathcal{O}(\ln(N))$.

Negated Sentences. Our regularity results provide theoretical grounding to recent observations about deep language models (e.g. Table 4 of Kassner and Schtze (2019)), where negated sentences are shown to give identical predictions to the original ones: for instance, both “A beagle is a type of [MASK]” and “A beagle is not a type of [MASK]” get a prediction of “dog”. Similarly, “Birds can [MASK]” and “Birds cannot [MASK]” returns “talk” with high probability.

7 Related Work

Given the somewhat unorthodox approach to studying attention taken in this paper, we will briefly overview two very different areas that are related to this work: attention models (with an emphasis on variety of domains where attention is used) and self-interacting measure-valued equations.

We first highlight some important successes of attention-based models across domains of machine learning. As noted by Smola and Zhang (2019), the original notion of attention appears in statistics in the form of the Watson-Nadaraya estimator (Watson, 1964; Nadaraya, 1964) which implements a data-dependent regression model. The term “attention” and the modern “query-key-value” formulation comes from Bahdanau et al. (2014) who use attention for sequence alignment in a recurrent neural translation model. A similar setup was used in Graves et al. (2014) for differentiable, content-based addressing of a memory array. In Sukhbaatar et al. (2015) and Seo et al. (2016), attention is used for question answering, machine reading comprehension, and language modelling. The extremely successful “Transformer” architecture was introduced in Vaswani et al. (2017) and demonstrated that one could build powerful neural networks using attention as the main component. This led to important developments in language modelling (Devlin et al., 2018; Radford et al., 2018), graph modelling (Velićković et al., 2017), image modelling (Parmar et al., 2018), and set modelling (Lee et al., 2018). Recently, Baker et al. (2019) used attention in the policy architecture of a multi-agent reinforcement learning problem.

Concurrent to our work, there has been a very recent flurry of activity in the study of the properties of attention-based networks from an empirical and theoretical perspective. As discussed in Section 6, Kim et al. (2020) studies the Lipschitz constant of self-attention as a map from $\mathbb{R}^{d \times N} \rightarrow \mathbb{R}^{d \times N}$. In Katharopoulos et al. (2020), the authors show that transformers with causal masks in the attention inputs can be written as a recurrent computation, linking this application with RNNs. In Bhattamishra et al. (2020), the authors study the computational power of Transformers as measured by Turing completeness. In Hron et al. (2020), the authors study the behaviour of attention-based networks as the number of heads tends to infinity and show that the self-attention architecture behaves as a Gaussian process in the limit. Finally, in Levine et al. (2020), the authors study a reduced form of deep self-attention networks to understand the interplay between depth and width.

The theory of self-interacting Markov chains and the associated measure-valued processes was developed extensively in Del Moral (2004), who studied so-called “Feynman-Kac models” using semi-group techniques. These systems model a wide array of self-interacting phenomena such as genetic

algorithms, nonlinear filtering equations, self-avoiding random walks, self-interacting particle systems, etc. (Del Moral, 2004). Such interacting particle systems have also appeared in the Markov Chain Monte Carlo literature (Andrieu et al., 2007) and the mean-field game literature (Huang et al., 2006; Lasry and Lions, 2006).

8 Conclusion

In summary, we have presented a model of attention using measure theory which is mathematically equivalent to the original formulation of attention from Bahdanau et al. (2014) and fully compatible with the self-attention Transformer from Vaswani et al. (2017). Moreover, this framework is flexible enough to model all of the input modalities where attention is used, from graphs to sentences.

In exchange for the increased complexity of working with measures, we are able to connect self-attention to a maximum entropy problem and prove that, in a maximum-entropy sense, self-attention is an optimal feature extraction model. We also derive contraction estimates for self-attention in the 1-Wasserstein distance. We then apply these insights to study three practical problems from attention-based neural networks, namely continuity w.r.t. input data, infinitely-deep transformers, and Lipschitz estimates when $E = \mathbb{R}^d$ for a particular choice of interaction potential.

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A The Transformer

We now show how to extend the measure-theoretic model of self-attention described in the main text to the full Transformer encoder architecture (Vaswani et al., 2017)⁶. This is a straightforward application of the techniques from the main text. For our purpose, we work with the model

$$\text{Transformer}(X) = \text{FFN} \circ \text{MultiHeadSelfAttention}(X) \quad (5)$$

where $X = \{x_1, \dots, x_N\} \subset \mathbb{R}^d$ and FFN represents a feedforward neural network. To incorporate this into our formalism above, first set $\tilde{a}(x, y) = x^T y / \sqrt{d}$. We can model a single head of the Transformer using the attention kernel from Definition 8 with:

$$a(x, y) = \tilde{a}((W^Q)^T x, W^K y), \quad L(k_i, dv) = \delta_{W^V v_i}(dv).$$

where W^Q, W^K, W^V are matrices in $\mathbb{R}^{d' \times d}$. To model multi-headed attention, we note that multi-headedness amounts to processing independent copies of the data X and combining them with concatenation and matrix multiplication. The “concat-and-matmult” operation can be written as

$$\begin{bmatrix} x_i^1 & \cdots & x_i^H \end{bmatrix} \begin{bmatrix} W_1^O \\ \vdots \\ W_H^O \end{bmatrix} = x_i^1 W_1^O + \cdots + x_i^H W_H^O$$

where each $W_h^O \in \mathbb{R}^{d' \times d}$. Hence, letting $\mathbf{O}^h(x, dy) := \delta_{x W_h^O \cdot H}(dy)$, where we have multiplied by the scalar H , and introducing the mixture kernel

$$\widehat{\mathbf{M}} := \frac{1}{H} \sum_{h=1}^H \mathbf{A}^h \mathbf{O}^h$$

where each h parameterizes its own collection of projection matrices, we can define the multi-headed attention kernel as

$$\mathbf{M} := \Pi \circ \widehat{\mathbf{M}}, \quad \mathbf{M}_\mu(x, dy) = \Pi(\widehat{\mathbf{M}}_\mu(x, \bullet))(dy).$$

Finally, letting $f : E \rightarrow E$ be the FFN in 5 and defining the FFN kernel as $\mathbf{F}(x, dy) = \delta_{f(x)}(dy)$, we see that $\mathbf{T} := \mathbf{M}\mathbf{F}$ implements the self-attention transformer as nonlinear measure transport.

Proposition 11. *Let $X = \{x_1, \dots, x_N\} \subset \mathbb{R}^d$ be a collection of inputs. The nonlinear Markov transport equation $\delta_{x_i} \mapsto \delta_{x_i} \mathbf{T}_{m(X)}$ implements the self-attention Transformer.*

Proof. Given the discussion about standard attention, the only new element to be checked is the multi-headed attention kernel. Consider a fixed X , then

$$m(X) \mathbf{M}_{m(X)}(dy) = \frac{1}{N} \sum_{i=1}^N \int \delta_{x_i} \mathbf{M}_{m(X)}(x, dy) = \frac{1}{N} \sum_{i=1}^N \mathbf{M}_{m(X)}(x_i, dy)$$

Hence considering a single x_i , we see that

$$\mathbf{M}_{m(X)}(x_i, dy) = \Pi \left(\widehat{\mathbf{M}}_{m(X)}(x_i, \bullet) \right) (dy).$$

The inner kernel is

$$\widehat{\mathbf{M}}_{m(X)}(x_i, dy) = \frac{1}{H} \sum_{h=1}^H \int \mathbf{A}_{m(X)}^h(x_i, dz) \mathbf{O}^h(z, dy) = \frac{1}{H} \sum_{h=1}^H \int \mathbf{A}_{m(X)}^h(x_i, dz) \delta_{z W_h^O \cdot H}(dy).$$

⁶Technically, the Transformer also contains layer normalization and residual connections, which we do not treat here.

The measure $\mathbf{A}_{m(X)}^h(x_i, dz)$ is a delta-measure concentrated on the point

$$\sum_{j=1}^N \frac{\exp[\tilde{a}((W_h^Q)^T x_i, W_h^K x_j)]}{\sum_{p=1}^N \exp[\tilde{a}((W_h^Q)^T x_i, W_h^K x_p)]} W_h^V x_j = \text{MultiHeadSelfAttention}(x_i, X, X)_h =: y_i^h$$

hence

$$\frac{1}{H} \sum_{h=1}^H \int \mathbf{A}_{m(X)}^h(x_i, dz) \delta_{z W_h^O \cdot H}(\mathrm{d}y) = \frac{1}{H} \sum_{h=1}^H \int \delta_{y_i^h}(\mathrm{d}z) \delta_{z W_h^O \cdot H}(\mathrm{d}y) = \frac{1}{H} \sum_{h=1}^H \delta_{y_i^h W_h^O \cdot H}(\mathrm{d}y).$$

Finally, applying the mapping Π we get a measure that is concentrated on the point

$$\begin{aligned} \int_E \frac{1}{H} \sum_{h=1}^H \delta_{y_i^h W_h^O \cdot H}(\mathrm{d}y) y &= \frac{1}{H} \sum_{h=1}^H y_i^h W_h^O \cdot H = [y_i^1 \quad \cdots \quad y_i^H] \begin{bmatrix} W_1^O \\ \vdots \\ W_H^O \end{bmatrix} \\ &= \text{MultiHeadSelfAttention}(x_i, X, X), \end{aligned}$$

which concludes the proof. \square

B Proofs From Section 4

Lemma 30. *Let $\nu \in \mathcal{P}(E)$ be fixed, where $E \subset \mathbb{R}^d$ is compact. The mapping $\Psi_\bullet(\nu) : L^1(\nu) \rightarrow (\mathcal{P}_1(E), W_1)$ is continuous.*

Proof. Suppose $\{F_n\} \subset L^1(\nu)$ converges to $G \in L^1(\nu)$, and let $f \in Lip(1)$. Then

$$\begin{aligned} |\Psi_G(\nu)(f) - \Psi_{F_n}(\nu)(f)| &= \left| \frac{\int f(x) G(x) \nu(\mathrm{d}x)}{\nu(G)} - \frac{\int f(x) F_n(x) \nu(\mathrm{d}x)}{\nu(F_n)} \right| \\ &= \left| \int \left[\frac{G(x)}{\nu(G)} - \frac{F_n(x)}{\nu(F_n)} \right] f(x) \nu(\mathrm{d}x) \right| \\ &\leq \left\| \frac{G}{\nu(G)} - \frac{F_n}{\nu(F_n)} \right\|_{L^1(\nu)} \|f\|_\infty \\ &\leq \left\| \frac{G}{\nu(G)} - \frac{F_n}{\nu(F_n)} \right\|_{L^1(\nu)} \text{diam}(E). \end{aligned}$$

In the last line, we used the fact that $\Psi_G(\nu)(\bar{f}) = \Psi_{F_n}(\nu)(\bar{f})$ for any constant function \bar{f} . This allows us to subtract from f any constant without changing the value of $|\Psi_G(\nu)(f) - \Psi_{F_n}(\nu)(f)|$. Hence, we can assume without loss of generality that $\|f\|_\infty \leq \text{diam}(E)$ (picking an arbitrary $x \in E$, we have $\forall y \in E, |f(y) - f(x)| \leq |y - x| \|f\|_{Lip} \leq \text{diam}(E)$). Taking the supremum over f gives us $W_1(\Psi_G(\nu), \Psi_{F_n}(\nu)) \leq \left\| \frac{G}{\nu(G)} - \frac{F_n}{\nu(F_n)} \right\|_{L^1(\nu)}$. Letting $n \rightarrow \infty$ concludes the proof. \square

Lemma 31 (Himmelberg et al. (1976), Theorem 2). *Let S and A be Borel spaces, and R be a Borel measurable compact-valued multi-function from $S \rightarrow A$ (i.e. $\forall s \in S, R(s) \subset A$ and is compact). With $GrR = \{(s, a) \in S \times A | a \in R(s)\}$, we let $u : GrR \rightarrow \mathbb{R}$ be a Borel measurable function such that $u(s, \bullet)$ is an u.s.c. function on $R(s)$ for each $s \in S$. Then, there exists a Borel measurable selector $f : S \rightarrow A$ for R such that*

$$u(s, f(s)) = \max_{a \in R(s)} u(s, a) \quad \forall s \in S.$$

Moreover, the function defined by $v(s) = \max_{a \in R(s)} u(s, a)$ is Borel measurable.

Lemma 32 (Van Erven and Harremoës (2014), Theorem 19). *Suppose that \mathcal{X} is a Polish space (which is true for E in particular). Then for $P, Q \in \mathcal{P}(\mathcal{X})$, $\text{KL}(P||Q)$ is a lower semi-continuous function of the pair (P, Q) in the weak topology.*

Lemma 33 (Aliprantis and Border (2013), Th. 18.17 p.603 (Filippov's Implicit Function Th)). *Let (S, Σ) be a measurable space and let X, Y be separable measurable spaces. Suppose that $f : S \times X \rightarrow Y$ is a Carathéodory function and that $\varphi : S \rightarrow X$ is a weakly measurable correspondence with nonempty compact values. Assume that $\pi : S \rightarrow Y$ is a measurable selector from the range of f on φ in the sense that π is measurable and for each $s \in S$ there exists $x \in \varphi(s)$ with $\pi(s) = f(s, x)$. Then the correspondence $\nu : S \rightarrow X$ defined by*

$$\nu(s) = \{x \in \varphi(s) \mid f(s, x) = \pi(s)\}$$

is measurable and admits a measurable selector, i.e. in addition to being measurable, there is a measurable function $\xi : S \rightarrow X$ s.t. $\xi(s) \in \nu(s)$ i.e. $\pi(s) = f(s, \xi(s))$ for each $s \in S$.

Theorem 13. *Let $k : E \times E \rightarrow E'$ be a bi-measurable bounded function, $f : E \rightarrow E'$ a measurable function, and $\nu \in \mathcal{W}_1$ be fixed. Define the set*

$$\mathcal{Q}(\nu, x) := \{\mu \in \mathcal{W}_1 \mid \mu \ll \nu, \quad \mu(k(x, \bullet)) = f(x)\}, \quad \forall x \in E.$$

Then for each $x \in E$, there exists a unique maximizer μ_x^ to the maximum entropy problem*

$$\max_{\mu_x \in \mathcal{Q}(\nu, x)} H_\nu(\mu_x) \tag{4}$$

given by $\mu_x^ = \Psi_{G(x, \bullet)}(\nu)$ with $G(x, y) = \exp \langle \lambda(x), k(x, y) \rangle$ for some $\lambda(x) \in \mathbb{R}^{d'}$. Furthermore, $x \mapsto \mu_x^*$ is measurable, so $(x, dy) \mapsto \mu_x^*(dy)$ is the Markov kernel $(x, dy) \mapsto \Psi_{G(x, \bullet)}(\nu)(dy)$.*

Proof. For the existence and uniqueness of the maximum entropy distribution, let $\gamma \in \mathcal{Q}(\nu, x)$ be any other measure, and denote by $m(x) := \frac{d\mu_x^*}{d\nu}$ and $n(x) := \frac{d\gamma}{d\nu}(x)$. Then

$$\begin{aligned} H_\nu(\gamma) &= - \int n(y) \log n(y) \nu(dy) \\ &= - \int n(y) \log \frac{n(y)}{m(y)} \nu(dy) - \int n(y) \log m(y) \nu(dy) \\ &= -\mathbb{KL}(\gamma \parallel \mu_x^*) - \int n(y) \log m(y) \nu(dy) \\ &= -\mathbb{KL}(\gamma \parallel \mu_x^*) - \int n(y) [\langle \lambda(x), k(x, y) \rangle - A(x)] \nu(dy) \\ &= -\mathbb{KL}(\gamma \parallel \mu_x^*) - \int [\langle \lambda(x), k(x, y) \rangle - A(x)] \gamma(dy) \\ &= -\mathbb{KL}(\gamma \parallel \mu_x^*) - [\langle \lambda(x), f(x) \rangle - A(x)] && \text{by linearity and } \gamma \in \mathcal{Q}(\nu, x) \\ &= -\mathbb{KL}(\gamma \parallel \mu_x^*) - \int [\langle \lambda(x), k(x, y) \rangle - A(x)] \mu_x^*(dy) && \text{by linearity and } \mu_x^* \in \mathcal{Q}(\nu, x) \\ &= -\mathbb{KL}(\gamma \parallel \mu_x^*) + H_\nu(\mu_x^*) \\ &\leq H_\nu(\mu_x^*). \end{aligned}$$

since $\mathbb{KL}(\nu \parallel \mu_x^*) \geq 0$ and where $A(x) = \log \int \exp \langle \lambda(x), k(x, y) \rangle \nu(dy)$. This proves that μ_x^* is indeed the maximum entropy distribution, and is unique since any other maximum verifies $\mathbb{KL}(\gamma \parallel \mu_x^*) = 0$.

The second statement is effectively a measurable selection theorem, for which we will apply Lemma 31 with:

- $S = E$ and $A = \mathcal{P}(E)$,
- $R(x) = \mathcal{Q}(\nu, x) \subset \mathcal{P}(E)$ (ν is fixed throughout this theorem and its proof), and
- $u(x, \mu) = H_\nu(\mu) = -\mathbb{KL}(\mu \parallel \nu) \in \mathbb{R}$ for $\mu \in \mathcal{Q}(\nu, x)$.

First, $S = E$ is straightforwardly a Borel space. As far as A is concerned, we are working on the 1-Wasserstein space $\mathcal{W}_1 = (\mathcal{P}_1(E), \mathbb{W}_1)$, which is a complete metric space since $E \subset \mathbb{R}^d$ and E is equipped with the Borel σ -algebra, hence $A = \mathcal{P}(E)$ is also Borel.

Second, by Lemma 32, $\mu \mapsto H_\nu(\mu) = -\text{KL}(\mu\|\nu)$ is u.s.c. on $\mathcal{Q}(\nu, x)$ for each $x \in E$. This implies in particular that $H_\nu^{-1}(]-\infty, a])$ is open in the weak (i.e. 1-Wasserstein) topology for any a . Since the rays $] -\infty, a[$ generate the Borel sets, we get that u is Borel-measurable.

In order to apply Lemma 31, we need to prove that $R = x \mapsto \mathcal{Q}(\nu, x)$ is measurable and compact-valued. This will conclude the proof as Lemma 31 guarantees that the selector, which corresponds to $x \mapsto \mu_x^*$, is measurable.

Let us thus prove that $x \mapsto \mathcal{Q}(\nu, x)$ is measurable and compact-valued. Define $AC(\nu) := \{\mu \in \mathcal{W}_1 \mid \mu \ll \nu\}$ and the mapping $\phi : E \times \mathcal{W}_1 \rightarrow E$ by $\phi(x, \mu) = \mu(k(x, \bullet))$; we can describe $\mathcal{Q}(\nu, x)$ as the following:

$$\mathcal{Q}(\nu, x) = AC(\nu) \cap \{\mu \in \mathcal{W}_1 \mid \phi(x, \mu) = f(x)\}.$$

We will show that $AC(\nu)$ is measurable and closed in \mathcal{W}_1 , and that $x \mapsto \{\mu \in \mathcal{W}_1 \mid \phi(x, \mu) = f(x)\}$ is a measurable, closed-valued correspondence, yielding the result.

For the first step, we have that $\{\mu = \Psi_X(\nu) \mid X \in L^1(\mathbb{R}_+; \nu)\} \subset AC(\nu)$. Conversely, $\mu \in AC(\nu) \implies \exists X \in L^1(\mathbb{R}_+; \nu)$ s.t. $\mu(dx) = \Psi_X(\nu)$ by the Radon-Nikodym Theorem. Therefore, $AC(\nu) = \{\Psi_X(\nu) \mid X \in L^1(\mathbb{R}_+; \nu)\}$. Moreover, by Lemma 30, $X \mapsto \Psi_X(\nu)$ is a continuous map from $L^1(\mathbb{R}_+; \nu) \rightarrow \mathcal{W}_1$, therefore $AC(\nu)$, which is the image of $L^1(\mathbb{R}_+; \nu)$ under $\Psi_\bullet(\nu)$, is Borel measurable. Moreover, as $L^1(\mathbb{R}_+; \nu)$ is closed, $AC(\nu)$ is also closed.

For the second step, we apply Lemma 33. $\phi : E \times \mathcal{W}_1 \rightarrow E$ is a Caratheodory function. Indeed, $\forall \mu, x \mapsto \phi(x, \mu)$ is measurable by Fubini's Theorem, and $\forall x, \mu \mapsto \phi(x, \mu)$ is continuous in the weak (i.e. Wasserstein) topology. The correspondence from Lemma 33, $\varphi : E \rightarrow \mathcal{W}_1$, is the constant correspondence $\varphi(x) = \mathcal{W}_1$. The selector $\pi : E \rightarrow E$ is the function $f : E \rightarrow E$ which is measurable by assumption. Therefore, by Lemma 33, the level-set correspondence

$$x \mapsto \{\mu \mid \phi(x, \mu) = f(x)\}$$

is measurable. Moreover, $\{f(x)\}$ is a closed set, and $\mu \mapsto \phi(x, \mu)$ is continuous so $\phi(x, \bullet)^{-1}(\{f(x)\})$ is a closed set. This proves that $\mathcal{Q}(\nu, x)$ is closed in \mathcal{W}_1 . Since \mathcal{W}_1 is compact by compactness of E (Villani, 2008, Ch 6), we have shown that $\mathcal{Q}(\nu, x)$ is compact which concludes the proof. \square

Proposition 15. *Let $E \subseteq \mathbb{R}^d$ and \mathcal{F} be a natural exponential family with sufficient statistics $F : E \rightarrow E' \subseteq \mathbb{R}^l$ and base measure λ supported on E as above. Suppose that, for $\mu \in \mathcal{P}(E)$, $\mu \sim \nu$, $\forall \nu \in \mathcal{F}$. Then $\Pi : \mathcal{P}(E) \rightarrow \mathcal{F}$ satisfies the projection-like equation*

$$\Pi(\mu) = \arg \min_{\nu \in \mathcal{F}} \text{KL}(\mu\|\nu).$$

Proof. This proof is straightforward and follows the lines of Koller and Friedman (2009), Theorem 8.6. Let $\theta_M = \mu(F)$ so that $\nu_{\theta_M} \in \mathcal{F}$ is the measure which satisfies

$$\nu_{\theta_M}(F) = \mu(F)$$

and let ν_θ be any other element of \mathcal{F} . Then,

$$\begin{aligned}
\text{KL}(\mu \parallel \nu_{\theta_M}) - \text{KL}(\mu \parallel \nu_\theta) &= \int \log \frac{d\mu}{d\nu_{\theta_M}} d\mu - \int \log \frac{d\mu}{d\nu_\theta} d\mu \\
&= \int \log \frac{d\nu_\theta}{d\nu_{\theta_M}} d\mu \\
&= \int \log \exp(\langle \theta_M - \theta, F(x) \rangle) d\mu(x) - \log \frac{\mathcal{Z}(\theta_M)}{\mathcal{Z}(\theta)} \\
&= \int \langle \theta_M - \theta, F(x) \rangle d\mu(x) - \log \frac{\mathcal{Z}(\theta_M)}{\mathcal{Z}(\theta)} \\
&= \langle \theta_M - \theta, \mu(F) \rangle - \log \frac{\mathcal{Z}(\theta_M)}{\mathcal{Z}(\theta)} \\
&= \langle \theta_M - \theta, \nu_{\theta_M}(F) \rangle - \log \frac{\mathcal{Z}(\theta_M)}{\mathcal{Z}(\theta)} \\
&= -\text{KL}(\nu_{\theta_M} \parallel \nu_\theta) \leq 0
\end{aligned}$$

where $\mathcal{Z}(\theta) = \exp(A(\theta))$ is the partition function. \square

Definition 34 (Measure Convolution). Let $\mu, \nu \in \mathcal{P}(\mathbb{R}^d)$ be measures. Then we define the **measure convolution** of μ and ν , denoted $\mu * \nu$, by

$$(\mu * \nu)(f) := \int f(x+y) \mu(dx) \nu(dy) \quad \forall f \in \mathcal{B}_b(\mathbb{R}^d).$$

Lemma 35. Let $\mu, \nu \in \mathcal{P}(\mathbb{R}^d)$, and assume that $F : \mathbb{R}^d \rightarrow \mathbb{R}$ is a measurable, linear function, with the additional stipulation that $F \in L^1(\mu) \cap L^1(\nu)$. Then we have

$$(\mu * \nu)(F) = \mu(F) + \nu(F).$$

Proof. We have:

$$\begin{aligned}
(\mu * \nu)(F) &= \int F(x+y) \mu(dx) \nu(dy) = \int [F(x) + F(y)] \mu(dx) \nu(dy) \\
&= \int F(x) \mu(dx) \nu(dy) + \int F(y) \mu(dx) \nu(dy) = \mu(F) + \nu(F),
\end{aligned}$$

which concludes the proof. \square

Lemma 36. Define $\rho_n := \mathcal{N}(0, \sigma_n^2 I)$ be a multivariate Gaussian on \mathbb{R}^d , $\sigma_n \rightarrow 0$, and let $\mu \in \mathcal{P}_1(\mathbb{R}^d)$. Then $\rho_n * \mu \in \mathcal{P}_1(\mathbb{R}^d)$ and $\mathbb{W}_1(\rho_n * \mu, \mu) \rightarrow 0$ as $n \rightarrow \infty$.

Proof. Let $x_0 \in \mathbb{R}^d$. A measure ν has finite 1st moment iff $\int \|x_0 - x\| \nu(dx) < \infty$. Firstly,

$$\begin{aligned}
\int \|x_0 - x\| \rho_n * \mu(dx) &= \iint \|x_0 - (x+y)\| \rho_n(dx) \mu(dy) \\
&\leq \iint (\|x_0/2 - x\| + \|x_0/2 - y\|) \rho_n(dx) \mu(dy) \\
&\leq \int \|x_0/2 - x\| \rho_n(dx) + \int \|x_0/2 - y\| \mu(dy) < \infty
\end{aligned}$$

so that $\rho_n * \mu \in \mathcal{P}_1(\mathbb{R}^d)$. Now let $f \in Lip(1)$, then

$$\begin{aligned} |(\rho_n * \mu)(f) - \mu(f)| &= \left| \iint [f(x+y) - f(y)] \rho_n(dx) \mu(dy) \right| \\ &\leq \iint |f(x+y) - f(y)| \rho_n(dx) \mu(dy) \\ &\leq \int \|x+y-y\| \mu(dy) \rho_n(dx) \\ &= \int \|x\| \rho_n(dx) \rightarrow \int \|x\| \delta_0(dx) = 0 \end{aligned}$$

as $n \rightarrow \infty$. Since the upper bound is independent of f , we are done. \square

Proposition 16. *Let $\mu \in \mathcal{W}_1$, and $F(x) = x$. Setting $\mathcal{F}_n := \{\rho_n * \delta_x \mid \delta_x \in \mathcal{P}_\delta(E)\}$ ($= \{\mathcal{N}(x, \sigma_n I), x \in E\}$), where $\rho_n := \mathcal{N}(0, \sigma_n I)$ with $\sigma_n \rightarrow 0$, then in the 1-Wasserstein topology:*

$$\Pi_{\mathcal{F}}(\mu) = \lim_{n \rightarrow \infty} \arg \min_{\nu \in \mathcal{F}_n} \text{KL}(\rho_n * \mu \parallel \nu).$$

Proof. Let $f := \mu(F)$. Below, we extend $\mu \in \mathcal{P}_1(E)$ to be a (compactly supported) element of $\mathcal{P}_1(\mathbb{R}^d)$ by simply setting $\mu(A) = \mu(A \cap E) \forall A \in \mathcal{B}(\mathbb{R}^d)$, and trivially extend F to \mathbb{R}^d .

1. We have that $\rho_n * \mu(F) = \mu(F) \forall n$ by Lemma 35 since $F(x) = x$ is linear and $\rho_n(F) = 0$. Therefore, $\Pi_{\mathcal{F}}(\rho_n * \mu) = \Pi_{\mathcal{F}}(\mu), \forall n$.
2. Let \mathcal{F}_n be as above. By the previous step, we have

$$\Pi_{\mathcal{F}_n}(\rho_n * \mu) = \Pi_{\mathcal{F}_n}(\mu) = (\rho_n * \nu)_f = \rho_n * \nu_f.$$

Moreover, since $\rho_n * \mu \sim \nu \forall \nu \in \mathcal{F}_n$ and \mathcal{F}_n is an exponential family, by Proposition 15

$$\Pi_{\mathcal{F}_n}(\rho_n * \mu) = \arg \min_{\nu \in \mathcal{F}_n} \text{KL}(\rho_n * \mu \parallel \nu).$$

3. Finally, $\nu_f := \Pi_{\mathcal{F}}(\mu)$ is equal to the limit

$$\nu_f \stackrel{(1)}{=} \lim_{n \rightarrow \infty} \rho_n * \nu_f \stackrel{(2)}{=} \lim_{n \rightarrow \infty} \Pi_{\mathcal{F}_n}(\rho_n * \mu) \stackrel{(3)}{=} \lim_{n \rightarrow \infty} \arg \min_{\nu \in \mathcal{F}_n} \text{KL}(\rho_n * \mu \parallel \nu)$$

where (1) is due to Lemma 36, and (2), (3) are due to step 2. Hence we can think of ν_f as the limit of the minimizers in the 1-Wasserstein sense. \square

C Proofs From Section 5

Proposition 18. *Suppose $\mu, \nu \in \mathcal{P}_1(E)$ and $G : E \times E \rightarrow \mathbb{R}$, $G(x, y) \geq \epsilon(G) > 0$ is an interaction potential s.t. $\|G\|_{\infty, Lip} < \infty$ and $\|G\|_{Lip, \infty} < \infty$. Then, $\forall x, y \in E$:*

$$\begin{aligned} W_1(\Psi_{G(x, \bullet)}(\mu), \Psi_{G(y, \bullet)}(\mu)) &\leq 2 \frac{\|G\|_{Lip, \infty} \text{diam}(E)}{\epsilon(G)} \cdot d(x, y), \\ W_1(\Psi_{G(x, \bullet)}(\mu), \Psi_{G(x, \bullet)}(\nu)) &\leq \frac{2\|G\|_{\infty, Lip} \text{diam}(E)}{\epsilon(G)} \cdot W_1(\mu, \nu). \end{aligned}$$

Proof. For the first inequality, let f be any 1-Lipschitz function, and $x, y \in E$. We have:

$$\begin{aligned} |\Psi_{G(x, \bullet)}(\mu)(f) - \Psi_{G(y, \bullet)}(\mu)(f)| &= \left| \int \frac{G(x, z)f(z)}{\mu(G(x, \bullet))} - \frac{G(y, z)f(z)}{\mu(G(y, \bullet))} \mu(dz) \right| \\ &\leq \left| \int \frac{G(x, z)f(z)}{\mu(G(x, \bullet))} - \frac{G(x, z)f(z)}{\mu(G(y, \bullet))} \mu(dz) \right| \\ &\quad + \left| \int \frac{G(x, z)f(z)}{\mu(G(y, \bullet))} - \frac{G(y, z)f(z)}{\mu(G(y, \bullet))} \mu(dz) \right|. \end{aligned}$$

Let us bound the first term:

$$\begin{aligned} \left| \int \frac{G(x, z)f(z)}{\mu(G(x, \bullet))} - \frac{G(x, z)f(z)}{\mu(G(y, \bullet))} \mu(dz) \right| &\leq \frac{|\mu(G(x, \bullet)) - \mu(G(y, \bullet))|}{\mu(G(x, \bullet))\mu(G(y, \bullet))} \int G(x, z)|f(z)|\mu(dz) \\ &\leq \frac{\int |G(x, z) - G(y, z)|\mu(dz)}{\mu(G(x, \bullet))\epsilon(G)} \mu(G(x, \bullet))\|f\|_\infty \\ &\leq \frac{\int |G(x, z) - G(y, z)|\mu(dz)\|f\|_\infty}{\epsilon(G)d(x, y)} d(x, y) \\ &\leq \frac{\|G\|_{Lip, \infty}\|f\|_\infty}{\epsilon(G)} d(x, y). \end{aligned}$$

Let us now bound the second term:

$$\begin{aligned} \left| \int \frac{G(x, z)f(z)}{\mu(G(y, \bullet))} - \frac{G(y, z)f(z)}{\mu(G(y, \bullet))} \mu(dz) \right| &\leq \frac{\|f\|_\infty}{\epsilon(G)} \int |G(x, z) - G(y, z)|\mu(dz) \\ &\leq \frac{\|G\|_{Lip, \infty}\|f\|_\infty}{\epsilon(G)} d(x, y). \end{aligned}$$

Using the fact that $\Psi_{G(x, \bullet)}(\mu)(\bar{f}) = \Psi_{G(y, \bullet)}(\mu)(\bar{f})$ for any constant function \bar{f} , we can subtract from f any constant without changing the value of $|\Psi_{G(x, \bullet)}(\mu)(f) - \Psi_{G(y, \bullet)}(\mu)(f)|$. This allows us to assume without loss of generality that $\|f\|_\infty \leq \text{diam}(E)$ (picking an arbitrary $x \in E$, we have $\forall y \in E$, $|f(y) - f(x)| \leq |y - x|\|f\|_{Lip} \leq \text{diam}(E)$). Combining everything, we get:

$$|\Psi_{G(x, \bullet)}(\mu)(f) - \Psi_{G(y, \bullet)}(\mu)(f)| \leq 2 \frac{\|G\|_{Lip, \infty} \text{diam}(E)}{\epsilon(G)} d(x, y).$$

Taking the supremum over 1-Lipschitz functions f concludes the first part of the proof.

Let us now prove the second inequality. Similarly, let f be any 1-Lipschitz function, and μ, ν two compactly supported distributions on (E, \mathcal{E}) . We use the notation $G(z) := G(x, z)$ for this part because x is fixed. We have:

$$\begin{aligned} |\Psi_G(\mu)(f) - \Psi_G(\nu)(f)| &= \left| \int \frac{G(z)f(z)}{\mu(G)} \mu(dz) - \int \frac{G(z)f(z)}{\nu(G)} \nu(dz) \right| \\ &\leq \left| \int \frac{G(z)f(z)}{\mu(G)} \mu(dz) - \int \frac{G(z)f(z)}{\nu(G)} \mu(dz) \right| \\ &\quad + \left| \int \frac{G(z)f(z)}{\nu(G)} \mu(dz) - \int \frac{G(z)f(z)}{\nu(G)} \nu(dz) \right|. \end{aligned}$$

Let us bound the first term:

$$\begin{aligned} \left| \int \left(\frac{G(z)f(z)}{\mu(G)} - \frac{G(z)f(z)}{\nu(G)} \right) \mu(dz) \right| &\leq \frac{|\mu(G) - \nu(G)|}{\mu(G)\nu(G)} \int G(z)|f(z)|\mu(dz) \\ &\leq \frac{\|G\|_{Lip} \mathbb{W}_1(\mu, \nu)}{\mu(G)\epsilon(G)} \mu(G)\|f\|_\infty \\ &\leq \frac{\|G\|_{Lip}\|f\|_\infty}{\epsilon(G)} \mathbb{W}_1(\mu, \nu). \end{aligned}$$

Let us now bound the second term:

$$\begin{aligned} \left| \int \frac{G(z)f(z)}{\nu(G)} \mu(dz) - \int \frac{G(z)f(z)}{\nu(G)} \nu(dz) \right| &\leq \frac{\|f\|_\infty}{\nu(G)} \left| \int G(z) \mu(dz) - \int G(z) \nu(dz) \right| \\ &\leq \frac{\|G\|_{Lip} \|f\|_\infty}{\epsilon(G)} \mathbb{W}_1(\mu, \nu). \end{aligned}$$

Using the same reasoning as above, we can assume without loss of generality that $\|f\|_\infty \leq \text{diam}(E)$, which gives:

$$|\Psi_G(\mu)(f) - \Psi_G(\nu)(f)| \leq 2 \frac{\|G\|_{Lip} \text{diam}(E)}{\epsilon(G)} \mathbb{W}_1(\mu, \nu).$$

Taking the supremum over all 1-Lipschitz functions f concludes the proof. \square

Proposition 19. *Suppose that $F(x) = x$, $\mathcal{F} = \mathcal{P}_\delta(E)$, and $\Pi := \Pi_{\mathcal{F}}$ is the moment projection onto \mathcal{F} . Then, for $\mu, \nu \in \mathcal{P}_1(E)$, $\mathbb{W}_1(\Pi(\mu), \Pi(\nu)) \leq d \cdot \mathbb{W}_1(\mu, \nu)$.*

Proof. Denote by $\pi_i : E \rightarrow \mathbb{R}$ the canonical projection onto the i -th coordinate of $E \subset \mathbb{R}^d$, and let $x_i := \pi_i(x)$. Then

$$\begin{aligned} \mathbb{W}_1(\Pi(\mu), \Pi(\nu)) &= \mathbb{W}_1(\delta_{\mu(F)}, \delta_{\nu(F)}) \\ &= \|\mu(F) - \nu(F)\|_1 \\ &= \sum_{i=1}^d |\mu(F)_i - \nu(F)_i| \\ &= \sum_{i=1}^d |\mu(\pi_i \circ F) - \nu(\pi_i \circ F)| \\ &\leq d \cdot \max_{i=1, \dots, d} \{|\mu(\pi_i \circ F) - \nu(\pi_i \circ F)|\} \\ &\leq d \cdot \sup_{f \in Lip(1)} |\mu(f) - \nu(f)| \\ &= d \cdot \mathbb{W}_1(\mu, \nu) \end{aligned}$$

since $\pi_i \circ F \in Lip(1)$ for $i = 1, \dots, d$ (we recall that here, F is the identity). \square

Proposition 20. *Suppose $L : E \times \mathcal{E} \rightarrow [0, 1]$ is a lookup kernel implementing a deterministic lookup function $\ell : E \rightarrow E$, (i.e. $L(x, dy) = \delta_{\ell(x)}(dy)$) and suppose that ℓ is K_ℓ -Lipschitz in the 1-norm, then $\mathbb{W}_1(\mu L, \gamma L) \leq K_\ell \mathbb{W}_1(\mu, \gamma)$.*

Proof.

$$\begin{aligned} \mathbb{W}_1(\mu L, \gamma L) &= \sup_{f \in Lip(1)} \left| \int f(x) \mu L(dx) - \int f(y) \gamma L(dy) \right| \\ &= \sup_{f \in Lip(1)} \left| \int f(x) \int \mu(dz) L(z, dx) - \int f(y) \int \gamma(dz) L(z, dy) \right| \\ &= \sup_{f \in Lip(1)} \left| \iint f(x) L(z, dx) \mu(dz) - \iint f(y) L(z, dy) \gamma(dz) \right| \\ &= \sup_{f \in Lip(1)} \left| \iint f(x) \delta_{\ell(z)}(dx) \mu(dz) - \iint f(y) \delta_{\ell(z)}(dy) \gamma(dz) \right| \\ &= \sup_{f \in Lip(1)} \left| \int f \circ \ell(z) \mu(dz) - \int f \circ \ell(z) \gamma(dz) \right|. \end{aligned}$$

Then since $\|f\|_{Lip} = 1$, we have $\|f \circ \ell\|_{Lip} \leq \|f\|_{Lip} \|\ell\|_{Lip} = K_\ell$. Hence, by our earlier estimation techniques:

$$\begin{aligned} W_1(\mu L, \gamma L) &= \sup_{f \in Lip(1)} \left| \int f \circ \ell(dz) \mu(dz) - \int f \circ \ell(z) \gamma(dz) \right| \\ &\leq K_\ell \sup_{g \in Lip(1)} \left| \int g(dz) \mu(dz) - \int g(z) \gamma(dz) \right| = K_\ell W_1(\mu, \gamma), \end{aligned}$$

which concludes the proof. \square

Lemma 37. 1. Suppose that $\Phi, \Gamma : \mathcal{P}(E) \rightarrow \mathcal{P}(E)$ are (possibly nonlinear) mappings. Then

$$\tau(\Phi \circ \Gamma) \leq \tau(\Phi) \tau(\Gamma).$$

2. Suppose $K : E \times \mathcal{E} \rightarrow [0, 1]$ is an integral kernel. Then

$$\tau(K) = \sup_{x \neq y} \frac{W_1(K(x, \bullet), K(y, \bullet))}{d(x, y)}.$$

3. Suppose $K_1, K_2 : E \times \mathcal{E} \rightarrow [0, 1]$ are two integral kernels and $\nu \in \mathcal{P}(E)$. Then:

$$W_1(\nu K_1, \nu K_2) \leq \int \nu(dx) W_1(K_1(x, \bullet), K_2(x, \bullet)).$$

Proof. 1. This is a standard result on Lipschitz constants. We include it for completeness:

$$\begin{aligned} \tau(\Phi \circ \Gamma) &= \sup_{\mu \neq \nu} \frac{W_1(\Phi \circ \Gamma(\mu), \Phi \circ \Gamma(\nu))}{W_1(\mu, \nu)} \\ &= \sup_{\mu \neq \nu} \frac{W_1(\Phi \circ \Gamma(\mu), \Phi \circ \Gamma(\nu))}{W_1(\Gamma(\mu), \Gamma(\nu))} \frac{W_1(\Gamma(\mu), \Gamma(\nu))}{W_1(\mu, \nu)} \\ &\leq \sup_{\eta \neq \gamma} \frac{W_1(\Phi(\eta), \Phi(\gamma))}{W_1(\eta, \gamma)} \cdot \sup_{\mu \neq \nu} \frac{W_1(\Gamma(\mu), \Gamma(\nu))}{W_1(\mu, \nu)} \\ &= \tau(\Phi) \tau(\Gamma). \end{aligned}$$

2. Since $W_1(\delta_x, \delta_y) = d(x, y)$ and $\delta_x K = K(x, \bullet)$ we have:

$$\sup_{x \neq y} \frac{W_1(K(x, \bullet), K(y, \bullet))}{d(x, y)} = \sup_{\delta_x \neq \delta_y} \frac{W_1(\delta_x K, \delta_y K)}{W_1(\delta_x, \delta_y)} \leq \sup_{\mu \neq \nu} \frac{W_1(\mu K, \nu K)}{W_1(\mu, \nu)}.$$

For the reverse inequality,

$$\begin{aligned} W_1(\mu K, \nu K) &= \sup_{f \in Lip(1)} |\mu K(f) - \nu K(f)| \\ &= \sup_{f \in Lip(1)} |\mu(Kf) - \nu(Kf)| \\ &\leq \sup_{f \in Lip(1)} \|Kf\|_{Lip(1)} \cdot \sup_{g \in Lip(1)} |\mu(g) - \nu(g)| \\ &\leq \sup_{f \in Lip(1)} \|Kf\|_{Lip(1)} \cdot W_1(\mu, \nu) \end{aligned}$$

and

$$\begin{aligned} \sup_{f \in Lip(1)} \|Kf\|_{Lip(1)} &= \sup_{f \in Lip(1)} \sup_{x \neq y} \frac{\int K(x, dz) f(z) - \int K(y, dz) f(z)}{d(x, y)} \\ &= \sup_{f \in Lip(1)} \sup_{x \neq y} \frac{\int [K(x, dz) - K(y, dz)] f(z)}{d(x, y)} \\ &= \sup_{x \neq y} \frac{W_1(K(x, \bullet), K(y, \bullet))}{d(x, y)}. \end{aligned}$$

Dividing by $W_1(\mu, \nu)$ gives us the reverse inequality and concludes the proof.

3. By definition, we have:

$$\begin{aligned}
W_1(\nu K_1, \nu K_2) &= \sup_{f \in Lip(1)} |\nu K_1(f) - \nu K_2(f)| \\
&= \sup_{f \in Lip(1)} \left| \iint \nu(dx) K_1(x, dy) f(y) - \iint \nu(dx) K_2(x, dy) f(y) \right| \\
&\leq \sup_{f \in Lip(1)} \int \nu(dx) \left| \int K_1(x, dy) f(y) - \int K_2(x, dy) f(y) \right| \\
&\leq \int \nu(dx) W_1(K_1(x, \bullet), K_2(x, \bullet)).
\end{aligned}$$

□

Using Propositions 18, 19 and 20 and Lemma 37, we can prove Theorem 22.

Theorem 22. *Let $E \subset \mathbb{R}^d$ be compact, $\mathcal{F} = \mathcal{P}_\delta(E)$, and $\Pi := \Pi_{\mathcal{F}}$. Let \mathbf{A} be the attention kernel from definition 8, with $L(x, dy) = \delta_{\ell(x)}(dy)$. Let G be an interaction potential such that $G(x, y) \geq \epsilon(G) > 0$, $\|G\|_{Lip, \infty} < \infty$ and $\|G\|_{\infty, Lip} < \infty$. Then, with $\tau(\mathbf{A})$ the 1-Wasserstein contraction coefficient of \mathbf{A} considered as a mapping on $\mathcal{P}(E)$ through $\mathbf{A} : \mu \rightarrow \mu \mathbf{A}_\mu$, we have:*

$$\tau(\mathbf{A}) \leq \tau(\Pi) \tau(\Psi_G) \tau(L)$$

where $\tau(\Pi) = d$, $\tau(\Psi_G) = \frac{2(\|G\|_{Lip, \infty} + \|G\|_{\infty, Lip}) \text{diam}(E)}{\epsilon(G)}$ and $\tau(L) = K_\ell$.

Proof. We want to bound $\sup_{\mu \neq \nu} \frac{W_1(\mu A_\mu, \nu A_\nu)}{W_1(\mu, \nu)}$. Let $\mu \neq \nu \in \mathcal{P}(E)$, we have:

$$\frac{W_1(\mu A_\mu, \nu A_\nu)}{W_1(\mu, \nu)} \leq \frac{W_1(\mu A_\mu, \nu A_\mu)}{W_1(\mu, \nu)} + \frac{W_1(\nu A_\mu, \nu A_\nu)}{W_1(\mu, \nu)}$$

Let us start with the first term:

$$\begin{aligned}
\frac{W_1(\mu A_\mu, \nu A_\mu)}{W_1(\mu, \nu)} &\leq \frac{W_1(\mu \Pi[\Psi_{G(\bullet, \bullet)}(\mu) L], \nu \Pi[\Psi_{G(\bullet, \bullet)}(\mu) L])}{W_1(\mu, \nu)} \\
&\leq \sup_{x \neq y} \frac{W_1(\Pi[\Psi_{G(x, \bullet)}(\mu) L], \Pi[\Psi_{G(y, \bullet)}(\mu) L])}{d(x, y)} \\
&\leq \tau_1(\Pi) \tau_1(L) \sup_{x \neq y} \frac{W_1(\Psi_{G(x, \bullet)}(\mu), \Psi_{G(y, \bullet)}(\mu))}{d(x, y)} \\
&\leq \tau_1(\Pi) \tau_1(L) \frac{2\|G\|_{Lip, \infty} \text{diam}(E)}{\epsilon(G)},
\end{aligned}$$

where we used Lemma 37 for the second and third lines, and Propositions 18, 19 and 20 for the third and last. As for the second term, we have:

$$\begin{aligned}
W_1(\nu A_\mu, \nu A_\nu) &= W_1(\nu \Pi[\Psi_G(\mu) L], \nu \Pi[\Psi_G(\nu) L]) \\
&\leq \int \nu(dx) W_1(\Pi[\Psi_{G(x, \bullet)}(\mu) L], \Pi[\Psi_{G(x, \bullet)}(\nu) L]) \\
&\leq \tau_1(\Pi) \tau_1(L) \int \nu(dx) W_1(\Psi_{G(x, \bullet)}(\mu), \Psi_{G(x, \bullet)}(\nu)) \\
&\leq \tau_1(\Pi) \tau_1(L) \int \nu(dx) \frac{2\|G(x, \bullet)\|_{Lip} \text{diam}(E)}{\epsilon(G)} W_1(\mu, \nu) \\
&\leq \tau_1(\Pi) \tau_1(L) \frac{2\|G\|_{\infty, Lip} \text{diam}(E)}{\epsilon(G)} W_1(\mu, \nu)
\end{aligned}$$

where we also used Lemma 37 for the second and third lines, and Propositions 18, 19 and 20 for the third and last. □

D Proofs for Section 6.3

Lemma 38. For any $f : \mathbb{R}^d \rightarrow \mathbb{R}$ with $\|f\|_{Lip} < \infty$:

$$\|f\|_{Lip} = \sup_{x \neq y, \|x-y\| \leq 1} \frac{|f(x) - f(y)|}{\|x - y\|}. \quad (6)$$

Proof. Let $x \neq y$ and $L = \sup_{x \neq y, \|x-y\| \leq 1} \frac{|f(x) - f(y)|}{\|x-y\|} \leq \|f\|_{Lip}$. We split the segment $[x, y]$ into the minimum number of chunks of lengths smaller than 1: $x = z_1 \rightarrow z_2 \rightarrow \dots \rightarrow z_k = y$ (in particular, if $\|x - y\| \leq 1$ then $z_2 = y$). Clearly:

$$\begin{aligned} |f(x) - f(y)| &\leq \sum_{1 \leq i \leq k-1} |f(z_i) - f(z_{i+1})| \\ &\leq L \sum_{1 \leq i \leq k-1} \|z_i - z_{i+1}\| = L\|x - y\|. \end{aligned}$$

This gives $\|f\|_{Lip} \leq L$ which concludes the proof. \square

Lemma 39. For any n and $(z_1, \dots, z_n) \in \mathbb{R}_+^n$:

$$f(z_1, \dots, z_n) := \frac{\sum_{i=1}^n z_i e^{-z_i^2}}{1 + \sum_{i=1}^n e^{-z_i^2}} \leq \sqrt{\ln n + \frac{1}{2e}}. \quad (7)$$

Proof. f is clearly bounded on \mathbb{R}_+^n ($z_i e^{-z_i^2} \rightarrow 0$ when $z_i \rightarrow \infty$). Let us now compute the partial derivatives of f . For a given z_i :

$$\frac{\partial f}{\partial z_i} = \frac{e^{-z_i^2}}{1 + \sum_{k=1}^n e^{-z_k^2}} [1 - 2z_i^2 + 2z_i f(z_1, \dots, z_n)].$$

There is only one positive solution of $1 - 2z_i^2 + 2z_i f^* = 0$, meaning that f reaches its maximum when all its coordinates are equal. We thus only need to study:

$$g(x) := \frac{nx e^{-x^2}}{1 + n e^{-x^2}} = \frac{x e^{\ln n - x^2}}{1 + e^{\ln n - x^2}}. \quad (8)$$

The change of variable $y = \ln n - x^2$ gives $g(y) = \frac{\sqrt{\ln n - y} e^y}{1 + e^y} \leq \frac{\sqrt{\ln n - y}}{1 + e^{-y}}$ with $y \in]-\infty, \ln n]$.

On $[0, \ln n]$, we clearly have $g(y) \leq \sqrt{\ln n}$. Let us consider $y \in]-\infty, 0]$. We get $g^2(y) = \frac{\ln n - y}{(1 + e^{-y})^2} \leq \frac{\ln n - y}{e^{-2y}} \leq \ln n + \frac{1}{2e}$ with since $(2e)^{-1}$ is the maximum of ze^{-2z} on \mathbb{R}_+ . This concludes the proof. \square

Lemma 40. Let $\mu_1, \mu_2, \nu_1, \nu_2 \in \mathcal{W}_1(\mathbb{R}^d)$. Then

$$\mathbb{W}_1(\mu_1 \otimes \mu_2, \nu_1 \otimes \nu_2) \leq \mathbb{W}_1(\mu_1, \nu_1) + \mathbb{W}_1(\mu_2, \nu_2)$$

Proof. Let $\gamma_1 \in \mathcal{C}(\mu_1, \nu_1), \gamma_2 \in \mathcal{C}(\mu_2, \nu_2)$ be optimal for $c(x, y) = \|x - y\|_1$. Note that $\gamma_1 \otimes \gamma_2 \in \mathcal{C}(\mu_1 \otimes \mu_2, \nu_1 \otimes \nu_2)$, i.e. $\gamma_1 \otimes \gamma_2$ is a transfer plan with the correct marginals, by considering

$$\begin{aligned} \int_{X \times X} d\gamma_1 \otimes \gamma_2(x_1, x_2, y_1, y_2) &= \int_{X \times X} d\gamma_1(x_1, y_1) d\gamma_2(x_2, y_2) \\ &= \int_X d\gamma_1(x_1, y_1) \int_X d\gamma_2(x_2, y_2) \\ &= \nu_1(dy_1) \nu_2(dy_2) = d\nu_1 \otimes \nu_2(y_1, y_2) \end{aligned}$$

and same for the other marginals.

Thus we have

$$\begin{aligned}
W_1(\mu_1 \otimes \mu_2, \nu_1 \otimes \nu_2) &= \inf_{\gamma \in \mathcal{C}(\mu_1 \otimes \mu_2, \nu_1 \otimes \nu_2)} \int \| (x_1, x_2) - (y_1, y_2) \| d\gamma(x_1, x_2, y_1, y_2) \\
&= \inf_{\gamma \in \mathcal{C}(\mu_1 \otimes \mu_2, \nu_1 \otimes \nu_2)} \int (\|x_1 - y_1\| + \|y_1, y_2\|) d\gamma(x_1, x_2, y_1, y_2) \\
&= \inf_{\gamma \in \mathcal{C}(\mu_1 \otimes \mu_2, \nu_1 \otimes \nu_2)} \int \|x_1 - y_1\| d\gamma(x_1, x_2, y_1, y_2) + \dots \\
&\quad \dots + \inf_{\gamma \in \mathcal{C}(\mu_1 \otimes \mu_2, \nu_1 \otimes \nu_2)} \int \|x_2 - y_2\| d\gamma(x_1, x_2, y_1, y_2) \\
&\leq \int \|x_1 - y_1\| d\gamma_1 \otimes \gamma_2(x_1, x_2, y_1, y_2) + \int \|x_2 - y_2\| d\gamma_1 \otimes \gamma_2(x_1, x_2, y_1, y_2) \\
&= \int \|x_1 - y_1\| d\gamma_1(x_1, y_1) + \int \|x_2 - y_2\| d\gamma_2(x_2, y_2) \\
&= W_1(\mu_1, \nu_1) + W_1(\mu_2, \nu_2)
\end{aligned}$$

□

Proposition 27. Let $E = \mathbb{R}^d$ and suppose $X = \{x_1, \dots, x_N\}$ and $Y = \{y_1, \dots, y_N\}$. Let $\mu = m(X)$, $\nu = m(Y)$. Then for $x \in \text{supp}(\mu)$ and $y \in \text{supp}(\nu)$, we have

$$W_1(\Psi_{G(x, \bullet)}(\mu), \Psi_{G(y, \bullet)}(\nu)) \leq \left[\sqrt{d} \sqrt{\ln N + \frac{1}{2e}} \|G\|_{Lip} + \|G\|_\infty + \sqrt{d} + 2 \right] (d(x, y) + W_1(\mu, \nu)).$$

Proof. We use the Kantorovich formulation of W_1 . Let f be a function with $\|f\|_{Lip} \leq 1$. Using the same kind of technique as in Section C, we can assume without loss of generality that $f(y) = 0$. For simplicity, we write $G(x, \bullet) = G_x$. We wish to upper-bound the quantity $|\Psi_{G_x}(\mu)(f) - \Psi_{G_y}(\nu)(f)|$.

Because Ψ_{G_x} and Ψ_{G_y} are homonegeous in their measure argument, and for the sake of simplicity, we write $\mu = \sum_i \delta_{x_i}$, $\nu = \sum_i \delta_{y_i}$ (which is equivalent to simplifying by $1/N$ in e.g. the numerator and denominator of Ψ_{G_x}). This guarantees in particular that $\mu(G_x) \geq 1$ and $\nu(G_y) \geq 1$ (x and y are in $\text{supp}(\mu)$ and $\text{supp}(\nu)$ resp.) and equivalently that $1/\mu(G_x) \leq 1$ and $1/\nu(G_y) \leq 1$.

Then:

$$\begin{aligned}
|\Psi_{G_x}(\mu)(f) - \Psi_{G_y}(\nu)(f)| &= \frac{1}{\mu(G_x)\nu(G_y)} |\nu(G_y)\mu(G_x f) - \mu(G_x)\nu(G_y f)| \\
&= \frac{1}{\mu(G_x)\nu(G_y)} |\nu(G_y)\mu(G_x f) - \nu(G_y)\nu(G_y f) + \nu(G_y)\nu(G_y f) - \mu(G_x)\nu(G_y f)| \\
&\leq \frac{\nu(G_y)}{\mu(G_x)\nu(G_y)} |\mu(G_x f) - \nu(G_y f)| + \frac{\nu(G_y f)}{\mu(G_x)\nu(G_y)} |\nu(G_y) - \mu(G_x)|. \tag{9}
\end{aligned}$$

We start by bounding the second term of (9). We have:

$$\begin{aligned}
\frac{\nu(G_y f)}{\mu(G_x)\nu(G_y)} |\nu(G_y) - \mu(G_x)| &= \frac{\nu(G_y f)}{\mu(G_x)\nu(G_y)} |(\delta_x \otimes \mu)(G) - (\delta_y \otimes \nu)(G)| \\
&\leq \frac{\nu(G_y f)}{\mu(G_x)\nu(G_y)} \|G\|_{Lip} W_1(\delta_x \otimes \mu, \delta_y \otimes \nu).
\end{aligned}$$

Here, $\delta_x \otimes \mu$ denotes the product of the two measures on $E \times E$. Since $f(y) = 0$, we see that $f(z) \leq f(y) + \|f\|_{Lip} \|y - z\|_1 \leq \|y - z\|_1$. This gives:

$$\begin{aligned}
\frac{\nu(G_y f)}{\nu(G_y)} &= \frac{\int G_y(z) f(z) \nu(dz)}{\int G_y(z) \nu(dz)} \leq \frac{\int G_y(z) \|y - z\|_1 \nu(dz)}{\int G_y(z) \nu(dz)} \\
&\leq \frac{\sum_{i=1}^N G(y, y_i) \|y - y_i\|_1}{\sum_{i=1}^N G(y, y_i)} \leq \sqrt{d} \frac{\sum_{i=1}^N e^{-\|y - y_i\|_2^2} \|y - y_i\|_2}{\sum_{i=1}^N e^{-\|y - y_i\|_2^2}},
\end{aligned}$$

where we applied Cauchy-Schwartz for the last inequality. Since $y = y_i$ for a given i , we are interested in the quantity $\frac{\sum_{i=1}^{N-1} z_i e^{-z_i^2}}{1 + \sum_{i=1}^{N-1} e^{-z_i^2}}$ for arbitrary $z_i \geq 0$. Applying Lemma 39 with $n = N - 1$ gives an upper-bound of $\sqrt{\ln N + \frac{1}{2e}}$.

Let us now consider the first term of (9):

$$\begin{aligned} \frac{\nu(G_y)}{\mu(G_x)\nu(G_y)} |\mu(G_x f) - \nu(G_y f)| &= \frac{1}{\mu(G_x)} |\mu(G_x f) - \nu(G_y f)| \\ &\leq \frac{1}{\mu(G_x)} \|Gf\|_{Lip} \mathbb{W}_1(\delta_x \otimes \mu, \delta_y \otimes \nu). \end{aligned}$$

To estimate $\|Gf\|_{Lip}$ we have

$$\|Gf\|_{Lip} = \sup_{(x,w) \neq (y,z)} \frac{|G(x,w)f(w) - G(y,z)f(z)|}{\|(x,w) - (y,z)\|_1}$$

where additionally, we can assume that $\|(x,w) - (y,z)\| \leq 1$ (see Lemma 38). We have:

$$\begin{aligned} |G(x,w)f(w) - G(y,z)f(z)| &= |G(x,w)f(w) - G(x,w)f(z) + G(x,w)f(z) - G(y,z)f(z)| \\ &\leq |G(x,w)||f(w) - f(z)| + |f(z)||G(x,w) - G(y,z)|. \end{aligned}$$

For the first term, we see that

$$\begin{aligned} |G(x,w)||f(w) - f(z)| &\leq \|G\|_{\infty, \infty} \|f\|_{Lip} d(w, z) \\ &\leq \|G\|_{\infty, \infty} \|f\|_{Lip} (d(w, z) + d(x, y)). \end{aligned}$$

For the second term, we have

$$\begin{aligned} |f(z)||G(x,w) - G(y,z)| &\leq \|y - z\|_1 |G(x,w) - G(y,z)| \\ &\leq \|y - z\|_1 \|\nabla G(t_1, t_2)\|_{\infty} \|(x,w) - (y,z)\|_1, \end{aligned}$$

for t_1 in the segment $[x, y]$ and t_2 in the segment $[w, z]$ (this follows directly from the mean value theorem, note that the gradient is taken with respect to both variables). We used $f(y) = 0$ and $f(z) \leq f(y) + \|f\|_{Lip} \|y - z\|_1 = \|y - z\|_1$ in the first line.

In the Gaussian case:

$$\begin{aligned} \|y - z\|_1 \|\nabla G(t_1, t_2)\|_{\infty} &\leq (\|y - t_1\|_1 + \|t_1 - t_2\|_1 + \|t_2 - z\|_1) 2 \|t_1 - t_2\|_{\infty} e^{-\|t_1 - t_2\|_2^2} \\ &\leq 2(2 + \|t_1 - t_2\|_1) \|t_1 - t_2\|_{\infty} e^{-\|t_1 - t_2\|_2^2}, \end{aligned}$$

where we used the fact that $\|y - t_1\|_1 \leq 1$ and $\|t_2 - z\|_1 \leq 1$ (t_1 is in the $[x, y]$ segment and $\|x - y\|_1 \leq 1$ by assumption). That upper bound is uniformly bounded with respect to t_1 and t_2 , we let C denote that constant. A loose upper-bound on C is $\sqrt{d} + 2$ (which we use in the statement of the proposition).

To conclude, it suffices to note that by Lemma 40 we have

$$\mathbb{W}_1(\delta_x \otimes \mu, \delta_y \otimes \nu) \leq \mathbb{W}_1(\delta_x, \delta_y) + \mathbb{W}_1(\mu, \nu).$$

□

Theorem 28. Let $E = \mathbb{R}^d$ and suppose $X = \{x_1, \dots, x_N\}$ and $Y = \{y_1, \dots, y_M\}$. Let $G(x, y) = \exp(-\|x - y\|_2^2)$, $L(x, dy) = \delta_{l(x)}(dy)$, and Π be the usual projection onto \mathcal{F}_{δ} . Then for $\mu = m(X)$ and $\nu = m(Y)$,

$$\mathbb{W}_1(\mu \mathbf{A}_{\mu}, \nu \mathbf{A}_{\nu}) \leq 2\tau(\Pi)\tau(L) \left[\sqrt{d} \sqrt{\ln(\min(N, M)) + \frac{1}{2e}} \|G\|_{Lip} + \|G\|_{\infty} + \sqrt{d} + 2 \right] \mathbb{W}_1(\mu, \nu).$$

Proof. Firstly, using Proposition 9, we know that $\mu \mathbf{A}_\mu$ is another empirical measure concentrated on $\{\text{Attention}(x_i, X, X)\}$, similarly, $\nu \mathbf{A}_\nu$ is concentrated on $\{\text{Attention}(y_i, Y, Y)\}$. This fact allows us to use the following result from Santambrogio (2015) Equation 6.2

$$\mathbb{W}_1(\mu, \nu) = \min \left\{ \sum_{i,j} \gamma_{ij} d(x_i, y_j) \mid \gamma_{i,j} \geq 0, \sum_i \gamma_{ij} = \frac{1}{M}, \sum_j \gamma_{ij} = \frac{1}{N} \right\},$$

Applied to $\mathbb{W}_1(\mu \mathbf{A}_\mu, \nu \mathbf{A}_\nu)$, it gives

$$\begin{aligned} \mathbb{W}_1(\mu \mathbf{A}_\mu, \nu \mathbf{A}_\nu) &= \min \left\{ \sum_{i,j} \gamma_{ij} d(\text{Attention}(x_i, X, X), \text{Attention}(y_j, Y, Y)) \mid \right. \\ &\quad \left. \gamma_{i,j} \geq 0, \sum_i \gamma_{ij} = \frac{1}{M}, \sum_j \gamma_{ij} = \frac{1}{N} \right\} \\ &= \min \left\{ \sum_{i,j} \gamma_{ij} \mathbb{W}_1(\mathbf{A}_\mu(x_i, \bullet), \mathbf{A}_\nu(y_j, \bullet)) \mid \right. \\ &\quad \left. \gamma_{i,j} \geq 0, \sum_i \gamma_{ij} = \frac{1}{M}, \sum_j \gamma_{ij} = \frac{1}{N} \right\}. \end{aligned}$$

Using Lemma 37 for each term, we have

$$\mathbb{W}_1(\mathbf{A}_\mu(x_i, \bullet), \mathbf{A}_\nu(y_j, \bullet)) \leq \tau(\Pi)\tau(L)\mathbb{W}_1(\Psi_{G(x_i, \bullet)}(\mu), \Psi_{G(y_j, \bullet)}(\nu)).$$

Now, from Proposition 27 (x_i belongs to $\text{supp}(\mu)$ and y_j to $\text{supp}(\nu)$), we get

$$\begin{aligned} &\mathbb{W}_1(\Psi_{G(x_i, \bullet)}(\mu), \Psi_{G(y_j, \bullet)}(\nu)) \\ &\leq \left[\sqrt{d} \sqrt{\ln N + \frac{1}{2e}} \|G\|_{Lip} + \|G\|_\infty + \sqrt{d} + 2 \right] (d(x_i, y_j) + \mathbb{W}_1(\mu, \nu)). \end{aligned}$$

Substituting this back into the above formula, we obtain

$$\begin{aligned} &\mathbb{W}_1(\mu \mathbf{A}_\mu, \nu \mathbf{A}_\nu) \\ &\leq \min \left\{ \sum_{i,j} \gamma_{ij} \mathbb{W}_1(\mathbf{A}_\mu(x_i, \bullet), \mathbf{A}_\nu(y_j, \bullet)) \mid \gamma_{i,j} \geq 0, \sum_i \gamma_{ij} = \frac{1}{M}, \sum_j \gamma_{ij} = \frac{1}{N} \right\} \\ &\leq \tau(\Pi)\tau(L) \min \left\{ \sum_{i,j} \gamma_{ij} \left[\sqrt{d} \sqrt{\ln N + \frac{1}{2e}} \|G\|_{Lip} + \|G\|_\infty + \sqrt{d} + 2 \right] (d(x_i, y_j) + \mathbb{W}_1(\mu, \nu)) \mid \right. \\ &\quad \left. \gamma_{i,j} \geq 0, \sum_i \gamma_{ij} = \frac{1}{M}, \sum_j \gamma_{ij} = \frac{1}{N} \right\} \\ &= \tau(\Pi)\tau(L) \left[\sqrt{d} \sqrt{\ln N + \frac{1}{2e}} \|G\|_{Lip} + \|G\|_\infty + \sqrt{d} + 2 \right] \left(\mathbb{W}_1(\mu, \nu) + \right. \\ &\quad \left. \min \left\{ \sum_{i,j} \gamma_{ij} d(x_i, y_j) \mid \gamma_{i,j} \geq 0, \sum_i \gamma_{ij} = \frac{1}{M}, \sum_j \gamma_{ij} = \frac{1}{N} \right\} \right) \\ &= \tau(\Pi)\tau(L) \left[\sqrt{d} \sqrt{\ln N + \frac{1}{2e}} \|G\|_{Lip} + \|G\|_\infty + \sqrt{d} + 2 \right] (\mathbb{W}_1(\mu, \nu) + \mathbb{W}_1(\mu, \nu)) \\ &= 2\tau(\Pi)\tau(L) \left[\sqrt{d} \sqrt{\ln N + \frac{1}{2e}} \|G\|_{Lip} + \|G\|_\infty + \sqrt{d} + 2 \right] \mathbb{W}_1(\mu, \nu), \end{aligned}$$

where we used in particular $\sum_{i,j} \gamma_{ij} = 1$. The inequality being valid for both M and N , taking the min gives the result. \square