

TRANSFORMERS THROUGH THE LENS OF SUPPORT-PRESERVING MAPS BETWEEN MEASURES

Anonymous authors

Paper under double-blind review

ABSTRACT

Transformers are deep architectures that define “in-context maps” which enable predicting new tokens based on a given set of tokens (such as a prompt in NLP applications or a set of patches for a vision transformer). Previous work has studied the ability of these architectures to handle an arbitrarily large number of context tokens. To mathematically, uniformly analyze their expressivity, previous work considered the case that the mappings are conditioned on a context represented by a probability distribution which becomes discrete for a finite number of tokens. Modeling neural networks as maps on probability measures has multiple applications, such as studying Wasserstein regularity, proving generalization bounds and doing a mean-field limit analysis of the dynamics of interacting particles as they go through the network. In this work, we study the question what kind of maps between measures are transformers. We fully characterize the properties of maps between measures that enable these to be represented in terms of in-context maps via a push forward. On the one hand, these include transformers; on the other hand, transformers universally approximate representations with any continuous in-context map. These properties are preserving the cardinality of support and that the regular part of their Fréchet derivative is uniformly continuous. Moreover, we show that the solution map of the Vlasov equation, which is of nonlocal transport type, for interacting particle systems in the mean-field regime for the Cauchy problem satisfies the conditions on the one hand and, hence, can be approximated by a transformer; on the other hand, we prove that the measure-theoretic self-attention has the properties that ensure that the infinite depth, mean-field measure-theoretic transformer can be identified with a Vlasov flow.

1 INTRODUCTION

Transformers have revolutionized the field of machine learning with their powerful attention mechanisms as introduced by Vaswani et al. (2017). The exceptional performance and expressivity of large-scale transformers have been empirically well established for both NLP (Brown et al. (2020)) and vision applications (Dosovitskiy et al. (2020)). One key property of these architectures is their ability to leverage contexts of arbitrary length, which enables the parameterization of “in-context” mappings with an arbitrarily large complexity. The previous work (Furuya et al. (2024)) studied this by analyzing the expressivity of mappings that are conditioned on a context represented by a probability distribution of tokens which becomes discrete for a finite number of these. By implication, transformers are viewed as maps between measures. Here, we present a full characterization of maps between measures that can be represented by these measure-theoretic transformers, that is, we address the question which class of mappings between measures can be identified with transformers.

Mathematical modeling of transformers. It is now customary to describe transformers as performing “in context” prediction, which means that it maps token to token, while this map depends on a set of previously seen tokens. The size of this context might be very long, possibly arbitrarily long, which has been addressed in Furuya et al. (2024) that concerns the transformers as universal in-context learners. The ability of trained transformers to effectively perform in-context computation has been supported by both empirical studies (von Oswald et al. (2023)) and theoretical ones (Ahn et al. (2024); Mahankali et al. (2023); Sander et al. (2024); Zhang et al. (2023)) on simplified

054 architectures (typically with linear attention) and specific data generation processes. The connection
055 between transformers and graph neural networks is exposed in Müller et al. (2023).

056
057 It has been noted that in order to make a comprehensive analysis of arbitrarily long token lengths,
058 and to describe a “mean-field” limit of an infinite number of tokens, it is natural to view attention
059 as operating over probability distributions of tokens (Vuckovic et al. (2020); Sander et al. (2022)).
060 The regularity (Lipschitz continuity) of the resulting attention layers was analyzed in Castin et al.
061 (2024).

062 Deep transformers (with residual or skip connections) have been described by a coupled system of
063 particles evolving across the layers. Such systems are fundamental in modeling phenomena across
064 physics, biology, and engineering. This connection has been exploited by Geshkovski et al. (2024)
065 who studied measure-to-measure interpolation using transformers. The analysis of the clustering
066 properties of such an evolution was studied in Geshkovski et al. (2023a;b). Biswal et al. (2024)
067 further investigate the use of transformers to approximate the mean-field dynamics of interacting
068 particle systems exhibiting collective behavior. They establish theoretical bounds on the distance
069 between the true mean-field dynamics and those obtained using a transformer, by lifting it from a
070 sequence-to-sequence map to a map on measures upon taking the expectation of a finite-dimensional
071 transformer with respect to a product measure. From a different viewpoint, this connection will
072 be further developed here, in general for mappings between measures satisfying the conditions to
073 be representable by measure-theoretic transformers. The structure of the interacting particle sys-
074 tem enables concrete connections to established mathematical topics, including nonlinear, nonlocal
075 transport equations, Wasserstein gradient flows, and collective behavior models.

076 **Universality of transformers.** Yun et al. (2019) provides, to the best of our knowledge, the most
077 detailed account of the universality of transformers. The authors rely on shallow transformers with
078 only two heads and require that the transformers operate over an embedding dimension which grows
079 with the number of tokens. This result is refined in Nath et al. (2024) and emphasizes the difficulty
080 of attention mechanisms to capture smooth functions.

081 We note that there exist variations of the original transformer’s architecture which enjoy universality
082 results, for instance, the Sumformer (Alberti et al. (2023)) and stochastic deep network (De Bie
083 et al. (2019)); these also require an embedding dimension that grows with the number of tokens. We
084 furthermore mention the introduction of probabilistic transformers (Kratsios et al. (2023)) which
085 can approximate embeddings of metric spaces. The work of Agrachev and Letrouit (2024) provides
086 an abstract universal interpolation result for equivariant architectures under genericity conditions;
087 however, it is not known whether there exist generic attention maps.

088 While this is not directly related to the analysis presented here, some works study the expressivity
089 of transformers when operating on a discrete set of tokens as formal systems (Chiang et al. (2023);
090 Merrill and Sabharwal (2023); Strobl et al. (2024); Elhage et al. (2021)). Another line of work
091 studies the impact of positional encoding on their expressivity (Luo et al. (2022)).

092 Furuya et al. (2024) provide a rigorous formalization of transformer expressivity and continuity
093 as operating over the space of probability distributions through its in-context mapping. The main
094 mathematical result is the universal approximation of in-context mappings for the unmasked and the
095 masked settings, considering deep transformers with a fixed embedding dimension, but which are
096 universal for an arbitrary number of tokens. A more constructive approach, although applicable to a
097 narrower class of functions, is proposed by Wang et al. (2024). Sander and Peyré (2024) introduce a
098 framework to analyze the expressivity of deep transformers in next-token prediction, while exploring
099 how successive attention layers solve a causal kernel least squares regression problem to predict the
100 next token accurately.

102 1.1 OUR CONTRIBUTIONS

103
104 The central question posed here, is whether a support-preserving map between measures can be
105 characterized as the push forward with an in-context map or not. We answer this question in the
106 affirmative by introducing a “certain” smoothness condition, which roughly entails that a “certain”
107 derivative of the map is uniformly continuous. We provide a counterexample, showing that this
condition is essential. Our proof is essentially constructive.

Applying this result and the underlying analysis, we prove that measure-theoretic transformers approximate such support-preserving maps, using the results of Furuya et al. (2024). This settles the full characterization of measure-theoretic transformers.

Finally, we show that the solution operator of the Vlasov equation, which is of nonlocal transport type, for the Cauchy problem satisfies the above mentioned condition(s) as a map between initial and final measures. This provides a bridge between interacting particle systems, in the mean-field regime, in the general context of measure-theoretic transformers. (A second-order generalization of measure-theoretic transformers yields a similar result for the solution operator of the kinetic Cucker-Smale equation (Biswal et al. (2024)).)

We first present the analysis relating support-preserving maps between measures with in-context maps that define measure-theoretic transformers. We later show, in an appendix, that “classical” transformers arise as a limiting case through (sub)sequences of discrete measures determined by tokens. The correspondence with Vlasov flows is established in the mean-field sense and is based on an infinite-depth limit.

1.2 NOTATION

Let $\Omega \subset \mathbb{R}^d$ be a compact set. We denote by $\mathcal{P}(\Omega)$ the space of probability measures on Ω . Below, all measures μ on subset Ω of \mathbb{R}^d are defined on the σ -algebra of the Borel sets of Ω . We denote by $C(\Omega)$ the space of continuous functions from Ω to \mathbb{R} , and the dual coupling between $\varphi \in C(\Omega)$ and $\mu \in \mathcal{P}(\Omega)$ by

$$\langle \varphi, \mu \rangle := \int_{\Omega} \varphi(x) d\mu(x).$$

We use the notations of Wasserstein distance as W_p for $1 \leq p < \infty$. We extend $\mathcal{P}(\Omega)$, that is, the set of all probability measures to the set of all strictly positive, finite measures

$$\mathcal{M}^+(\Omega) = \{s\mu : \mu \in \mathcal{P}(\Omega), s > 0\}.$$

We also extend the W_1 distance to $\mathcal{M}^+(\Omega)$ by defining for $\mu_1, \mu_2 \in \mathcal{P}(\Omega)$ and $s_1, s_2 > 0$

$$W_1(s_1\mu_1, s_2\mu_2) = W_1(\mu_1, \mu_2) + |s_1 - s_2|,$$

see Lombardini and Rossi (2022). We write

$$\mathcal{M}_{fin,(n)}^+(\Omega) := \left\{ \sum_{i=1}^n a_i \delta_{x_i} \in \mathcal{M}^+(\Omega) : x_i \in X, a_i > 0 \right\},$$

$$\mathcal{M}_{fin}^+(\Omega) := \bigcup_{n=1}^{\infty} \mathcal{M}_{fin,(n)}^+(\Omega) = \left\{ \sum_{i=1}^n a_i \delta_{x_i} \in \mathcal{M}^+(\Omega) : x_i \in \Omega, a_i > 0, n \in \mathbb{N} \right\}.$$

Finally, we denote by $\mathcal{M}_{fin,dif,(n)}^+(\Omega)$ the measures of the form $\mu = \sum_{i=1}^n a_i \delta_{x_i} \in \mathcal{M}_{fin,(n)}^+(\Omega)$, where $a_j > 0$ and for all non-empty subsets $J, K \subset \{1, 2, \dots, n\}$ satisfying $J \cap K = \emptyset$ it holds that

$$\sum_{j \in J} a_j \neq \sum_{k \in K} a_k.$$

We set $\mathcal{M}_{fin,dif}^+(\Omega) = \bigcup_{n=1}^{\infty} \mathcal{M}_{fin,dif,(n)}^+(\Omega)$. For a continuous map $g : \Omega \rightarrow \Omega$ and a measure μ the push-forward measure of μ in the map g is the measure $g_{\#}\mu(A) := \mu(g^{-1}(A))$, where $A \subset \Omega$ is an open set. For further details pertaining to these notions, we refer to Appendix A.1.

We state the following lemma, which is proved in Appendix B.1.

Lemma 1. $\mathcal{M}_{fin,dif}^+(\Omega)$ is dense in $\mathcal{M}^+(\Omega)$ in the 1-Wasserstein topology.

2 DEFINITIONS AND PROPERTIES OF THE RELEVANT MAPS

2.1 SUPPORT-PRESERVING MAPS AND IN-CONTEXT MAPS

Definition 1. We say that $f : \mathcal{M}^+(\Omega) \rightarrow \mathcal{M}^+(\mathbb{R}^d)$ is a support-preserving map if for all finitely supported measures of the form,

$$\mu = \sum_{i=1}^n a_i \delta_{x_i} \in \mathcal{M}_{fin}^+(\Omega), \quad (1)$$

where $a_i = \frac{c}{n}$, $c \in \mathbb{R}_+$, and $x_i \in \Omega$, there exist $y_1, \dots, y_n \in \mathbb{R}^{d'}$ such that

$$f(\mu) = \sum_{i=1}^n a_i \delta_{y_i} \in \mathcal{M}_{fin}^+(\mathbb{R}^{d'}) \quad (2)$$

and satisfy the condition

$$\text{if } x_j = x_i \text{ then } y_j = y_i. \quad (3)$$

The consideration of support-preserving maps to study transformers is natural; see Section 4.1 and formula (23) in Appendix A.3 and A.4 for a detailed discussion. Let $(x_1, x_2, \dots, x_n) \in \Omega^n$ be the sequences of n tokens in $\Omega \subset \mathbb{R}^d$, and let the union of all these be $X_d = \bigcup_{n=1}^{\infty} \Omega^n$. A sequence (x_1, x_2, \dots, x_n) can be identified with the probability measure $\mu = \sum_{i=1}^n \frac{1}{n} \delta_{x_i}$. We denote the corresponding identification map by $\iota : X_d \rightarrow \mathcal{P}_{fin}(\Omega)$,

$$\iota : (x_1, x_2, \dots, x_n) \rightarrow \sum_{i=1}^n \frac{1}{n} \delta_{x_i}. \quad (4)$$

Then a map $F : X_d \rightarrow X_{d'}$ that for any n maps a sequence (x_1, x_2, \dots, x_n) of d -dimensional tokens to a sequence (y_1, y_2, \dots, y_n) of d' -dimensional tokens so that the condition (3) is satisfied, defines a support-preserving map $f : \mathcal{M}_{fin}^+(\Omega) \rightarrow \mathcal{M}_{fin}^+(\mathbb{R}^{d'})$ that is the zero-homogeneous extension of the map $f = \iota \circ F \circ \iota^{-1} : \mathcal{P}_{fin}(\Omega) \rightarrow \mathcal{P}_{fin}(\mathbb{R}^{d'})$. This map satisfies $f(\sum_{i=1}^n \frac{1}{n} \delta_{x_i}) = \sum_{i=1}^n \frac{1}{n} \delta_{y_i}$. We consider the Wasserstein distance, which is a generalization of the permutation invariant distance of sequences of tokens. We recall that the 1-Wasserstein distance of the measures $\mu = \sum_{i=1}^n \frac{1}{n} \delta_{x_i}$ and $\mu' = \sum_{i=1}^n \frac{1}{n} \delta_{x'_i}$ is given by

$$W_1(\mu, \mu') = \min_{\sigma} \frac{1}{n} \sum_{i=1}^n |x_i - x'_{\sigma(i)}|,$$

where the minimum is taken over the permutations, $\sigma : \{1, 2, \dots, n\} \rightarrow \{1, 2, \dots, n\}$. For background material on basic transformers, we refer the reader to Appendix A.4. The convergence of the point measures toward continuous measures as $n \rightarrow \infty$, is discussed in Appendix A.3.

Lemma 2. *Let $f : \mathcal{M}^+(\Omega) \rightarrow \mathcal{M}^+(\mathbb{R}^{d'})$ be a support-preserving map that is continuous in the 1-Wasserstein metric. Then, for any measure of the form (1) with $a_i > 0$ we have that $f(\mu)$ is of the form (2) and satisfies condition (3).*

Lemma 2 can be proved by using sequences of points x_i of which several are equal and simply approximating a_i by rational numbers. The details of the proof Lemma 2 are given in Appendix B.2.

Definition 2. *We say that $f : \mathcal{M}^+(\Omega) \rightarrow \mathcal{M}^+(\mathbb{R}^{d'})$ is a support-preserving map given by an in-context map, $G : \mathcal{M}^+(\Omega) \times \Omega \rightarrow \mathbb{R}^{d'}$, if there exists such a map such that*

$$f(\mu) = G(\mu)_{\#}\mu,$$

where $G(\mu)$ is regarded as the map $x \mapsto G(\mu)(x) = G(\mu, x)$. We sometimes write $f = f_G$.

Note that for a measure $\mu = \sum_{i=1}^n \frac{1}{n} \delta_{x_i}$ it holds that $f_G(\mu) = \sum_{i=1}^n \frac{1}{n} \delta_{y_i}$, where $y_i = G(\mu, x_i)$. A particularly interesting example of such a map is $f_{\Gamma} : \mu \rightarrow \Gamma(\mu)_{\#}\mu$, where the function Γ is a multi-head self attention; see Section 4.1.

In Corollary 1, we revisit the connection between the maps in this definition and transformers. Our goal is to show that a support-preserving map f under a ‘‘certain’’ smoothness condition can be written in the form, f_G , with an in-context map, G . In the following subsection, we specify this ‘‘certain’’ smoothness in detail.

2.2 REGULAR PART OF THE DERIVATIVE

Definition 3. *Let $\eta, \rho > 0$. We consider triplets $(\mu, x, \psi) \in \mathcal{X}$, with*

$$\mathcal{X} = \mathcal{X}_{\Omega, \rho, \eta} := \{\mu \in \mathcal{M}^+(\Omega) : \mu(\Omega) \leq \rho\} \times \Omega \times \{\psi \in C_0^1(\mathbb{R}^{d'}) : \text{Lip}(\psi) \leq \eta\},$$

which is endowed with the distance function

$$D_{\mathcal{X}}((\mu_1, x_1, \psi_1), (\mu_2, x_2, \psi_2)) = W_1(\mu_1, \mu_2) + |x_1 - x_2| + \|\psi_1 - \psi_2\|_{L^\infty(\mathbb{R}^{d'})}. \quad (5)$$

We observe that $(\mathcal{X}, D_{\mathcal{X}})$ is not a complete metric space (i.e., the Cauchy sequences may not converge in \mathcal{X}), as the functions ψ are assumed to be in the space $C_0^1(\mathbb{R}^{d'})$, but we consider their convergence in $L^\infty(\mathbb{R}^{d'})$.

Definition 4. Let $f : \mathcal{M}^+(\Omega) \rightarrow \mathcal{M}^+(\mathbb{R}^{d'})$, and $(\mu, x, \psi) \in \mathcal{X}$. We define the L^∞ -regular part of the Fréchet derivative of f at (μ, x, ψ) by the limit

$$\overline{D}_f(\mu, x, \psi) := \lim_{k \rightarrow \infty} \lim_{\epsilon \rightarrow +0} \frac{\langle \psi_k, f(\mu_k + \epsilon \delta_x) - f(\mu_k) \rangle}{\epsilon} \quad (6)$$

for all $\psi_k \in C_0^1(\mathbb{R}^{d'})$ and $\mu_k \in \mathcal{M}^+(\Omega)$ such that

$$\psi_k \text{ is constant in an open neighborhood of } \text{supp}(f(\mu_k)) \quad (7)$$

and

$$\lim_{n \rightarrow \infty} W_1(\mu_k, \mu) = 0, \quad \lim_{n \rightarrow \infty} \|\psi_k - \psi\|_{L^\infty(\mathbb{R}^{d'})} = 0.$$

We note that the existence of the limit $\overline{D}_f(\mu, x, \psi)$ means that for all μ and ψ , the limits in (6) exist independently of the chosen sequences μ_k and ψ_k .

2.2.1. Motivational observations. Let f_G be a support-preserving map given by in-context map $G : \mathcal{M}^+(\Omega) \times \Omega \rightarrow \mathbb{R}^{d'}$, where $(\mu, x) \mapsto G(\mu, x)$ is continuous. We observe that for $\mu \in \mathcal{M}^+(\Omega)$, $x \in \Omega$ and $\psi \in C_0^1(\mathbb{R}^{d'})$,

$$\frac{\langle \psi, f_G(\mu + \epsilon \delta_x) - f_G(\mu) \rangle}{\epsilon} = \psi(G(\mu + \epsilon \delta_x, x)) + \int \frac{\psi(G(\mu + \epsilon \delta_x, y)) - \psi(G(\mu, y))}{\epsilon} d\mu(y).$$

Thus the limit as $\epsilon \rightarrow +0$ can be written as a sum of two terms

$$\lim_{\epsilon \rightarrow +0} \frac{\langle \psi, f_G(\mu + \epsilon \delta_x) - f_G(\mu) \rangle}{\epsilon} = D_{f_G}^{reg}(\mu, x, \psi) + D_{f_G}^{irreg}(\mu, x, \psi),$$

where

$$D_{f_G}^{reg}(\mu, x, \psi) := \lim_{\epsilon \rightarrow +0} \psi(G(\mu + \epsilon \delta_x, x)) = \psi(G(\mu, x))$$

and (if the limit exists)

$$D_{f_G}^{irreg}(\mu, x, \psi) := \lim_{\epsilon \rightarrow +0} \int \frac{\psi(G(\mu + \epsilon \delta_x, y)) - \psi(G(\mu, y))}{\epsilon} d\mu(y).$$

We call $D_{f_G}^{reg}(\mu, x, \psi)$ the L^∞ -regular part of the Fréchet derivative of f_G and $D_{f_G}^{irreg}(\mu, x, \psi)$ the L^∞ -irregular part of the Fréchet derivative. This terminology reflects the fact that $\psi \rightarrow D_{f_G}^{reg}(\mu, x, \psi)$ is continuous in the L^∞ -topology whereas $\psi \rightarrow D_{f_G}^{irreg}(\mu, x, \psi)$ is not. The lemma below states that $\overline{D}_{f_G}(\mu, x, \psi)$ is an extension of the regular part of the derivative $D_{f_G}^{reg}(\mu, x, \psi)$ for functions G .

In what follows, we refer to the L^∞ -regular part of the Fréchet derivative as the regular part of the derivative. The following lemma is proved in Appendix B.3.

Lemma 3. Let $\Omega \subset \mathbb{R}^d$ be a compact set and let a support-preserving map be given by the in-context map $G : \mathcal{M}^+(\Omega) \times \Omega \rightarrow \mathbb{R}^{d'}$, where $(\mu, x) \mapsto G(\mu, x)$ is continuous. Then, for $(\mu, x, \psi) \in \mathcal{X}$,

$$\overline{D}_{f_G}(\mu, x, \psi) = D_{f_G}^{reg}(\mu, x, \psi) = \psi(G(\mu, x))$$

and the map $\mathcal{X} \ni (\mu, x, \psi) \mapsto \overline{D}_{f_G}(\mu, x, \psi) \in \mathbb{R}$ is uniformly continuous with respect to the metric $D_{\mathcal{X}}$ defined in equation (5).

As we see in Lemma 3, for map f_G defined with a uniformly continuous in-context function G , the regular part of derivative $\overline{D}_{f_G}(\mu, x, \psi)$ coincides with the above defined object, $D_{f_G}^{reg}(\mu, x, \psi)$ on \mathcal{X} . So we consider $D_{f_G}^{reg}(\mu, x, \psi)$ as a new object that is different from the classical Fréchet derivative, and show that the definition of $D_{f_G}^{reg}(\mu, x, \psi)$ can be extended as a generalized regular part of the derivative, $\overline{D}_f(\mu, x, \psi)$, for a class of functions f , for which we do not assume that the classical Fréchet derivative is well-defined. For further remarks on the regular part of derivative $\overline{D}_f(\mu, x, \psi)$, see Appendix D.

3 MAIN RESULT

Our goal is to prove

Theorem 1. *Let $\Omega \subset \mathbb{R}^d$ be a compact set. Let $f : \mathcal{M}^+(\Omega) \rightarrow \mathcal{M}^+(\mathbb{R}^{d'})$ be a continuous map in the 1-Wasserstein topology. Then,*

(A1) *f is a map given by some in-context map G in the sense of Definition 2, i.e., $f = f_G$ with some function $G : \mathcal{M}^+(\Omega) \times \Omega \rightarrow \mathbb{R}^{d'}$; and*

(A2) *the function $(\mu, x) \rightarrow G(\mu, x)$ is continuous,*

if and only if

(B1) *f is a support-preserving map in the sense of Definition 1; and*

(B2) *the regular part of the derivative of f , $\overline{\mathcal{D}}_f(\mu, x, \psi)$, exists for all $(\mu, x, \psi) \in \mathcal{X}$, and the map $\mathcal{X} \ni (\mu, x, \psi) \rightarrow \overline{\mathcal{D}}_f(\mu, x, \psi) \in \mathbb{R}$ is uniformly continuous with respect to the metric $D_{\mathcal{X}}$ given by Definition 5.*

Moreover, the map $(\mu, x) \rightarrow G(\mu, x)$ is Lipschitz if and only if the map $\mathcal{X} \ni (\mu, x, \psi) \rightarrow \overline{\mathcal{D}}_f(\mu, x, \psi) \in \mathbb{R}$ is a Lipschitz map with respect to the metric $D_{\mathcal{X}}$.

Theorem 1 provides the characterization of support-preserving maps that can be represented by in-context maps through a push forward. Condition (B2) can be roughly described as the uniform continuity of a ‘‘certain’’ derivative of f , derived from Definition 4. The continuity of f is not sufficient for the theorem to hold as shown in the following proposition, that is proved in Appendix F.

Proposition 1. *Let $d = 1$ and $\Omega = [-3, 3] \subset \mathbb{R}$ and consider the set $\mathcal{P}(\Omega)$ endowed with the 1-Wasserstein topology. There exists a continuous, support-preserving map $f : \mathcal{P}(\Omega) \rightarrow \mathcal{P}(\Omega)$ such that there does not exist a continuous map $G : \mathcal{P}(\Omega) \times \Omega \rightarrow \Omega$ for which $f = f_G$.*

3.1 SKETCH OF THE PROOF OF THEOREM 1: (A1)-(A2) IMPLY (B1)-(B2)

In this section, we give a sketch of the main ideas of proof: Assume that (A1) and (A2) hold true. Then, let $f_G : \mathcal{M}^+(\Omega) \rightarrow \mathcal{M}^+(\mathbb{R}^{d'})$ be the map, $f_G(\mu) = G(\mu)_{\#}\mu$, with $G : \mathcal{M}^+(\Omega) \times \Omega \rightarrow \mathbb{R}^{d'}$. It is straightforward to prove (B1) and, hence, we will focus on proving that (B2) holds. We assume that $\psi_k, \psi \in C_0^1(\mathbb{R}^{d'})$ and $\mu_k, \mu \in \mathcal{M}_+(\Omega)$, $k = 1, 2, \dots$ are sequences with ψ_k is constant in an open neighborhood of $\text{supp}(f(\mu_k))$ and $\lim_{k \rightarrow \infty} W_1(\mu_k, \mu) = 0$, and $\lim_{k \rightarrow \infty} \|\psi_k - \psi\|_{L^\infty(\mathbb{R}^{d'})} = 0$. Let

$$\mu_{k,x}^\epsilon := \mu_k + \epsilon \delta_x.$$

Then, by a simple computation,

$$\langle f_G(\mu_{k,x}^\epsilon), \psi \rangle = \int_{\mathbb{R}^d} \psi_k(G(\mu_{k,x}^\epsilon, y)) d\mu_k(y) + \epsilon \psi_k(G(\mu_{k,x}^\epsilon, x)).$$

As the set $\Omega \subset \mathbb{R}^d$ is compact,

$$\mathcal{M}_\rho^+(\Omega) := \{\mu \in \mathcal{M}^+(\Omega) : \mu(\Omega) \leq \rho\},$$

is also compact by the Prokhorov’s theorem. Then the map $G : \mathcal{M}_\rho^+(\Omega) \times \Omega \rightarrow \mathbb{R}^{d'}$ is uniformly continuous. As $G(\mu_{k,x}^\epsilon, \cdot) \rightarrow G(\mu_k, \cdot)$ uniformly in $\Omega \subset \mathbb{R}^d$ as $\epsilon \rightarrow 0$, we see that

$$\sup_{y \in \text{supp}(\mu_k)} |G(\mu_{k,x}^\epsilon, y) - G(\mu_k, y)| \rightarrow 0 \quad \text{as } \epsilon \rightarrow 0.$$

Thus, we find that for sufficiently small $\epsilon \in (0, 1)$

$$\psi_k(G(\mu_{k,x}^\epsilon, y)) = \psi_k(G(\mu_k, y))$$

for all $y \in \text{supp}(\mu_k)$, and

$$\langle f_G(\mu_{k,x}^\epsilon), \psi_k \rangle = \int_{\mathbb{R}^d} \psi_k(G(\mu_k, y)) d\mu_k(y) + \epsilon \psi_k(G(\mu_k, x)).$$

This implies that

$$\overline{D}_{f_G}(\mu_k, x, \psi_k) = \lim_{\epsilon \rightarrow +0} \frac{\langle f_G(\mu_{k,x}^\epsilon), \psi_k \rangle - \langle f_G(\mu_k), \psi_k \rangle}{\epsilon} = \psi_k(G(\mu_k, y)).$$

Upon taking the limit $k \rightarrow \infty$, we obtain

$$\overline{D}_{f_G}(\mu, x, \psi) = \psi(G(\mu, y)).$$

From the uniform (Lipschitz) continuity of ψ and G , we can show that the regular part \overline{D}_{f_G} is uniformly (Lipschitz) continuous with respect to the metric $D_{\mathcal{X}}$. For the details of the proof, see Appendix C.1.

3.2 SKETCH OF THE PROOF OF THEOREM 1: (B1)-(B2) IMPLY (A1)-(A2)

Again, here, we give a sketch of the main ideas of the proof. Assume that (B1) and (B2) hold true. Since f is a support-preserving map, $f : \mathcal{M}^+(\Omega) \rightarrow \mathcal{M}^+(\mathbb{R}^{d'})$, there are (possibly non-continuous) functions,

$$y_i : \Omega^n \times (0, \infty)^n \rightarrow \mathbb{R}^{d'}, \quad (\mathbf{x}, \mathbf{a}) \rightarrow y_i(\mathbf{x}; \mathbf{a}), \quad i = 1, 2, \dots, n,$$

where $\mathbf{x} = (x_1, \dots, x_n)$ and $\mathbf{a} = (a_1, \dots, a_n)$, such that the following holds: Let $\mu = \sum_{i=1}^n a_i \delta_{x_i} \in \mathcal{M}_{fin}(\Omega)$, $a_i > 0$; then the functions $y_i(\mathbf{x}; \mathbf{a})$ satisfy

$$f(\mu) = \sum_{i=1}^n a_i \delta_{y_i(\mathbf{x}; \mathbf{a})}.$$

When $\mu \in \mathcal{M}_{fin, dif, (n)}^+(\Omega)$ (which is a refinement of the property that if $j \neq i$ then $a_j \neq a_i$), the functions $(\mathbf{x}; \mathbf{a}) \rightarrow y_i(\mathbf{x}; \mathbf{a})$ must have the property that if $x_j = x_i$ then $y_j(\mathbf{x}; \mathbf{a}) = y_i(\mathbf{x}; \mathbf{a})$.

We have the following lemma, which is proved in Appendix B.4.

Lemma 4. *Let $\mu_0 = \sum_{i=1}^n a_i^0 \delta_{x_i^0} \in \mathcal{M}_{fin, dif, (n)}^+(\Omega)$ and $\mu_p = \sum_{i=1}^n a_i^p \delta_{x_i^p} \in \mathcal{M}_{fin, (n)}^+(\Omega)$. Assume that for all $i = 1, 2, \dots, n$, it holds that $x_i^p \rightarrow x_i^0$ and $a_i^p \rightarrow a_i^0$ as $p \rightarrow \infty$. Then it holds for all $j \in [n]$, that*

$$\lim_{p \rightarrow \infty} y_j(\mathbf{x}^p; \mathbf{a}^p) = y_j(\mathbf{x}^0; \mathbf{a}^0).$$

We now return to the proof of Theorem 1. Let $\mu \in \mathcal{M}^+(\Omega)$ and $x \in \Omega$, and $\alpha \in C_0^\infty(\mathbb{R}^d)$ be a cutoff function such that $\alpha(x) = 1$ for all $x \in \Omega$ and $\text{Lip}(\alpha(x) \cdot x) \leq \eta$. We define

$$G(\mu, x) := \begin{pmatrix} \overline{D}_f(\mu, x, \alpha\pi_1) \\ \vdots \\ \overline{D}_f(\mu, x, \alpha\pi_{d'}) \end{pmatrix},$$

where $\pi_\ell : \mathbb{R}^d \rightarrow \mathbb{R}$ is the projection $\pi_\ell(x) = x_\ell$ onto the ℓ -th component. By (B2), the map $(\mu, x) \mapsto G(\mu, x)$ is continuous, which proves (A2). In what follows, we will prove (A1).

When $\mu \in \mathcal{M}_{fin, dif, (n)}^+(\Omega)$, using Lemma 4, we can prove that for each $j \in [n]$,

$$G(\mu, x_j) = y_j(\mathbf{x}; \mathbf{a}),$$

which is equivalent to

$$f(\mu) = (G_\mu)_\# \mu \quad \text{for } \mu \in \mathcal{M}_{fin, dif, (n)}^+(\Omega).$$

For the case $\mu \in \mathcal{M}^+(\Omega)$, we choose the sequence $(\tilde{\mu}_k)_{k \in \mathbb{N}} \subset \mathcal{M}_{fin, dif}^+(\Omega)$ such that $\tilde{\mu}_k \rightarrow \mu$ as $k \rightarrow \infty$, where the limit is considered in the 1-Wasserstein topology (which is possible by Lemma 1). We have already shown that for $\tilde{\mu}_k \in \mathcal{M}_{fin, dif}^+(\Omega)$,

$$f(\tilde{\mu}_k) = (G_{\tilde{\mu}_k})_\#(\tilde{\mu}_k).$$

Hence, by the uniform continuity of $(\mu, x) \mapsto G(\mu, x)$, the limit $k \rightarrow \infty$ converges,

$$f(\mu) = \lim_{k \rightarrow \infty} (G_{\tilde{\mu}_k})_\#(\tilde{\mu}_k) = (G_\mu)_\# \mu \quad \text{for } \mu \in \mathcal{M}^+(\Omega).$$

For the details of the proof, see Appendix C.2.

4 VLASOV FLOWS

Here, we present the close connections between support-preserving maps satisfying (B1) and (B2) in Theorem 1, Vlasov flows and measure-theoretic transformers.

4.1 INFINITELY DEEP MEASURE-THEORETIC TRANSFORMERS: UNIVERSAL APPROXIMATION AND THE VLASOV EQUATION

An in-context map as it appears in a single-layer ‘‘measure-theoretic’’ transformer Furuya et al. (2024); Castin et al. (2024) based on multi-head self attention, is of the form,

$$\Gamma : \mathcal{P}(\mathbb{R}^d) \times \mathbb{R}^d \rightarrow \mathbb{R}^d, \quad \Gamma(\mu, x) := x + \sum_{h=1}^H W^h \int_{\mathbb{R}^d} \frac{\exp\left(\frac{1}{\sqrt{k}}\langle Q^h x, K^h y \rangle\right)}{\int_{\mathbb{R}^d} \exp\left(\frac{1}{\sqrt{k}}\langle Q^h x, K^h z \rangle\right) d\mu(z)} V^h y d\mu(y),$$

see Appendix A.4 for corresponding functions operating to discrete measures and sequences of tokens. Here, K^h and Q^h are the multi-head key and query matrices in $\mathbb{R}^{k \times d}$, V^h are the multi-head value matrices in $\mathbb{R}^{d_{head} \times d}$, and W^h are the multi-head weight matrices in $\mathbb{R}^{d \times d_{head}}$, respectively. By abuse of notation, $\Gamma(\mu)(x) = \Gamma(\mu, x)$ defines a map $\mathbb{R}^d \rightarrow \mathbb{R}^d$. For two in-context maps, Γ_1 and Γ_2 , the composition $\Gamma_2 \diamond \Gamma_1$ is defined as

$$(\mu, x) \mapsto (\Gamma_2 \diamond \Gamma_1)(\mu, x) := \Gamma_2(\nu, \Gamma_1(\mu, x)), \quad \nu := \Gamma_1(\mu) \# \mu. \quad (8)$$

With this composition, the in-context map, G_{tran} say, for a multi-layer measure-theoretic transformer is obtained. To be precise, the composition should alternate between in-context maps and context-free MLPs, $F(\mu, x) = F(x)$ say. When restricted to finite discrete empirical measures of the form $\frac{1}{n} \sum_{i=1}^n \delta_{x_i}$, $f_{\text{tran}} := f_{G_{\text{tran}}}$ (cf. Definition 2) reduces to a classical transformer acting on a sequence of tokens, (x_1, \dots, x_n) rather than on a measure μ . For more details, see (Furuya et al., 2024, Section 2). Being based on multi-head self attention, G_{tran} is (locally) Lipschitz Castin et al. (2024), and, hence, satisfies (A2) in Theorem 1.

As a consequence of Theorem 1, f_{tran} satisfies (B1) and (B2), while using (Furuya et al., 2024, Theorem 1), we obtain the following universal approximation result that is prove in Appendix B.5.

Corollary 1. *Let $f : \mathcal{M}^+(\Omega) \rightarrow \mathcal{M}^+(\mathbb{R}^d)$ satisfy (B1) and (B2) in Theorem 1. Then, for any $\epsilon \in (0, 1)$, there exists a sufficiently deep measure-theoretic transformer, f_{tran} , (that is, a deep composition of multi-head self attention maps and MLPs), such that*

$$\sup_{\mu \in \mathcal{P}(\Omega)} W_1(f_{\text{tran}}(\mu), f(\mu)) \leq \epsilon.$$

Next, we consider a MLP $F_\eta : \mathbb{R}^d \rightarrow \mathbb{R}^d$, see (54) in Appendix A.4, and the attention function

$$\text{Att}_\xi : \mathcal{P}(\mathbb{R}^d) \times \mathbb{R}^d \rightarrow \mathbb{R}^d, \quad \text{Att}_\xi(\mu, x) := \sum_{h=1}^H W^h \int_{\mathbb{R}^d} \frac{\exp\left(\frac{1}{\sqrt{k}}\langle Q^h x, K^h y \rangle\right)}{\int_{\mathbb{R}^d} \exp\left(\frac{1}{\sqrt{k}}\langle Q^h x, K^h z \rangle\right) d\mu(z)} V^h y d\mu(y).$$

where η and ξ are sets of parameter matrices for MLPs and the attention, respectively. Let us write the MLP F_η as $F_\eta = Id_x + H_\eta$, and define $\mathcal{V} = \text{Att}_\xi + H_\eta \circ (Id_x + \text{Att}_\xi)$, so that $F_\eta(\Gamma_\xi(\mu, x)) = x + \mathcal{V}(\mu, x)$, see formulas (59) and (60) in Appendix E for detailed formulas. Again, by abuse of notation, $\mathcal{V}(\mu)(x) = \mathcal{V}(\mu, x)$ defines a map or vector field, $\mathbb{R}^d \rightarrow \mathbb{R}^d$. We consider layers, $x_i(\tau + 1) = F_{\eta_\tau}(\Gamma_{\xi_\tau}(\mu_i(\tau), x_i(\tau)))$, where the sets η_τ and ξ_τ of parameter matrices depend on τ . Then, we find that

$$x_i(\tau + 1) - x_i(\tau) = \mathcal{V}_\tau(\mu_\tau)(x_i(\tau)), \quad \text{where } \mu_\tau(\cdot) = \frac{1}{n} \sum_{i=1}^n \delta_{x_i(\tau)}(\cdot) \text{ and } \tau = 0, 1, 2, \dots, T.$$

Taking the continuum limit, scaling \mathcal{V}_τ with $1/T$, where T signifies the number of layers, and identifying the layer index, τ , with $t \in [0, 1]$ that corresponds to the limit of values τ/T as $T \rightarrow \infty$, the tokens that evolve according to an infinitely deep transformer satisfy

$$\dot{x}_i(t) = \mathcal{V}_t(\mu_t)(x_i(t)) \quad (9)$$

for all $i \in [n]$, where $\mu_t(\cdot) = \frac{1}{n} \sum_{i=1}^n \delta_{x_i(t)}(\cdot)$, and $t \in [0, 1]$; see also Zhong et al. (2022). This is extended to positive measures by the partial differential, nonlocal transport equation,

$$\partial_t \mu_t + \operatorname{div}(\mathcal{V}_t(\mu_t)\mu_t) = 0 \quad \text{on } [0, 1] \times \mathbb{R}^d, \quad (10)$$

$$\mu_t|_{t=0} = \mu_0 \quad \text{on } \mathbb{R}^d \quad (11)$$

in the sense of distributions, replacing the (neural) ODE in (9); see Renardy and Rogers (2004). It basically follows from

$$\begin{aligned} \frac{d}{dt} \int_{\mathbb{R}^d} \varphi(t, x) d\mu_t(x) &= \frac{d}{dt} \frac{1}{n} \sum_{i=1}^n \varphi(t, x_i(t)) \\ &= \int_{\mathbb{R}^d} (\partial_t \varphi(t, x) + \langle \nabla_x \varphi(t, x), \mathcal{V}_t(\mu_t)(x) \rangle) d\mu_t(x) \end{aligned} \quad (12)$$

for all $\varphi \in C_c^\infty([0, 1] \times \mathbb{R}^d)$, and integrating by parts. Thus, an infinitely deep measure-theoretic transformer without MLPs, with $\mu_t := f_{\text{tran};t}^\infty(\mu_0)$, $t \in (0, 1]$, is argued to satisfy the Vlasov equation; see Piccoli et al. (2015) and Paul and Trélat (2024). Some prior work Sander et al. (2022); Geshkovski et al. (2025); Castin et al. (2025) already discussed that the mean-field (with respect to tokens) and deep transformers are associated with nonlocal transport PDEs. Moreover, the infinitely deep in-context map, $G_{\text{tran};t}^\infty$, satisfies an evolution equation in spacetime that generalizes the equation (9) for the point measures,

$$\partial_t G_{\text{tran};t}^\infty(\mu_0, x) = \mathcal{V}_t(\mu_t)(G_{\text{tran};t}^\infty(\mu_0, x)), \quad G_{\text{tran};0}^\infty(\mu_0, x) = x.$$

4.2 THE SOLUTION MAP OF THE VLASOV EQUATION SATISFIES (B1) AND (B2) OF THEOREM 1

Piccoli et al. (2015) studied the well-posedness of nonlocal transport PDEs having the form,

$$\partial_t \mu_t + \operatorname{div}(V(t, \mu_t)\mu_t) = 0, \quad \mu_t|_{t=0} = \mu_0, \quad (13)$$

where $\mu = \mu_t = \mu(t)$ is a time-dependent probability measure on \mathbb{R}^d and $V(\cdot, \mu) : \mathbb{R} \times \mathbb{R}^d \rightarrow \mathbb{R}^d$ is a C^1 -smooth vector field that depends on $(t, x) \in \mathbb{R} \times \mathbb{R}^d \rightarrow \mathbb{R}^d$ and the measure μ . The vector field $V(\mu)$ is called the velocity field.

Under the assumptions on V required by (Piccoli et al., 2015, Theorem 2.3), there exists a unique solution of (13). Moreover, the solution at time t , μ_t can be written as

$$\mu_t = G_t(\mu_0) \# \mu_0,$$

where G_t is defined as the unique solution of the following Cauchy problem,

$$\partial_t G_t(\mu_0, x) = V(t, \mu_t)(G_t(\mu_0, x)), \quad G_0(\mu_0, x) = x.$$

Thus, we can define the solution map $f_T : \mathcal{P}(\Omega) \rightarrow \mathcal{P}(\mathbb{R}^d)$ (the solution at time $t = T$) by

$$f_T(\mu_0) := \mu_T. \quad (14)$$

The map, f_T , is a support-preserving map given by the in-context map, G_T . The following proposition is proved Appendix B.6.

Proposition 2. *Under the assumptions for V required by (Piccoli et al., 2015, Theorem 2.3), the solution map, f_T , defined by (14) satisfies (B1) and (B2). That is, the solution map f_T of the Vlasov flow can be represented as a map $f_{G_T} : \mu \rightarrow G_T(\mu) \# \mu$ with a continuous in-context map G_T .*

5 CONCLUSION AND DISCUSSION

In this work, we fully characterize mappings between measures that can be universally approximated by measure-theoretic transformers. To this end, we introduce a ‘‘certain’’ smoothness condition, which roughly entails that a ‘‘certain’’ derivative of the mapping is uniformly continuous. A limitation of our method is that it is not quantitative. We make rigorous a connection between particle systems and mappings between measures through measure-theoretic transformers in the mean-field regime, which connection has been discussed in various works before. This has implications in the framing of LLMs. Beyond the Vlasov equation, it will be interesting to study the BBGKY hierarchy describing the dynamics of a system of a large number of interacting particles (see, for example, Golse (2016)) with measure-theoretic transformers.

REFERENCES

- 486
487
488 Andrei Agrachev and Cyril Letrouit. Generic controllability of equivariant systems and applications
489 to particle systems and neural networks. *arXiv preprint arXiv:2404.08289*, 2024.
- 490 Kwangjun Ahn, Xiang Cheng, Hadi Daneshmand, and Suvrit Sra. Transformers learn to imple-
491 ment preconditioned gradient descent for in-context learning. *Advances in Neural Information*
492 *Processing Systems*, 36, 2024.
- 493
494 Silas Alberti, Niclas Dern, Laura Thesing, and Gitta Kutyniok. Sumformer: Universal approxi-
495 mation for efficient transformers. In *Topological, Algebraic and Geometric Learning Workshops*
496 *2023*, pages 72–86. PMLR, 2023.
- 497 Patrick Billingsley. *Convergence of probability measures*. Wiley Series in Probability and Statis-
498 tics: Probability and Statistics. John Wiley & Sons, Inc., New York, second edition, 1999.
499 ISBN 0-471-19745-9. doi: 10.1002/9780470316962. URL [https://doi.org/10.1002/](https://doi.org/10.1002/9780470316962)
500 [9780470316962](https://doi.org/10.1002/9780470316962). A Wiley-Interscience Publication.
- 501
502 Shiba Biswal, Karthik Elamvazhuthi, and Rishi Sonthalia. Universal approximation of mean-field
503 models via transformers. *arXiv preprint arXiv:2410.16295*, 2024.
- 504 Tom Brown, Benjamin Mann, Nick Ryder, Melanie Subbiah, Jared D Kaplan, Prafulla Dhariwal,
505 Arvind Neelakantan, Pranav Shyam, Girish Sastry, Amanda Askell, et al. Language models are
506 few-shot learners. *Advances in neural information processing systems*, 33:1877–1901, 2020.
- 507
508 Valérie Castin, Pierre Ablin, and Gabriel Peyré. How smooth is attention? In *ICML 2024*, 2024.
- 509 Valérie Castin, Pierre Ablin, José Antonio Carrillo, and Gabriel Peyré. A unified perspective on the
510 dynamics of deep transformers. *arXiv preprint arXiv:2501.18322*, 2025.
- 511
512 David Chiang, Peter Cholak, and Anand Pillay. Tighter bounds on the expressivity of transformer
513 encoders. In *International Conference on Machine Learning*, pages 5544–5562. PMLR, 2023.
- 514
515 Gwendoline De Bie, Gabriel Peyré, and Marco Cuturi. Stochastic deep networks. In *International*
516 *Conference on Machine Learning*, pages 1556–1565. PMLR, 2019.
- 517 Alexey Dosovitskiy, Lucas Beyer, Alexander Kolesnikov, Dirk Weissenborn, Xiaohua Zhai, Thomas
518 Unterthiner, Mostafa Dehghani, Matthias Minderer, Georg Heigold, Sylvain Gelly, et al. An
519 image is worth 16x16 words: Transformers for image recognition at scale. *arXiv preprint*
520 *arXiv:2010.11929*, 2020.
- 521
522 Nelson Elhage, Neel Nanda, Catherine Olsson, Tom Henighan, Nicholas Joseph, Ben Mann,
523 Amanda Askell, Yuntao Bai, Anna Chen, Tom Conerly, et al. A mathematical framework for
524 transformer circuits. *Transformer Circuits Thread*, 1(1):12, 2021.
- 525 Takashi Furuya, Maarten V de Hoop, and Gabriel Peyré. Transformers are universal in-context
526 learners. *arXiv preprint arXiv:2408.01367*, 2024.
- 527
528 Borjan Geshkovski, Cyril Letrouit, Yury Polyanskiy, and Philippe Rigollet. The emergence of clus-
529 ters in self-attention dynamics. *arXiv preprint arXiv:2305.05465*, 2023a.
- 530 Borjan Geshkovski, Cyril Letrouit, Yury Polyanskiy, and Philippe Rigollet. A mathematical per-
531 spective on transformers. *arXiv preprint arXiv:2312.10794*, 2023b.
- 532
533 Borjan Geshkovski, Philippe Rigollet, and Domènec Ruiz-Balet. Measure-to-measure interpolation
534 using transformers. *arXiv preprint arXiv:2411.04551*, 2024.
- 535
536 Borjan Geshkovski, Cyril Letrouit, Yury Polyanskiy, and Philippe Rigollet. A mathematical per-
537 spective on transformers. *Bulletin of the American Mathematical Society*, 62(3):427–479, 2025.
- 538 François Golse. On the dynamics of large particle systems in the mean field limit. In *Macroscopic*
539 *and large scale phenomena: coarse graining, mean field limits and ergodicity*, pages 1–144.
Springer, 2016.

- 540 Achim Klenke. *Probability theory—a comprehensive course*. Universitext. Springer, Cham, 2020.
 541 ISBN 978-3-030-56402-5. doi: 10.1007/978-3-030-56402-5. URL [https://doi.org/10.](https://doi.org/10.1007/978-3-030-56402-5)
 542 [1007/978-3-030-56402-5](https://doi.org/10.1007/978-3-030-56402-5). Third edition [of 2372119].
 543
- 544 Konik Kothari, AmirEhsan Khorashadizadeh, Maarten V. de Hoop, and Ivan Dokmanić. Trum-
 545 pets: Injective flows for inference and inverse problems. In *Conference on Uncertainty in*
 546 *Artificial Intelligence*, 2021. URL [https://api.semanticscholar.org/CorpusID:](https://api.semanticscholar.org/CorpusID:231985888)
 547 [231985888](https://api.semanticscholar.org/CorpusID:231985888).
- 548 Anastasis Kratsios, Valentin Debarnot, and Ivan Dokmanić. Small transformers compute universal
 549 metric embeddings. *Journal of Machine Learning Research*, 24(170):1–48, 2023.
 550
- 551 Luca Lombardini and Francesco Rossi. Obstructions to extension of Wasserstein distances for
 552 variable masses. *Proc. Amer. Math. Soc.*, 150(11):4879–4890, 2022. ISSN 0002-9939. doi:
 553 [10.1090/proc/16030](https://doi.org/10.1090/proc/16030). URL <https://doi.org/10.1090/proc/16030>.
- 554 Shengjie Luo, Shanda Li, Shuxin Zheng, Tie-Yan Liu, Liwei Wang, and Di He. Your transformer
 555 may not be as powerful as you expect. *Advances in Neural Information Processing Systems*, 35:
 556 4301–4315, 2022.
 557
- 558 Arvind Mahankali, Tatsunori B Hashimoto, and Tengyu Ma. One step of gradient descent is
 559 provably the optimal in-context learner with one layer of linear self-attention. *arXiv preprint*
 560 *arXiv:2307.03576*, 2023.
- 561 William Merrill and Ashish Sabharwal. The expressive power of transformers with chain of
 562 thought. *arXiv preprint arXiv:2310.07923*, 2023.
 563
- 564 Luis Müller, Mikhail Galkin, Christopher Morris, and Ladislav Rampásek. Attending to graph
 565 transformers. *arXiv preprint arXiv:2302.04181*, 2023.
 566
- 567 Swaroop Nath, Harshad Khadilkar, and Pushpak Bhattacharyya. Transformers are expressive, but
 568 are they expressive enough for regression? *arXiv preprint arXiv:2402.15478*, 2024.
- 569 Thierry Paul and Emmanuel Trélat. From microscopic to macroscopic scale equations: mean field,
 570 hydrodynamic and graph limits, 2024. URL <https://arxiv.org/abs/2209.08832>.
 571
- 572 Benedetto Piccoli, Francesco Rossi, and Emmanuel Trélat. Control to flocking of the kinetic cucker-
 573 smale model. *SIAM Journal on Mathematical Analysis*, 47(6):4685–4719, 2015.
- 574 Michael Reed and Barry Simon. *Methods of modern mathematical physics. I*. Academic Press, Inc.
 575 [Harcourt Brace Jovanovich, Publishers], New York, second edition, 1980. ISBN 0-12-585050-6.
 576 Functional analysis.
 577
- 578 Michael Renardy and Robert C Rogers. *An introduction to partial differential equations*. Springer,
 579 2004.
 580
- 581 Michael E Sander and Gabriel Peyré. Towards understanding the universality of transformers for
 582 next-token prediction. *arXiv preprint arXiv:2410.03011*, 2024.
- 583 Michael E Sander, Pierre Ablin, Mathieu Blondel, and Gabriel Peyré. Sinkformers: Transform-
 584 ers with doubly stochastic attention. In *International Conference on Artificial Intelligence and*
 585 *Statistics*, pages 3515–3530. PMLR, 2022.
 586
- 587 Michael E Sander, Raja Giryes, Taiji Suzuki, Mathieu Blondel, and Gabriel Peyré. How do trans-
 588 formers perform in-context autoregressive learning? *arXiv preprint arXiv:2402.05787*, 2024.
- 589 Filippo Santambrogio. Optimal transport for applied mathematicians. *Birkäuser, NY*, 55(58-63):94,
 590 2015.
 591
- 592 Lena Strobl, William Merrill, Gail Weiss, David Chiang, and Dana Angluin. What formal lan-
 593 guages can transformers express? a survey. *Transactions of the Association for Computational*
Linguistics, 12:543–561, 2024.

594 S. S. Vallender. Calculation of the wasserstein distance between probability distributions on the
595 line. *Theory of Probability & Its Applications*, 18(4):784–786, 1974. doi: 10.1137/1118101.
596 URL <https://doi.org/10.1137/1118101>.
597

598 Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N Gomez,
599 Łukasz Kaiser, and Illia Polosukhin. Attention is all you need. *Advances in neural informa-*
600 *tion processing systems*, 30, 2017.

601 Johannes von Oswald, Eyvind Niklasson, Maximilian Schlegel, Seijin Kobayashi, Nicolas Zucchet,
602 Nino Scherrer, Nolan Miller, Mark Sandler, Max Vladymyrov, Razvan Pascanu, et al. Uncovering
603 mesa-optimization algorithms in transformers. *arXiv preprint arXiv:2309.05858*, 2023.
604

605 James Vuckovic, Aristide Baratin, and Remi Tachet des Combes. A mathematical theory of atten-
606 tion. *arXiv preprint arXiv:2007.02876*, 2020.

607 Mingze Wang et al. Understanding the expressive power and mechanisms of transformer for se-
608 quence modeling. *Advances in Neural Information Processing Systems*, 37:25781–25856, 2024.
609

610 Chulhee Yun, Srinadh Bhojanapalli, Ankit Singh Rawat, Sashank J Reddi, and Sanjiv Kumar.
611 Are transformers universal approximators of sequence-to-sequence functions? *arXiv preprint*
612 *arXiv:1912.10077*, 2019.

613 Ruiqi Zhang, Spencer Frei, and Peter L Bartlett. Trained transformers learn linear models in-context.
614 *arXiv preprint arXiv:2306.09927*, 2023.

615

616 Yaofeng Desmond Zhong, Tongtao Zhang, Amit Chakraborty, and Biswadip Dey. A neural ode
617 interpretation of transformer layers. *arXiv preprint arXiv:2212.06011*, 2022.
618
619
620
621
622
623
624
625
626
627
628
629
630
631
632
633
634
635
636
637
638
639
640
641
642
643
644
645
646
647

648 A NOTATION AND A SUMMARY OF RESULTS OF MEASURE THEORY

649 A.1 NOTATIONS

650 Let $\Omega \subset \mathbb{R}^d$ be a compact set. We denote by $\mathcal{P}(\Omega)$ the space of probability measures on Ω . Below,
651 all measures μ on subset Ω of \mathbb{R}^d are defined on the σ -algebra of the Borel sets of Ω . We denote by
652 $C(\Omega)$ the space of continuous functions from Ω to \mathbb{R} , and the dual coupling between $\varphi \in C(\Omega)$ and
653 $\mu \in \mathcal{P}(\Omega)$ by

$$654 \langle \varphi, \mu \rangle := \int_{\Omega} \varphi(x) d\mu(x).$$

655 With the weak* topology on $\mathcal{P}(\Omega)$, we have the convergence of sequences of measures,

$$656 \mu_k \rightharpoonup^* \mu \Leftrightarrow \left(\forall \varphi \in C_0(\Omega), \langle \varphi, \mu_k \rangle \rightarrow \langle \varphi, \mu \rangle \right).$$

657 In the case when Ω is compact, the weak* topology is equivalent to the topology of the Wasserstein
658 distance W_p ($1 \leq p < \infty$), meaning that

$$659 \mu_k \rightharpoonup^* \mu \Leftrightarrow W_p(\mu_k, \mu) \rightarrow 0,$$

660 see e.g., (Santambrogio, 2015, Theorem 5.10). By the duality theorem of Kantorovich and Rubin-
661 stein, when $\mu, \nu \in \mathcal{P}(\Omega)$, where Ω is compact, we have that

$$662 W_1(\mu, \nu) = \sup \left\{ \int_{\Omega} \varphi(x) d(\mu - \nu)(x) \mid \varphi : \Omega \rightarrow \mathbb{R} \text{ continuous, } \text{Lip}(\varphi) \leq 1 \right\},$$

663 where

$$664 \text{Lip}(\varphi) := \sup_{x \neq y} \frac{|\varphi(x) - \varphi(y)|}{|x - y|}$$

665 denotes the Lipschitz constant for $\varphi : \Omega \rightarrow \mathbb{R}$.

666 We extend $\mathcal{P}(\Omega)$, that is, the set of all probability measures to the set of all strictly positive, finite
667 measures

$$668 \mathcal{M}^+(\Omega) = \{s\mu : \mu \in \mathcal{P}(\Omega), s > 0\}.$$

669 We also extend the W_1 distance to $\mathcal{M}^+(\Omega)$ by defining for $\mu_1, \mu_2 \in \mathcal{P}(\Omega)$ and $s_1, s_2 > 0$

$$670 W_1(s_1\mu_1, s_2\mu_2) = W_1(\mu_1, \mu_2) + |s_1 - s_2|,$$

671 see Lombardini and Rossi (2022). Using this extension, we can extend the map $f : \mathcal{P}(\Omega) \rightarrow \mathcal{P}(\mathbb{R}^d)$
672 to a map between positive measures invoking m -homogeneity ($m \in \mathbb{N}_0$) according to

$$673 f(s\mu) = s^m f(\mu) \quad \text{for all } s \in \mathbb{R}_+.$$

674 We write

$$675 \mathcal{M}_{fin}^+(\Omega) := \left\{ \sum_{i=1}^n a_i \delta_{x_i} \in \mathcal{M}^+(\Omega) : x_i \in \Omega, a_i > 0, n \in \mathbb{N} \right\},$$

676 and

$$677 \mathcal{M}_{fin,(n)}^+(\Omega) := \left\{ \sum_{i=1}^n a_i \delta_{x_i} \in \mathcal{M}^+(\Omega) : x_i \in X, a_i > 0 \right\}.$$

678 Finally, we denote by $\mathcal{M}_{fin,dif,(n)}^+(\Omega)$ the measures of the form

$$679 \mu = \sum_{i=1}^n a_i \delta_{x_i} \in \mathcal{M}_{fin,(n)}^+(\Omega),$$

680 where $a_j > 0$ and for all non-empty subsets $J, K \subset \{1, 2, \dots, n\}$ satisfying $J \cap K = \emptyset$ it holds that

$$681 \sum_{j \in J} a_j \neq \sum_{k \in K} a_k.$$

682 We set $\mathcal{M}_{fin,dif}^+(\Omega) = \bigcup_{n=1}^{\infty} \mathcal{M}_{fin,dif,(n)}^+(\Omega)$. For $\mu \in \mathcal{M}_{fin,dif,(n)}^+(\Omega)$ we define the minimal
683 gap

$$684 \text{gap}(\mu) = \min_{J, K \subset \{1, 2, \dots, n\}, J \cap K = \emptyset, J \neq \emptyset} \left| \sum_{j \in J} a_j - \sum_{k \in K} a_k \right|. \quad (15)$$

702 A.2 PUSH FORWARDS OF MEASURES

703
704 We will consider push forwards of measures in various maps. When ν is a general Borel measure
705 on set $\Omega \subset \mathbb{R}^d$ and $F : \Omega \rightarrow \mathbb{R}^{d'}$ is a continuous map, the push-forward measure of ν in the map F ,
706 denoted by $F_{\#}\nu$, is the measure that for an open (or Borel measurable) set A is defined to be

$$707 F_{\#}\nu(A) = \nu(F^{-1}(A)).$$

708
709 When $\mu = \sum_{j=1}^n a_j \delta_{x_j}$ is a discrete measure supported at points x_1, \dots, x_n , we have

$$710 F_{\#}\mu = \sum_{j=1}^n a_j \delta_{y_j}, \quad y_j = F(x_j).$$

711
712 When $\nu = \rho(x)dx$ is a continuous measure where $\rho : \mathbb{R}^d \rightarrow [0, \infty)$ is a continuous function and dx
713 is the Lebesgue measure on \mathbb{R}^d and $F : \mathbb{R}^d \rightarrow \mathbb{R}^d$ is a differentiable map which inverse function
714 $F^{-1} : \mathbb{R}^d \rightarrow \mathbb{R}^d$ is differentiable, then

$$715 F_{\#}(\rho(x)dx) = \tau(x)dx, \quad \text{where } \tau(x) = \rho(F^{-1}(x)) \cdot \left| \det \left(\frac{\partial F}{\partial x}(F^{-1}(x)) \right) \right|,$$

716
717 where $\det \left(\frac{\partial F}{\partial x}(F^{-1}(x)) \right)$ is the determinant of the Jacobian matrix of the function F evaluated at
718 the point $F^{-1}(x)$.

719
720 When $F : \mathbb{R}^d \rightarrow \mathbb{R}^{d'}$ is a smooth injective map and $d' > d$, the push forward of the measures μ
721 on \mathbb{R}^d to the d -dimensional image manifold $M = F(\mathbb{R}^d)$ of F are discussed e.g. in Kothari et al.
722 (2021).

723 A.3 CONVERGENCE OF POINT MEASURES TO A GENERAL MEASURE

724
725 Let us consider the convergence of discrete measures $\mu_n = \sum_{j=1}^n a_{n,j} \delta_{x_{n,j}}$ to continuous measures.
726 Let $\Omega \subset \mathbb{R}^d$ be a compact set, $x_{n,j} \in \Omega$, and $a_{n,j} > 0$ are such that $\sum_{j=1}^n a_{n,j} = 1$. If for all
727 relatively open subsets $U \subset \Omega$ there exists limits

$$728 m(U) = \lim_{n \rightarrow \infty} \mu_n(U), \quad \text{where } \mu_n(U) = \sum_{x_{n,j} \in U} a_{n,j}, \quad (16)$$

729 then the limits $m(U)$ define a (Borel) probability measure in $m \in \mathcal{P}(\Omega)$ and the measures μ_n
730 converge in the 1-Wasserstein topology to the measure m .

731
732 By the Portmanteau theorem, see Klenke (2020), Theorem 13.16 (see also Remark 13.14), the existence
733 of limits (16) is equivalent to following conditions:

734 (C1) There is a probability measure $m \in \mathcal{P}(\Omega)$ such that $m(U) \geq \liminf_{n \rightarrow \infty} \mu_n(U)$ for all
735 relatively open sets $U \subset \Omega$

736 (C2) There is a probability measure $m \in \mathcal{P}(\Omega)$ such that for all Lipschitz functions $\phi : \Omega \rightarrow \mathbb{R}$

$$737 \int_{\Omega} \phi d\mu_n = \sum_{j=1}^n a_{n,j} \phi(x_{n,j}) \rightarrow \int_{\Omega} \phi dm, \quad \text{as } n \rightarrow \infty, \quad (17)$$

738
739 that is, the existence of limits $m(U)$ in (16) and the conditions (C1) and (C2) are all equivalent to
740 that μ_n converge weakly to m that is further equivalent to that μ_n converge to m in the 1-Wasserstein
741 topology.

742
743 In particular, consider the case when $x_{n,j} = x_j$ are independent of n and $a_{n,j} = 1/n$. Also, let us
744 consider the Lipschitz functions $\phi : \Omega \rightarrow \mathbb{R}$ as feature functions. That is the measures, μ_n are the
745 point measures

$$746 \mu_n = \sum_{j=1}^n \frac{1}{n} \delta_{x_j}$$

747
748 that correspond to prompts $X_n = (x_1, x_2, \dots, x_n)$, that is, sequences of n tokens. Then, if the
749 the prompt length n goes to infinity, it follows from Prokhorov's theorem (Klenke, 2020, Theorem

13.29 and Corollary 13.30), that there is at least one sub-sequence X_{n_k} of prompts, where $n_k \rightarrow \infty$ as $k \rightarrow \infty$ such that for all feature functions $\phi \in C^{0,1}(\Omega)$ the averages of the features

$$\int_{\Omega} \phi d\mu_{n_k} = \sum_{j=1}^{n_k} \frac{1}{n_k} \phi(x_j)$$

converge to some limit

$$\lim_{k \rightarrow \infty} \int_{\Omega} \phi d\mu_{n_k} = \int_{\Omega} \phi d\mu,$$

These limits define a probability measure $\mu \in \mathcal{P}(\Omega)$ such that

$$\lim_{k \rightarrow \infty} W_1(\mu_{n_k}, \mu) = 0. \quad (18)$$

Moreover, by (Reed and Simon, 1980, Theorems I.13 and I.14), the measure μ can be written as a sum of three measures,

$$\mu = \nu_1 + \nu_2 + \nu_3, \quad \nu_1 = \sum_{i=1}^N a_j \delta_{y_j}, \quad \nu_2 = \rho(x) dx, \quad \nu_3 \perp dx \quad (19)$$

where ν_1 is a pure point measure supported at the points $y_j \in \Omega$ with $N \in \mathbb{N} \cup \{\infty\}$ and $a_j > 0$, ν_2 is an absolutely continuous measure having the density $\rho(x)$ with respect to the Lebesgue measure dx of \mathbb{R}^d , and ν_3 is a singular continuous measure, that is, there is a set $S \subset \Omega$ which the Lebesgue measure is zero such that $\nu_3(\Omega \setminus S) = 0$ and $\nu_3(\{p\}) = 0$ for all singleton sets with $p \in \Omega$.

A.4 ATTENTION AND TRANSFORMERS

Finally we recall notations related to attention functions. The multi-head self attention is the function

$$\begin{aligned} \Gamma : \mathcal{P}(\mathbb{R}^d) \times \mathbb{R}^d &\rightarrow \mathbb{R}^d, \\ \Gamma(\mu, x) &= x + \sum_{h=1}^H W^h \int_{\mathbb{R}^d} \frac{\exp\left(\frac{1}{\sqrt{k}} \langle Q^h x, K^h y \rangle\right)}{\int_{\mathbb{R}^d} \exp\left(\frac{1}{\sqrt{k}} \langle Q^h x, K^h z \rangle\right) d\mu(z)} V^h y d\mu(y) \\ &= x + \text{Att}(\mu, x). \end{aligned} \quad (20)$$

We recall that here K^h and Q^h are the multi-head key and query matrices in $\mathbb{R}^{k \times d}$, V^h are the multi-head value matrices in $\mathbb{R}^{d_{head} \times d}$, and W^h are the multi-head weight matrices in $\mathbb{R}^{d \times d_{head}}$, respectively. When

$$\mu = \sum_{i=1}^n \frac{1}{n} \delta_{x_i} \quad (21)$$

is a discrete measure corresponding to a sequence x_1, x_2, \dots, x_n of points in $\Omega \subset \mathbb{R}^d$, it holds that

$$\begin{aligned} \Gamma(\mu, x) &= x + \sum_{h=1}^H W^h \int_{\mathbb{R}^d} \frac{\exp\left(\frac{1}{\sqrt{k}} \langle Q^h x, K^h y \rangle\right)}{\int_{\mathbb{R}^d} \exp\left(\frac{1}{\sqrt{k}} \langle Q^h x, K^h z \rangle\right) d\mu(z)} V^h y d\mu(y) \\ &= x + \sum_{h=1}^H W^h \sum_{\ell=1}^n \frac{\exp\left(\frac{1}{\sqrt{k}} (Q^h x)^\top (K^h x_\ell)\right)}{\sum_{j=1}^n \exp\left(\frac{1}{\sqrt{k}} (Q^h x)^\top (K^h x_j)\right)} V^h x_\ell, \end{aligned} \quad (22)$$

where v^\top denotes the transpose of a column vector $v \in \mathbb{R}^k$.

For the measure μ given in (21) it holds that

$$f_\Gamma\left(\sum_{i=1}^n \frac{1}{n} \delta_{x_i}\right) = \Gamma(\mu, \cdot) \# \mu = \sum_{i=1}^n \frac{1}{n} \delta_{y_i}, \quad (23)$$

where $y_i = \Gamma(\mu, x_i)$.

In the case that the measures $\mu_{n_k} = \sum_{i=1}^{n_k} \frac{1}{n} \delta_{x_i}$ converge in 1-Wasserstein topology to a measure μ as $k \rightarrow \infty$, we have pointwise limits

$$\lim_{k \rightarrow \infty} \Gamma(\mu_{n_k}, x) = \Gamma(\mu, x), \quad (24)$$

where $\Gamma(\mu_{n_k}, x)$ and $\Gamma(\mu, x)$ are given in formulas (22) and (20), respectively. Moreover, it holds that the push forwards of the measures satisfy the limit

$$\lim_{k \rightarrow \infty} \Gamma(\mu_{n_k}, \cdot) \# \mu_{n_k} = \Gamma(\mu, \cdot) \# \mu \quad (25)$$

in the 1-Wasserstein topology.

Let us next consider the prompts (x_1, x_2, \dots, x_n) and the corresponding discrete measures $\mu_n = \sum_{i=1}^n \frac{1}{n} \delta_{x_i}$. As seen above, then there exists at least one sub-sequence μ_{n_k} that converge to a general probability measure $\mu \in \mathcal{P}(\Omega)$, that is a sum of a point measure, a continuous measure, and a measure that are singular with respect to the standard measure of \mathbb{R}^d , see formula (19). Thus, to understand properties of transformers it is useful to consider mappings between general probability measures that have the same properties of the transformers.

B PROOFS FOR TECHNICAL PARTS

B.1 PROOF OF LEMMA 1

Proof. Let $\mu \in \mathcal{M}^+(\Omega)$ and let $\epsilon \in (0, 1)$. Since $\mathcal{M}_{fin}^+(\Omega)$ is dense in $\mathcal{M}^+(\Omega)$ in 1-Wasserstein topology, there is $\mu_k \in \mathcal{M}_{fin,dif}^+(\Omega)$ with $\mu_k = \sum_{i=1}^n a_i \delta_{x_i}$, $a_i > 0$ such that

$$W_1(\mu_k, \mu) \leq \epsilon.$$

We can choose $\tilde{a}_1, \dots, \tilde{a}_n > 0$ such that $|\tilde{a}_j - a_j| < \epsilon/n$ and, for any non-empty disjoint subsets $J, K \subset \{1, \dots, n\}$, it holds that

$$\sum_{i \in J} \tilde{a}_i \neq \sum_{i \in K} \tilde{a}_i.$$

Indeed, setting $\tilde{a}_i = a_i + \eta_i$, the equality

$$\sum_{i \in J} \tilde{a}_i = \sum_{i \in K} \tilde{a}_i,$$

is equivalent to

$$\sum_{i \in J} \eta_i - \sum_{i \in K} \eta_i = \underbrace{\sum_{i \in K} a_i - \sum_{i \in J} a_i}_{=:\Delta_{J,K}}.$$

Since the set $\cup_{J,K} \{\eta \in \mathbb{R}^n : \sum_{i \in J} \eta_i - \sum_{i \in K} \eta_i = \Delta_{J,K}\}$ of affine hyperplanes are measure-zero set, we can choose small $|\eta_i| < \epsilon/n$ so that

$$\eta \notin \bigcup_{J,K} \left\{ \eta \in \mathbb{R}^n : \sum_{i \in J} \eta_i - \sum_{i \in K} \eta_i = \Delta_{J,K} \right\}.$$

Thus, defining by $\tilde{\mu}_n = \sum_{i=1}^n \tilde{a}_i \delta_{x_i} \in \mathcal{M}_{fin,dif}^+(\Omega)$, we see that

$$W_1(\mu_k, \tilde{\mu}_n) < \epsilon.$$

We have proved Lemma 1. □

B.2 PROOF OF LEMMA 2

Proof. When $\tilde{x}_j \in \Omega$, $\tilde{a}_j > 0$, $j = 1, 2, \dots, \tilde{n}$ are of the form $\tilde{a}_j = cm_j$ where $c > 0$ and $m_j \in \mathbb{Z}_+$, we can write the measure

$$\mu = \sum_{j=1}^{\tilde{n}} \tilde{a}_j \delta_{\tilde{x}_j} \quad (26)$$

864 in the form

$$865 \mu = \sum_{i=1}^n \frac{\mu(\Omega)}{n} \delta_{x_i}, \quad (27)$$

866 where $n = \sum_{j=1}^{\tilde{n}} m_j$ and x_1, x_2, \dots, x_n is a sequence where each point \tilde{x}_j appears m_j times. As f
867 is a support preserving map, there are $y_i \in \mathbb{R}^{d'}$, $i = 1, 2, \dots, n$, such that

$$871 f(\mu) = \sum_{i=1}^n \frac{\mu(\Omega)}{n} \delta_{y_i}. \quad (28)$$

872 Moreover, $y_{i_1} = y_{i_2}$ if $x_{i_1} = x_{i_2}$. Hence, we can write $f(\mu)$ in the form

$$876 f(\mu) = \sum_{j=1}^{\tilde{n}} \left(\sum_{i: x_i = \tilde{x}_j} \frac{\mu(\Omega)}{n} \right) \delta_{y_i} \\ 877 = \sum_{j=1}^{\tilde{n}} \frac{cm_j}{n} \delta_{\tilde{y}_j} \quad (29)$$

882 where $c = \mu(\Omega)$ and the set $\{\tilde{y}_1, \dots, \tilde{y}_{\tilde{n}}\}$ contains the same points as the set $\{y_1, \dots, y_n\}$. Below,
883 we denote $\tilde{X} = (\tilde{x}_1, \dots, \tilde{x}_{\tilde{n}})$ and $Y_j(\tilde{X}, \mu) := \tilde{y}_j$. The above shows that the claim is valid when the
884 a_j are of the form $a_j = cm_j$, $m_j \in \mathbb{Z}_+$.

885 We now consider general values, $a_i > 0$, and points, $x_i \in \Omega$, $i = 1, \dots, n$ and let $c = \sum_{i=1}^n a_i$. We
886 let $N_k, m_{k,i} \in \mathbb{Z}_+$, $i = 1, \dots, n$, $k \in \mathbb{Z}_+$ be such that

$$888 \lim_{k \rightarrow \infty} \frac{m_{k,i}}{N_k} = a_i \quad \text{for all } i = 1, 2, \dots, n.$$

889 Also, we let $c_k = c/N_k$ and

$$891 \mu_k = \sum_{i=1}^n c_k m_{k,i} \delta_{x_i}. \quad (30)$$

894 We write $X = (x_1, \dots, x_n)$. Then, as we have already shown that the claim is valid for measures
895 μ_k of the form (30), we can write $f(\mu_k)$ as

$$897 f(\mu_k) = \sum_{i=1}^n c_k m_{k,i} \delta_{Y_i(X, \mu_k)} = \sum_{i=1}^n \frac{m_{k,i}}{N_k} \delta_{Y_i(X, \mu_k)} \in \mathcal{M}_{fin, (n)}^+(\Omega). \quad (31)$$

899 As f is a continuous map in the 1-Wasserstein topology and the set $\mathcal{M}_{fin, (n)}^+(\Omega)$ is a closed subset
900 of $\mathcal{M}^+(\Omega)$ in the same topology and $\mathcal{M}^+(\Omega)$ is a complete space, we conclude that there exists a
901 limit

$$903 f(\mu) = \lim_{k \rightarrow \infty} f(\mu_k) \in \mathcal{M}_{fin, (n)}^+(\Omega). \quad (32)$$

904 Thus we can write $f(\mu)$ in the form,

$$906 f(\mu) = \sum_{j=1}^{n'} b_j \delta_{z_j}, \quad (33)$$

907 with some $n' \leq n$, $z_j \in \Omega$ and $b_j > 0$. We choose

$$911 \rho = \min\{|z_{j_1} - z_{j_2}| : j_1, j_2 \in [n'], j_1 \neq j_2\} > 0$$

912 and let $A = \min_j a_j > 0$. Moreover, as $f(\mu_k) \rightarrow f(\mu)$ in the 1-Wasserstein metric as $k \rightarrow \infty$,
913 we observe that for each k there is a partition of the set $\{1, 2, \dots, n\}$ to a union of disjoint sets,
914 $I_{1,k}, \dots, I_{n',k}$, such that when k is sufficiently large,

$$916 \sum_{j=1}^{n'} \frac{A}{4} \min_{i \in I_{j,k}} \text{dist}(Y_i(X, \mu_k), z_j) + \frac{1}{4} \sum_{j=1}^{n'} \left| \left(\sum_{i \in I_{j,k}} \frac{m_{k,i}}{N_k} \right) - b_j \right| \leq W_1(f(\mu_k), f(\mu)).$$

As $W_1(f(\mu_k), f(\mu)) \rightarrow 0$ as $k \rightarrow \infty$, we find that by replacing μ_k by its suitable subsequence, we can assume that the partition $I_{1,k}, \dots, I_{n',k}$ is equal to a partition $I_1, \dots, I_{n'}$ that is independent of k , and

$$Y_i(X, \mu_k) \rightarrow z_i, \quad \text{as } k \rightarrow \infty. \quad (34)$$

Moreover,

$$\sum_{i \in I_j} a_i = \sum_{i \in I_j} \lim_{k \rightarrow \infty} \frac{m_{k,i}}{N_k} = b_j \quad (35)$$

for $j = 1, 2, \dots, n'$. Then $b_j = \sum_{i \in I_j} a_i$, and

$$f(\mu) = \sum_{j=1}^{n'} \left(\sum_{i \in I_j} a_i \right) \delta_{z_j} = \sum_{i=1}^n a_i \delta_{y_i}, \quad (36)$$

where y_1, \dots, y_n is a sequence of the points $z_1, \dots, z_{n'}$ where each z_j appears $|I_j|$ times. This proves the claim for general weights $a_i > 0$. \square

B.3 PROOF OF LEMMA 3

Proof. Let $f_G : \mathcal{M}^+(\Omega) \rightarrow \mathcal{M}^+(\mathbb{R}^{d'})$ be the map, $f_G(\mu) = G(\mu) \# \mu$, with a continuous map $G : \mathcal{M}^+(\Omega) \times \Omega \rightarrow \mathbb{R}^{d'}$. We assume that $\psi_k, \psi \in C_0^1(\mathbb{R}^{d'})$ and $\mu_k, \mu \in \mathcal{M}_+(\Omega)$, $k = 1, 2, \dots$ are sequences with

$$\psi_k \text{ is constant in an open neighborhood of } \text{supp}(f(\mu_k))$$

and

$$\lim_{k \rightarrow \infty} W_1(\mu_k, \mu) = 0, \quad \lim_{k \rightarrow \infty} \|\psi_k - \psi\|_{L^\infty(\mathbb{R}^{d'})} = 0.$$

Let

$$\mu_{k,x}^\epsilon := \mu_k + \epsilon \delta_x.$$

Then, by the simple computation,

$$\langle f_G(\mu_{k,x}^\epsilon), \psi \rangle = \int_{\mathbb{R}^d} \psi_k(G(\mu_{k,x}^\epsilon, y)) d\mu_k(y) + \epsilon \psi_k(G(\mu_{k,x}^\epsilon, x)).$$

As the set $\Omega \subset \mathbb{R}^d$ is compact,

$$\mathcal{M}_\rho^+(\Omega) := \{\mu \in \mathcal{M}^+(\Omega) : \mu(\Omega) \leq \rho\}$$

is also compact by the Prokhorov's theorem. Then, the map $G : \mathcal{M}_\rho^+(\Omega) \times \Omega \rightarrow \mathbb{R}^{d'}$ is uniformly continuous. As $G(\mu_{k,x}^\epsilon, \cdot) \rightarrow G(\mu_k, \cdot)$ uniformly in $\Omega \subset \mathbb{R}^d$ as $\epsilon \rightarrow 0$, we see that

$$\sup_{y \in \text{supp}(\mu_k)} |G(\mu_{k,x}^\epsilon, y) - G(\mu_k, y)| \rightarrow 0 \quad \text{as } \epsilon \rightarrow 0.$$

Thus, we find that for sufficiently small $\epsilon \in (0, 1)$

$$\psi_k(G(\mu_{k,x}^\epsilon, y)) = \psi_k(G(\mu_k, y))$$

for all $y \in \text{supp}(\mu_k)$, and

$$\langle f_G(\mu_{k,x}^\epsilon), \psi_k \rangle = \int_{\mathbb{R}^d} \psi_k(G(\mu_k, y)) d\mu_k(y) + \epsilon \psi_k(G(\mu_k, x)).$$

This implies that

$$\overline{D}_{f_G}(\mu_k, x, \psi_k) = \lim_{\epsilon \rightarrow +0} \frac{\langle f_G(\mu_{k,x}^\epsilon), \psi_k \rangle - \langle f_G(\mu_k), \psi_k \rangle}{\epsilon} = \psi_k(G(\mu_k, x)).$$

Upon taking the limit $k \rightarrow \infty$, we obtain

$$\overline{D}_{f_G}(\mu, x, \psi) = \psi(G(\mu, x)).$$

Next, we prove that the map $(\mu, y, \psi) \rightarrow \overline{\mathcal{D}}_{f_G}(\mu, y, \psi)$ is uniformly continuous. Let $\epsilon_1 > 0$. By the uniform continuity of G , there is a $\delta_1 = \delta_1(\epsilon_1) \in (0, \epsilon_1)$ such that if $W_1(\mu_1, \mu_2) < \delta_1(\epsilon_1)$ and $|y_1 - y_2| < \delta_1(\epsilon_1)$ then $|G(\mu_1, y_1) - G(\mu_2, y_2)| < \epsilon_1/2$. Let $(\mu_1, y_1, \psi_1), (\mu_2, y_2, \psi_2) \in \mathcal{X}$ so that $\text{Lip}(\psi_j) \leq \eta$ for $j = 1, 2$. Also, assume that $\|\psi_1 - \psi_2\|_{L^\infty} < \delta_1(\epsilon_1)$. We then see that

$$\begin{aligned} |\overline{\mathcal{D}}_{f_G}(\mu_1, y_1, \psi_1) - \overline{\mathcal{D}}_{f_G}(\mu_2, y_2, \psi_2)| &= |\psi_1(G(\mu_1, y_1)) - \psi_2(G(\mu_2, y_2))| \\ &\leq |\psi_1(G(\mu_1, y_1)) - \psi_1(G(\mu_2, y_2))| \\ &\quad + |\psi_1(G(\mu_2, y_2)) - \psi_2(G(\mu_2, y_2))| \\ &\leq \text{Lip}(\psi_1)|G(\mu_1, y_1) - G(\mu_2, y_2)| + \|\psi_1 - \psi_2\|_{L^\infty} \\ &\leq \text{Lip}(\psi_1)\epsilon_1 + \delta_1(\epsilon_1) \\ &\leq (\eta + 1)\epsilon_1. \end{aligned}$$

We observe that if $D_{\mathcal{X}}((\mu_1, y_1, \psi_1), (\mu_2, y_2, \psi_2)) < \delta_1(\epsilon_1)$ then $W_1(\mu_1, \mu_2) < \delta_1(\epsilon_1)$ and $|y_1 - y_2| < \delta_1(\epsilon_1)$, and moreover that $\|\psi_1 - \psi_2\|_{L^\infty} < \delta_1(\epsilon_1)$. We conclude that $(\mu, y, \psi) \rightarrow \overline{\mathcal{D}}_{f_G}(\mu, y, \psi)$ is uniformly continuous. \square

B.4 PROOF OF LEMMA 4

Proof. The assumptions imply that $W_1(\mu_p, \mu_0) \rightarrow 0$ as $p \rightarrow \infty$. Hence, as f is continuous in the 1-Wasserstein distance, it holds that $W_1(f(\mu_p), f(\mu_0)) \rightarrow 0$ as $p \rightarrow \infty$. If the claim is not valid, there are k and $(\mathbf{x}^p, \mathbf{a}^p)$ such that $(\mathbf{x}^p, \mathbf{a}^p) \rightarrow (\mathbf{x}^0, \mathbf{a}^0)$ as $p \rightarrow \infty$ and $\mu_0 = \sum_{i=1}^n a_i^0 \delta_{x_i^0} \in \mathcal{M}_{f \text{ in, dif, } (n)}(\Omega)$, and the sequence $y_k(\mathbf{x}^p; \mathbf{a}^p)$, $p \in \mathbb{Z}_+$, does not converge to the value $y_k(\mathbf{x}^0; \mathbf{a}^0)$ as $p \rightarrow \infty$. By replacing $(\mathbf{x}^p; \mathbf{a}^p)$ by its suitable subsequence, we can assume that there exists $z \in \mathbb{R}^{d'}$ such that

$$\lim_{p \rightarrow \infty} y_k(\mathbf{x}^p; \mathbf{a}^p) = z \neq y_k(\mathbf{x}^0; \mathbf{a}^0). \quad (37)$$

As all a_i^0 are strictly positive and $a_i^p \rightarrow a_i^0$, there are $b > 0$ and p_0 such that we have $a_i^p > b$ for all $p > p_0$ and i . As $f(\mu_p) = \sum_{k=1}^n a_k^p \delta_{y_k(\mathbf{x}^p; \mathbf{a}^p)} \rightarrow f(\mu_0)$ in 1-Wasserstein distance, we see that

$$\lim_{p \rightarrow \infty} \sup_{y \in \text{supp}(f(\mu_p))} \text{dist}(y, \text{supp}(f(\mu_0))) = 0.$$

This and (37) imply that there is $k_0 \neq k$ such that

$$\lim_{p \rightarrow \infty} y_{k_0}(\mathbf{x}^p; \mathbf{a}^p) = y_{k_0}(\mathbf{x}^0; \mathbf{a}^0) \neq y_k(\mathbf{x}^0; \mathbf{a}^0). \quad (38)$$

Then, as (38) holds, we find that

$$\lim_{p \rightarrow \infty} |y_k(\mathbf{x}^p; \mathbf{a}^p) - y_k(\mathbf{x}^0; \mathbf{a}^0)| \geq \min\{|y - y'| : y, y' \in \text{supp}(f(\mu_0)), y \neq y'\} > 0$$

and that the measures $\mu_p = \sum_{i=1}^n a_i^p \delta_{x_i^p}$ and $\mu_0 = \sum_{i=1}^n a_i^0 \delta_{x_i^0}$ and their images under f , that is,

$$f(\mu_p) = \sum_{i=1}^n a_i^p \delta_{y_i(\mathbf{x}^p; \mathbf{a}^p)} \quad \text{and} \quad f(\mu_0) = \sum_{i=1}^n a_i^0 \delta_{y_i(\mathbf{x}^0; \mathbf{a}^0)},$$

satisfy the inequality

$$\lim_{p \rightarrow \infty} W_1(f(\mu_p), f(\mu_0)) \geq \text{gap}(\mu_0) \min\{|y - y'| : y, y' \in \text{supp}(f(\mu_0)), y \neq y'\} > 0,$$

where $\text{gap}(\mu_0)$ is defined in (15). This is not possible in view of the 1-Wasserstein continuity of f . Thus, the claim follows. \square

B.5 PROOF OF COROLLARY 1

Proof. Using Theorem 1, there is an in-context map G such that $f(\mu) = G(\mu)_{\#}\mu$. Since the map G is continuous, by using (Furuya et al., 2024, Theorem 1), for any $\epsilon \in (0, 1)$, there is a measure-theoretic transformer-style in-context mapping $G_{\text{tran}} := F_{\xi_L} \diamond \Gamma_{\theta_L} \diamond \dots \diamond F_{\xi_1} \diamond \Gamma_{\theta_1}$ such that

$$\sup_{(\mu, x) \in \mathcal{P}(\Omega) \times \Omega} |G_{\text{tran}}(\mu, x) - G(\mu, x)| \leq \epsilon,$$

1026 which implies that, by the duality theorem of Kantorovich and Rubinstein,
1027

$$1028 \quad W_1(f_{\text{tran}}(\mu), f(\mu)) = \sup_{\text{Lip}(\varphi) \leq 1} \int \varphi(G_{\text{tran}}(\mu, x)) - \varphi(G(\mu, x)) d\mu(x)$$

$$1029 \quad \leq \int |G_{\text{tran}}(\mu, x) - G(\mu, x)| d\mu(x) \leq \epsilon.$$

1030
1031
1032 We have proved Corollary 1. □

1033 B.6 PROOF OF PROPOSITION 2

1034
1035
1036 *Proof.* By (Piccoli et al., 2015, Theorem 2.3), there exists $G_t : \mathcal{P}(\Omega) \times \Omega \rightarrow \mathbb{R}^d$ such that

$$1037 \quad \mu_t = G_t(\mu_0) \# \mu_0,$$

1038 where G_t is defined by the unique solution of the following Cauchy problem

$$1039 \quad \partial_t G_t(\mu_0, x) = V[\mu(t)](t, G_t(\mu_0, x)), \quad G_0(\mu_0, x) = x. \quad (39)$$

1040 This is a push forward, thus the solution map, f , satisfies (B1). Moreover, if the map $(\mu, x) \mapsto$
1041 $G_T(\mu, x)$ is Lipschitz continuous, by Lemma 3 the map $(\mu, x, \psi) \mapsto \bar{\mathcal{D}}_{f_T}(\mu, x, \psi)$ is Lipschitz
1042 continuous with respect to the metric $D_{\mathcal{X}}$. This implies (B2). In what follows, we will prove that
1043 the map $(\mu, x) \mapsto G_T(\mu, x)$ is Lipschitz continuous.

1044 We estimate, for $\mu_0, \nu_0 \in \mathcal{P}(\Omega)$ and $x, y \in \Omega$,

$$1045 \quad \frac{d}{dt} \|G_t(\mu_0, x) - G_t(\nu_0, y)\|_2$$

$$1046 \quad \leq \left\| \frac{d}{dt} G_t(\mu_0, x) - \frac{d}{dt} G_t(\nu_0, y) \right\|_2 = \|V[\mu(t)](t, G_t(\mu_0, x)) - V[\nu(t)](t, G_t(\nu_0, x))\|_2$$

$$1047 \quad \leq \|V[\mu(t)](t, G_t(\mu_0, x)) - V[\mu(t)](t, G_t(\nu_0, x))\|_2$$

$$1048 \quad \quad + \|V[\mu(t)](t, G_t(\nu_0, x)) - V[\nu(t)](t, G_t(\nu_0, x))\|_2$$

$$1049 \quad \leq L(t) \|G_t(\mu_0, x) - G_t(\nu_0, x)\|_2 + K(t) W_1(\mu(t), \nu(t))$$

$$1050 \quad \leq L(t) \|G_t(\mu_0, x) - G_t(\nu_0, x)\|_2 + K(t) e^{C_T t} W_1(\mu_0, \nu_0),$$

1051 for some $K, L \in L_{loc}^\infty(\mathbb{R})$ and some $C_T > 0$. Here, we have used the assumption of Lipschitz
1052 continuity required in (Piccoli et al., 2015, Theorem 2.3), and the stability estimate (Piccoli et al.,
1053 2015, (2.3)). By Gronwall's inequality, we find that

$$1054 \quad \|G_t(\mu_0, x) - G_t(\nu_0, x)\|_2$$

$$1055 \quad \leq e^{A(t)} \underbrace{\|G_0(\mu_0, x) - G_0(\nu_0, x)\|_2}_{=\|x-y\|_2} + \left(\int_0^t e^{A(t)-A(s)} K(s) e^{C_T s} ds \right) W_1(\mu_0, \nu_0),$$

1056 where $A(t) = \int_0^t L(s) ds$. Thus, substituting $t = T$, there exists $C'_T > 0$ such that

$$1057 \quad \|G_T(\mu_0, x) - G_T(\nu_0, x)\|_2 \leq C'_T (W_1(\mu_0, \nu_0) + \|x - y\|_2),$$

1058 which implies that the map $(\mu, x) \mapsto G_T(\mu, x)$ is Lipschitz continuous. □

1059 C PROOF OF THEOREM 1

1060 C.1 PART 1 : (A1)-(A2) IMPLY (B1)-(B2)

1061 Assume that (A1) and (A2) hold true. Then, let $f_G : \mathcal{M}^+(\Omega) \rightarrow \mathcal{M}^+(\mathbb{R}^{d'})$ be the map, $f_G(\mu) =$
1062 $G(\mu) \# \mu$, with $G : \mathcal{M}^+(\Omega) \times \Omega \rightarrow \mathbb{R}^{d'}$. It is straightforward to prove (B1) and, hence, we will focus
1063 on proving that (B2) holds. We assume that $\psi_k, \psi \in C_0^1(\mathbb{R}^{d'})$ and $\mu_k, \mu \in \mathcal{M}_+(\Omega)$, $k = 1, 2, \dots$
1064 are sequences with

$$1065 \quad \psi_k \text{ is constant in an open neighborhood of } \text{supp}(f(\mu_k))$$

1080 and

$$1081 \quad \lim_{k \rightarrow \infty} W_1(\mu_k, \mu) = 0, \quad \lim_{k \rightarrow \infty} \|\psi_k - \psi\|_{L^\infty(\mathbb{R}^{d'})} = 0.$$

1082 Let

$$1083 \quad \mu_{k,x}^\epsilon := \mu_k + \epsilon \delta_x.$$

1084 Then

$$1085 \quad \begin{aligned} 1086 \quad \langle f_G(\mu_{k,x}^\epsilon), \psi \rangle &= \langle (G(\mu_{k,x}^\epsilon)) \# \mu_{k,x}^\epsilon, \psi_k \rangle \\ 1087 &= \langle \mu_{k,x}^\epsilon, \psi_k \circ G(\mu_{k,x}^\epsilon, \cdot) \rangle \\ 1088 &= \int_{\mathbb{R}^d} \psi_k(G(\mu_{k,x}^\epsilon, y)) d\mu_{k,x}^\epsilon(y) \\ 1089 &= \int_{\mathbb{R}^d} \psi_k(G(\mu_{k,x}^\epsilon, y)) d\mu_k(y) + \epsilon \psi_k(G(\mu_{k,x}^\epsilon, x)). \end{aligned}$$

1090 By (A2), $(\mu, x) \rightarrow G(\mu, x)$ is a continuous function. As the set $\Omega \subset \mathbb{R}^d$ is compact, for any $\rho > 0$
1091 the set

$$1092 \quad \mathcal{M}_\rho^+(\Omega) := \{\mu \in \mathcal{M}^+(\Omega) : \mu(\Omega) \leq \rho\},$$

1093 consists of measures that are uniformly bounded and supported in the same compact set Ω . There-
1094 fore, the set $\mathcal{M}_\rho^+(\Omega)$ is tight (see (Billingsley, 1999, Chapter 1, Section 1)). The set $\mathcal{M}_\rho^+(\Omega)$ is
1095 also closed in the weak* topology of measures as it is closed in the 1-Wasserstein topology. By
1096 Prokhorov's theorem (see (Billingsley, 1999, Chapter 5, Theorem 5.1)), the set $\mathcal{M}_\rho^+(\Omega)$ is com-
1097 pact in the 1-Wasserstein topology. As a continuous map defined in a compact metric space is
1098 uniformly continuous, the map $G : \mathcal{M}_\rho^+(\Omega) \times \Omega \rightarrow \mathbb{R}^{d'}$ is uniformly continuous. Moreover, by
1099 our assumptions, the derivative of ψ_k is zero in some neighborhood, $V \subset \mathbb{R}^{d'}$, of the finite set
1100 $\{G(\mu_k, x) : x \in \text{supp}(\mu_k)\}$. As $G(\mu_{k,x}^\epsilon, \cdot) \rightarrow G(\mu_k, \cdot)$ uniformly in $\Omega \subset \mathbb{R}^d$ as $\epsilon \rightarrow 0$, we see that

$$1101 \quad \sup_{y \in \text{supp}(\mu_k)} |G(\mu_{k,x}^\epsilon, y) - G(\mu_k, y)| \rightarrow 0 \quad \text{as } \epsilon \rightarrow 0. \quad (40)$$

1102 Thus, we find that for sufficiently small $\epsilon \in (0, 1)$, for all $y \in \text{supp}(\mu_k)$ the point $G(\mu_{k,x}^\epsilon, y)$ belongs
1103 to the set V , and, hence,

$$1104 \quad \psi_k(G(\mu_{k,x}^\epsilon, y)) = \psi_k(G(\mu_k, y))$$

1105 for all $y \in \text{supp}(\mu_k)$, and

$$1106 \quad \langle f_G(\mu_{k,x}^\epsilon), \psi_k \rangle = \int_{\mathbb{R}^d} \psi_k(G(\mu_k, y)) d\mu_k(y) + \epsilon \psi_k(G(\mu_k, x)).$$

1107 This implies that

$$1108 \quad \left. \frac{d}{d\epsilon} \right|_{\epsilon=0} \langle f_G(\mu_{k,x}^\epsilon), \psi_k \rangle = 0 + \psi_k(G(\mu_k, y)) = \psi_k(G(\mu_k, y)). \quad (41)$$

1109 Thus,

$$1110 \quad \overline{\mathcal{D}}_{f_G}(\mu_k, x, \psi_k) = \psi_k(G(\mu_k, x)).$$

1111 We see that

$$1112 \quad \lim_{k \rightarrow \infty} |\psi_k(G(\mu_k, x)) - \psi_k(G(\mu_k, x))| \leq \lim_{n \rightarrow \infty} \|\psi_k - \psi\|_{L^\infty(\mathbb{R}^{d'})} = 0,$$

1113 and as $\mu \rightarrow G(\mu, x)$ is continuous, we have

$$1114 \quad \lim_{k \rightarrow \infty} \psi(G(\mu_k, x)) = \psi(G(\mu, x)).$$

1115 But then

$$1116 \quad \lim_{k \rightarrow \infty} \psi_k(G(\mu_k, x)) = \psi(G(\mu, x)).$$

1117 As the above holds for all μ_k and ψ_k that converge to μ and ψ in the way stated in Definition 1, we
1118 conclude that the regular part of the derivative $\overline{\mathcal{D}}_{f_G}(\mu, y, \psi)$ exists and is equal to

$$1119 \quad \overline{\mathcal{D}}_{f_G}(\mu, x, \psi) = \psi(G(\mu, y)). \quad (42)$$

This proves the existence of the regular part of the derivative. Moreover, these arguments prove Lemma 3.

Next, we prove that the map $(\mu, y, \psi) \rightarrow \overline{D}_{f_G}(\mu, y, \psi)$ is uniformly continuous when (A1) and (A2) are valid. To this end, let $\epsilon_1 > 0$. By (A2), there is a $\delta_1 = \delta_1(\epsilon_1) \in (0, \epsilon_1)$ such that if $W_1(\mu_1, \mu_2) < \delta_1(\epsilon_1)$ and $|y_1 - y_2| < \delta_1(\epsilon_1)$ then $|G(\mu_1, y_1) - G(\mu_2, y_2)| < \epsilon_1/2$. Let $(\mu_1, y_1, \psi_1), (\mu_2, y_2, \psi_2) \in \mathcal{X}$ so that $\text{Lip}(\psi_j) \leq \eta$ for $j = 1, 2$. Also, assume that $\|\psi_1 - \psi_2\|_{L^\infty} < \delta_1(\epsilon_1)$. Equation (42) implies that

$$\begin{aligned} |\overline{D}_{f_G}(\mu_1, y_1, \psi_1) - \overline{D}_{f_G}(\mu_2, y_2, \psi_2)| &= |\psi_1(G(\mu_1, y_1)) - \psi_2(G(\mu_2, y_2))| \\ &\leq |\psi_1(G(\mu_1, y_1)) - \psi_1(G(\mu_2, y_2))| \\ &\quad + |\psi_1(G(\mu_2, y_2)) - \psi_2(G(\mu_2, y_2))| \\ &\leq \text{Lip}(\psi_1)|G(\mu_1, y_1) - G(\mu_2, y_2)| + \|\psi_1 - \psi_2\|_{L^\infty} \\ &\leq \text{Lip}(\psi_1)\epsilon_1 + \delta_1(\epsilon_1) \\ &\leq (\eta + 1)\epsilon_1. \end{aligned}$$

We observe that if $D_{\mathcal{X}}((\mu_1, y_1, \psi_1), (\mu_2, y_2, \psi_2)) < \delta_1(\epsilon_1)$ then $W_1(\mu_1, \mu_2) < \delta_1(\epsilon_1)$ and $|y_1 - y_2| < \delta_1(\epsilon_1)$, and moreover that $\|\psi_1 - \psi_2\|_{L^\infty} < \delta_1(\epsilon_1)$. We conclude that $(\mu, y, \psi) \rightarrow \overline{D}_{f_G}(\mu, y, \psi)$ is uniformly continuous. This proves (B2).

We continue with proving one direction of the final statement of the theorem. Let $G(\mu, y)$ be a Lipschitz map. Equation (42) implies that for all $(\mu_1, y_1, \psi_1), (\mu_2, y_2, \psi_2) \in \mathcal{X}$,

$$\begin{aligned} |\overline{D}_{f_G}(\mu_1, y_1, \psi_1) - \overline{D}_{f_G}(\mu_2, y_2, \psi_2)| &= |\psi_1(G(\mu_1, y_1)) - \psi_2(G(\mu_2, y_2))| \\ &\leq |\psi_1(G(\mu_1, y_1)) - \psi_1(G(\mu_2, y_2))| \\ &\quad + |\psi_1(G(\mu_2, y_2)) - \psi_2(G(\mu_2, y_2))| \\ &\leq \text{Lip}(\psi_1)|G(\mu_1, y_1) - G(\mu_2, y_2)| + \|\psi_1 - \psi_2\|_{L^\infty} \\ &\leq (\text{Lip}(\psi_1)\text{Lip}(G) + 1)D_{\mathcal{X}}((\mu_1, y_1, \psi_1), (\mu_2, y_2, \psi_2)) \\ &\leq (\eta\text{Lip}(G) + 1)D_{\mathcal{X}}((\mu_1, y_1, \psi_1), (\mu_2, y_2, \psi_2)). \end{aligned}$$

Hence, $(\mu, y, \psi) \rightarrow \overline{D}_{f_G}(\mu, y, \psi)$ is a Lipschitz map.

C.2 PART 2 : (B1)-(B2) IMPLY (A1)-(A2)

Assume that (B1) and (B2) hold true. Since f is a support-preserving map, $f : \mathcal{M}^+(\Omega) \rightarrow \mathcal{M}^+(\mathbb{R}^d)$, there are (possibly non-continuous) functions,

$$y_i : \Omega^n \times (0, \infty)^n \rightarrow \mathbb{R}^d, \quad (\mathbf{x}, \mathbf{a}) \rightarrow y_i(\mathbf{x}; \mathbf{a}), \quad i = 1, 2, \dots, n,$$

where

$$\mathbf{x} = (x_1, \dots, x_n) \quad \text{and} \quad \mathbf{a} = (a_1, \dots, a_n),$$

such that the following holds: Let

$$\mu = \sum_{i=1}^n a_i \delta_{x_i} \in \mathcal{M}_{fin}(\Omega), \quad a_i > 0;$$

then the functions $y_i(\mathbf{x}; \mathbf{a})$ satisfy

$$f(\mu) = \sum_{i=1}^n a_i \delta_{y_i(\mathbf{x}; \mathbf{a})}.$$

When $\mu \in \mathcal{M}_{fin, dif, (n)}^+(\Omega)$ (which is a refinement of the property that if $j \neq i$ then $a_j \neq a_i$), the functions $(\mathbf{x}; \mathbf{a}) \rightarrow y_i(\mathbf{x}; \mathbf{a})$ must have the following property,

$$\text{if } x_j = x_i \text{ then } y_j(\mathbf{x}; \mathbf{a}) = y_i(\mathbf{x}; \mathbf{a}). \quad (43)$$

Let $\mu \in \mathcal{M}^+(\Omega)$ and $x \in \Omega$, and $\alpha \in C_0^\infty(\mathbb{R}^d)$ be a cutoff function such that $\alpha(x) = 1$ for all $x \in \Omega$ and $\text{Lip}(\alpha(x) \cdot x) \leq \eta$. We define

$$G(\mu, x) := \begin{pmatrix} \overline{D}_f(\mu, x, \alpha\pi_1) \\ \vdots \\ \overline{D}_f(\mu, x, \alpha\pi_d) \end{pmatrix}, \quad (44)$$

where $\pi_\ell : \mathbb{R}^d \rightarrow \mathbb{R}$ is the projection $\pi_\ell(x) = x_\ell$ onto the ℓ -th component. By (B2), the map $(\mu, x) \mapsto G(\mu, x)$ is continuous, which proves (A2). In what follows, we will prove (A1).

The case when $\mu \in \mathcal{M}_{fin,dif,(n)}^+(\Omega)$. We let

$$\mu = \sum_{i=1}^n a_i \delta_{x_i} \in \mathcal{M}_{fin,dif,(n)}^+(\Omega)$$

and

$$f(\mu) = \sum_{i=1}^n a_i \delta_{y_i(\mathbf{x}; \mathbf{a})}.$$

We define the measures,

$$\mu_x^\epsilon = \epsilon \delta_x + \sum_{i=1}^n a_i \delta_{x_i}.$$

We observe that when $\epsilon > 0$ is small enough, it holds that $\mu_x^\epsilon \in \mathcal{M}_{fin,dif,(n)}^+(\Omega)$ if $x \in \{x_1, \dots, x_n\}$, or $\mu_x^\epsilon \in \mathcal{M}_{fin,dif,(n+1)}^+(\Omega)$ if $x \notin \{x_1, \dots, x_n\}$.

With the notation, $(\mathbf{x}, x) = (x_1, \dots, x_n, x)$, $(\mathbf{a}, \epsilon) = (a_1, \dots, a_n, \epsilon)$ and sometimes indicating the number, n say, of variables in the function y_i as $y_i^{(n)}$, we find that

$$f(\mu_x^\epsilon) = \epsilon \delta_{y_{n+1}^{(n+1)}(\mathbf{x}, x; \mathbf{a}, \epsilon)} + \sum_{i=1}^n a_i \delta_{y_i^{(n+1)}(\mathbf{x}, x; \mathbf{a}, \epsilon)}. \quad (45)$$

We consider the case when $x = x_j$. Then,

$$\left(\sum_{i=1}^n a_i \delta_{x_i} + \epsilon \delta_x \right) \Big|_{x=x_j} = \sum_{i \in \{1, \dots, n\} \setminus \{j\}} a_i \delta_{x_i} + (a_j + \epsilon) \delta_{x_j} \in \mathcal{M}_{fin,(n)}^+(\mathbb{R}). \quad (46)$$

Thus, when we write $x = x_{n+1} = x_j$, it holds that

$$y_{n+1}^{(n+1)}(\mathbf{x}, x; \mathbf{a}, \epsilon) \Big|_{x=x_j} = y_{n+1}^{(n+1)}(\mathbf{x}, x_{n+1}; \mathbf{a}, \epsilon) \Big|_{x_{n+1}=x_j} = y_j^{(n)}(\mathbf{x}; \mathbf{a} + \epsilon e_j), \quad (47)$$

where $e_j = (0, 0, \dots, 0, 1, 0, \dots, 0) = (\delta_{ij})_{i=1}^n$, whence

$$\mathbf{a} + \epsilon e_j = (a_1, \dots, a_{j-1}, a_j + \epsilon, a_{j+1}, \dots, a_n).$$

By Lemma 4, and using equations (46)-(47), we arrive at

$$\lim_{\epsilon \rightarrow 0^+} y_{n+1}^{(n+1)}(\mathbf{x}, x; \mathbf{a}, \epsilon) \Big|_{x=x_j} = y_j^{(n)}(\mathbf{x}; \mathbf{a}). \quad (48)$$

Let $\ell \in [d']$. We choose $\psi_k^{(\ell)} \in C_0^1(\mathbb{R}^{d'})$ such that

$$\psi_k^{(\ell)} \text{ is constant in an open neighborhood of } \text{supp}(f(\mu))$$

and

$$\text{Lip}(\psi_k^{(\ell)}) \leq \eta \text{ together with } \lim_{n \rightarrow \infty} \|\psi_k^{(\ell)} - \alpha \pi_\ell\|_{L^\infty(\mathbb{R}^{d'})} = 0.$$

Thus, by using equation (48), we obtain

$$\begin{aligned} \overline{\mathcal{D}}_f(\mu, x, \psi_k^{(\ell)}) \Big|_{x=x_j} &= \overline{\mathcal{D}}_f(\mu, x_{n+1}, \psi_k^{(\ell)}) \Big|_{x_{n+1}=x_j} \\ &= \lim_{\epsilon \rightarrow 0^+} \langle \psi_k^{(\ell)}, \delta_{y_{n+1}^{(n+1)}(\mathbf{x}, x_{n+1}; \mathbf{a}, \epsilon)} \rangle \Big|_{x_{n+1}=x_j} \\ &= \lim_{\epsilon \rightarrow 0^+} \psi_k^{(\ell)}(y_{n+1}^{(n+1)}(\mathbf{x}, x_{n+1}; \mathbf{a}, \epsilon)) \Big|_{x_{n+1}=x_j} \\ &= \lim_{\epsilon \rightarrow 0^+} \psi_k^{(\ell)}(y_j^{(n)}(\mathbf{x}; \mathbf{a} + \epsilon e_j)) \\ &= \psi_k^{(\ell)}(y_j^{(n)}(\mathbf{x}; \mathbf{a})) = \psi_k^{(\ell)}(y_j(\mathbf{x}; \mathbf{a})). \end{aligned}$$

By the definition of $\overline{\mathcal{D}}_f(\mu, x, \alpha\pi_\ell)$ and that $\psi_k^{(\ell)} \rightarrow \alpha\pi_\ell$ in $L^\infty(\mathbb{R}^{d'})$ as $n \rightarrow \infty$, we observe that for $x = x_j$,

$$\begin{aligned}\pi_\ell(G(\mu, x_j)) &= \overline{\mathcal{D}}_f(\mu, x_j, \alpha\pi_\ell) = \lim_{n \rightarrow \infty} \overline{\mathcal{D}}_f(\mu, x_j, \psi_k^{(\ell)}) \\ &= \lim_{n \rightarrow \infty} \psi_k^{(\ell)}(y_j(\mathbf{x}; \mathbf{a})) = (\alpha\pi_\ell)(y_j(\mathbf{x}; \mathbf{a})) = \pi_\ell(y_j).\end{aligned}$$

This proves that, for each $j \in [n]$,

$$G(\mu, x_j) = y_j(\mathbf{x}; \mathbf{a}), \quad (49)$$

which is equivalent to

$$f(\mu) = (G_\mu)_\# \mu \quad \text{for } \mu \in \mathcal{M}_{fin, dif, (n)}^+(\Omega).$$

The case when $\mu \in \mathcal{M}^+(\Omega)$. Let μ be a (possibly not-discretely supported) measure $\mu \in \mathcal{M}^+(\Omega)$. By Lemma 1, we choose the sequence $(\tilde{\mu}_k)_{k \in \mathbb{N}} \subset \mathcal{M}_{fin, dif}^+(\Omega)$ such that $\tilde{\mu}_k \rightarrow \mu$ as $k \rightarrow \infty$, where the limit is considered in the 1-Wasserstein topology. We have already shown that for $\tilde{\mu}_k \in \mathcal{M}_{fin, dif}^+(\Omega)$,

$$f(\tilde{\mu}_k) = (G_{\tilde{\mu}_k})_\#(\tilde{\mu}_k).$$

Hence, taking the limit,

$$f(\mu) = \lim_{m \rightarrow \infty} (G_{\tilde{\mu}_k})_\#(\tilde{\mu}_k). \quad (50)$$

That is, for all $\psi \in C_0^1(\mathbb{R}^{d'})$,

$$\langle \psi, f(\mu) \rangle = \lim_{m \rightarrow \infty} \langle \psi, (G_{\tilde{\mu}_k})_\#(\tilde{\mu}_k) \rangle, \quad (51)$$

where

$$\langle \psi, (G_{\tilde{\mu}_k})_\#(\tilde{\mu}_k) \rangle = \langle \psi \circ G_{\tilde{\mu}_k}, \tilde{\mu}_k \rangle = \int_{\mathbb{R}^{d'}} \psi(G_{\tilde{\mu}_k}(x)) d\tilde{\mu}_k(x).$$

But then

$$\begin{aligned}\lim_{k \rightarrow \infty} \langle \psi, (G_{\tilde{\mu}_k})_\#(\tilde{\mu}_k) \rangle &= \lim_{k \rightarrow \infty} \int_{\mathbb{R}} \psi(G_{\tilde{\mu}_k}(x)) d\tilde{\mu}_k(x) \\ &= \lim_{k \rightarrow \infty} \int_{\mathbb{R}} (\psi(G(\tilde{\mu}_k, x)) - \psi(G(\mu, x))) d\tilde{\mu}_k(x) + \int_{\mathbb{R}} \psi(G(\mu, x)) d\tilde{\mu}_k(x).\end{aligned} \quad (52)$$

By condition (B2), $(\mu, x) \rightarrow G(\mu, x)$ is uniformly continuous so that, using the compactness of Ω ,

$$\|\psi(G(\tilde{\mu}_k, \cdot)) - \psi(G(\mu, \cdot))\|_{L^\infty(\Omega)} \leq \|\psi\|_{C^1} \|G(\tilde{\mu}_k, \cdot) - G(\mu, \cdot)\|_{L^\infty(\Omega)} \rightarrow 0 \text{ as } k \rightarrow \infty.$$

Hence, equations (51) and (52) imply that

$$\begin{aligned}\langle \psi, f(\mu) \rangle &= 0 + \lim_{k \rightarrow \infty} \int_{\mathbb{R}} \psi(G(\mu, x)) d\tilde{\mu}_k(x) \\ &= \lim_{k \rightarrow \infty} \langle \psi(G(\mu, \cdot)), \tilde{\mu}_k \rangle = \langle \psi(G(\mu, \cdot)), \mu \rangle = \langle \psi, (G_\mu)_\# \mu \rangle\end{aligned} \quad (53)$$

for all $\psi \in C_0^1(\mathbb{R}^{d'})$, $\text{Lip}(\psi) \leq \eta$. As both sides of (53) are linear in ψ , we see that (53) holds for all $\psi \in C_0^1(\mathbb{R}^{d'})$ and, therefore, for all $\psi \in C_0(\mathbb{R}^{d'})$. Thus,

$$f(\mu) = (G_\mu)_\# \mu \quad \text{for } \mu \in \mathcal{M}^+(\Omega).$$

This implies (A1).

Finally, we observe that if $(\mu, y, \psi) \rightarrow \overline{\mathcal{D}}_{f_G}(\mu, y, \psi)$ is a Lipschitz map then $(\mu, y) \rightarrow G(\mu, y) = (\overline{\mathcal{D}}_f(\mu, y, \alpha\pi_j))_{j=1}^{d'}$ is also Lipschitz.

D THE REGULAR PART OF THE DERIVATIVE

We provide some perspectives on the regular part of the derivative introduced in the main text, in the following remarks.

Remark 1. *A similar situation occurs when one defines the generalization of a derivative for a Lipschitz function $h : \mathbb{R}^d \rightarrow \mathbb{R}$. By the Rademacher theorem, the classical derivative of h exists outside a zero-measurable set; to overcome this, one defines a weak derivative that is a function in $L^1_{loc}(\mathbb{R}^d)$ and is defined almost everywhere. We recall that the weak derivative is defined, in the sense of distributions, by the formula*

$$\langle \partial_{x_i} h, \psi \rangle = - \int_{\mathbb{R}^d} h(x) \partial_{x_i} \psi(x) dx, \quad \text{for } \psi \in C_0^\infty(\mathbb{R}^d).$$

In the case when h is a C^1 -function, the classical derivative coincides with the weak derivative and the distributional duality coincides with the L^2 -inner product

$$\langle \partial_{x_i} h, \psi \rangle = \int_{\mathbb{R}^d} \partial_{x_i} h(x) \psi(x) dx.$$

In this setting, the weak derivative is defined for a larger class of functions as a “new” generalized function.

Our definition of the regular part of the derivative is defined as a new generalized function using duality (or, in the weak sense). This definition is formally quite different from the classical one of Fréchet derivative. However, as we see in Lemma 3, for map f_G defined with a smooth in-context function G , the regular part of derivative $\overline{D}_{f_G}(\mu, x, \psi)$ coincides with the above defined object, $D_{f_G}^{reg}(\mu, x, \psi)$. So, we consider $D_{f_G}^{reg}(\mu, x, \psi)$ as a new object that is different from the classical Fréchet derivative, and show that the definition of $D_{f_G}^{reg}(\mu, x, \psi)$ can be extended as a generalized regular part of the derivative, $\overline{D}_f(\mu, x, \psi)$, for a class of functions f for which we do not assume that the classical Fréchet derivative is well-defined.

Remark 2. *We point out that for any support preserving map $f : \mathcal{M}^+(\Omega) \rightarrow \mathcal{M}^+(\mathbb{R}^{d'})$, $\mu \in \mathcal{M}^+(\Omega)$, and $\psi \in C_0^1(\mathbb{R}^{d'})$, we can find a sequence of finitely supported measures, $\mu_k \in \mathcal{M}_{fin}^+(\Omega)$, that converges in the 1-Wasserstein topology to μ as $n \rightarrow \infty$. Then also $\text{supp}(f(\mu_k))$ is finitely supported, and we can denote $\text{supp}(f(\mu_k)) = \{y_{1,n}, y_{2,n}, \dots, y_{m_n,n}\}$. We can modify the function ψ in a small neighborhood of each point, $y_{j,n}$, so that we obtain a function $\psi_k \in C_0^1(\mathbb{R}^{d'})$ that satisfies (7) and ψ_k converges in the L^∞ topology to ψ as $n \rightarrow \infty$. Thus, we see that for all measures $\mu \in \mathcal{M}^+(\Omega)$ and $\psi \in C_0^1(\mathbb{R}^{d'})$, we can find sequences μ_k and ψ_k that satisfy the conditions in Definition 4. The existence of $\overline{D}_f(\mu, x, \psi)$ thus means that for all μ, x , and ψ , the limits (6) exist and are independent of the chosen sequences μ_k and ψ_k .*

Remark 3. *We can come up with an alternative version of the definition for the regular part of the Fréchet derivative of f and of Definition 4. Let us consider the triplets of measures μ , points x and test functions ψ having the property that the test functions are locally constant in the support of $f(\mu)$. We denote this set by*

$$\mathcal{P}_{lc} = \mathcal{P}_{lc}(f, \Omega, \rho, \eta) = \{(\mu, x, \psi) \in \mathcal{M}^+(\Omega) \times \Omega \times C_0^1(\mathbb{R}^{d'}) : \mu(\Omega) \leq \rho, \psi \text{ is constant in an open neighborhood of } f(\mu), \|\psi\|_{C^1} \leq \eta\}.$$

Let

$$\mathcal{L}_f(\mu, x, \psi) = \langle \psi, D_\mu f(\mu)[\delta_x] \rangle,$$

be the duality of the Fréchet derivative $D_\mu f(\mu)[\delta_x]$ and the test function ψ . Then the restriction of \mathcal{L}_f to the set \mathcal{P}_{lc} , that is,

$$\mathcal{L}_f|_{\mathcal{P}_{lc}} : \mathcal{P}_{lc} \rightarrow \mathbb{R},$$

coincides with the regular part of the derivative $\overline{D}_f(\mu, x, \psi)$ of f . When the regular part of the derivative of f exists, this map has a continuous extension to the set \mathcal{X} ,

$$\mathcal{L}_f^{ext} : \mathcal{X} \rightarrow \mathbb{R},$$

in the topology determined by the metric, $D_{\mathcal{X}}$. This extension is the map $(\mu, x, \psi) \rightarrow \overline{D}_f(\mu, x, \psi)$. Hence, $\overline{D}_f(\mu, x, \psi)$ given in Definition 4 can also be defined as the extension of the usual Fréchet derivative from the set \mathcal{P}_{lc} to the completion of this set in the appropriate topology.

E MLPs WITH SKIP CONNECTIONS AND COMPOSITION FORMING AN IN-CONTEXT MAP

We consider MLPs with possible skip connections, denoted by F_η , that are given by the function

$$F_\eta : \mathbb{R}^d \rightarrow \mathbb{R}^d, \quad F_\eta = c_\eta \cdot Id_x + \sigma \circ (A_\eta^L + b_\eta^L) \circ \cdots \circ \sigma \circ (A_\eta^1 + b_\eta^1), \quad (54)$$

where $c_\eta \in \mathbb{R}$, $A_\eta^j \in \mathbb{R}^{d_j \times d_{j-1}}$ are the weight matrices, $b_\eta^j \in \mathbb{R}^{d_j}$ are bias vectors, σ is an activation function, for example the sigmoid function, and $d_0 = d_L = d$. This defines a map for measures, $f_{F_\eta} = (F_\eta)_\# : \mathcal{M}^+(\mathbb{R}^d) \rightarrow \mathcal{M}^+(\mathbb{R}^d)$ that for discrete measure $\nu = \sum_{i=1}^n \frac{1}{n} \delta_{y_i}$ is given by

$$f_{F_\eta}(\nu) = (F_\eta)_\# \left(\sum_{i=1}^n \frac{1}{n} \delta_{y_i} \right) = \sum_{i=1}^n \frac{1}{n} \delta_{z_i} \quad (55)$$

where

$$z_i = F_\eta(y_i). \quad (56)$$

The composition $f_{F_\eta} \diamond f_{\Gamma_\xi} : \mathcal{M}^+(\Omega) \rightarrow \mathcal{M}^+(\mathbb{R}^d)$ of the maps f_{F_η} and f_{Γ_ξ} , see (8), maps the discrete measure μ , given in (21), to

$$(f_{F_\eta} \diamond f_{\Gamma_\xi}) \left(\sum_{i=1}^n \frac{1}{n} \delta_{x_i} \right) = \sum_{i=1}^n \frac{1}{n} \delta_{z_i}, \quad z_i = F_\eta(\Gamma_\xi(\mu, x_i)). \quad (57)$$

We write

$$H_\eta(x) := F_\eta(x) - x.$$

We note that as $\Gamma_\xi(\mu, x) = x + \text{Att}_\xi(\mu, x)$ and $F_\eta(x) = x + H_\eta(x)$, we can write

$$F_\eta(\Gamma_\xi(\mu, x)) = x + \mathcal{V}(\mu, x) \quad (58)$$

and

$$f_{F_\eta} \diamond f_{\Gamma_\xi} = Id_x + f_{\mathcal{V}}, \quad (59)$$

where $\mathcal{V} : \mathcal{M}^+(\Omega) \times \mathbb{R}^d \rightarrow \mathbb{R}^d$ is the map $\mathcal{V} = \text{Att}_\xi + H_\eta \circ \Gamma_\xi$, that is,

$$\mathcal{V}(\mu, x) = \text{Att}_\xi(\mu, x) + H_\eta(\Gamma_\xi(\mu, x)) = \text{Att}_\xi(\mu, x) + H_\eta \circ (Id_x + \text{Att}_\xi(\mu, \cdot))(x). \quad (60)$$

F A COUNTEREXAMPLE FOR THE CHARACTERIZATION OF SUPPORT-PRESERVING MAPS USING ONLY CONTINUITY

In this section, we construct a map $f : \mathcal{P}(\Omega) \rightarrow \mathcal{P}(\Omega)$ that is support preserving and continuous in the 1-Wasserstein topology, but which cannot be represented as f_G using a continuous in-context map, G . Such a map, f , is given in formulas (63)-(65) below. This shows the importance of the assumptions on the derivative of the map f in the main theorem.

Let us next prove Proposition 1. We recall the statement:

Proposition 3. *Let $d = 1$ and $\Omega = [-3, 3] \subset \mathbb{R}$ and consider the set $\mathcal{P}(\Omega)$ endowed with the 1-Wasserstein topology. There exists a continuous, support preserving map $f : \mathcal{P}(\Omega) \rightarrow \mathcal{P}(\Omega)$ such that there does not exist a continuous map $G : \mathcal{P}(\Omega) \times \Omega \rightarrow \Omega$ for which $f = f_G$.*

Proof. For $0 \leq a \leq 1$, we define

$$R_a : [-3, 3] \rightarrow [-3, 3], \quad (61)$$

$$R_a(x) = \begin{cases} x, & \text{for } x \leq -1 \text{ or } x \geq 1, \\ x + \frac{1}{10} \cos^2(\frac{1}{2}\pi x) \cos(ax), & \text{for } -1 < x < 1. \end{cases}$$

We note that the derivative of R_a is given by

$$R'_a : [-3, 3] \rightarrow \mathbb{R}, \quad (62)$$

$$R'_a(x) = \begin{cases} 0, & \text{for } x \leq -1 \text{ or } x \geq 1, \\ 1 - \frac{\pi}{10} \cos(\frac{1}{2}\pi x) \sin(\frac{1}{2}\pi x) \cos(ax) - \frac{a}{10} \cos^2(\frac{1}{2}\pi x) \sin(ax), & \text{for } -1 < x < 1 \end{cases}$$

and that $R_a : [-3, 3] \rightarrow [-3, 3]$ is a C^1 function that maps $R_a : [-3, 3] \rightarrow [-3, 3]$. Moreover, we point out that when $a = 0$, $R_0(x) = x$.

Next, we consider the map

$$f(\mu) = (R_{a(\mu)})\#\mu, \quad (63)$$

where

$$a(\mu) = \begin{cases} \frac{1}{\kappa(\mu)} & \text{if } \kappa(\mu) > 0, \\ 0 & \text{if } \kappa(\mu) = 0 \end{cases} \quad (64)$$

and

$$\kappa(\mu) = \int_{-2}^{-1} (2 - |x|)d\mu(x) + \int_{-1}^1 d\mu(x) + \int_1^2 (2 - x)d\mu(x). \quad (65)$$

The function $\mu \rightarrow \kappa(\mu)$ is a continuous map $\mathcal{P}([-3, 3]) \rightarrow \mathbb{R}$ but $\mu \rightarrow a(\mu)$ is not continuous.

By Vallender (1974), the 1-Wasserstein distance satisfies,

$$W_1(\mu_1, \mu_2) = \int_{[-3, 3]} |F_1(x) - F_2(x)| dx, \quad (66)$$

where $F_1(x) = \mu_1([-3, x])$ and $F_2(x) = \mu_2([-3, x])$ are the cumulative distribution functions of μ_1 and μ_2 , respectively. Thus, as $R_{a(\mu)}(x)$ is the identity map for $x \in [-3, 3] \setminus [-\frac{3}{2}, \frac{3}{2}]$ and $R_{a(\kappa)}$ maps the interval $[-\frac{3}{2}, \frac{3}{2}]$ to itself, we find that

$$\begin{aligned} W_1(f(\mu_1), f(\mu_2)) &\leq \text{diam}\left(\left[-\frac{3}{2}, \frac{3}{2}\right]\right) \left| \mu_1\left(\left[-\frac{3}{2}, \frac{3}{2}\right]\right) - \mu_2\left(\left[-\frac{3}{2}, \frac{3}{2}\right]\right) \right| + W_1(\mu_1, \mu_2) \\ &\leq 3 \left(\mu_1\left(\left[-\frac{3}{2}, \frac{3}{2}\right]\right) + \mu_2\left(\left[-\frac{3}{2}, \frac{3}{2}\right]\right) \right) + W_1(\mu_1, \mu_2). \end{aligned} \quad (67)$$

Lemma 5. *The map, $f : \mathcal{P}([-3, 3]) \rightarrow \mathcal{P}([-3, 3])$, is continuous in the 1-Wasserstein topology and is a support-preserving map.*

Proof. When $\nu = \sum_{i=1}^n \frac{1}{n} \delta_{x_i}$, we have by the definition of f (cf. (63)) that

$$f(\nu) = (R_{a_0})\#\nu,$$

where $a_0 = a(\nu)$. As R_{a_0} is a C^1 -map, we see that

$$f(\nu) = \sum_{i=1}^n \frac{1}{n} \delta_{y_i}, \quad y_i = R_{a_0}(x_i). \quad (68)$$

This shows that f is a support-preserving map.

Let $\mu_k, \mu \in \mathcal{P}([-3, 3])$ satisfy

$$\lim_{k \rightarrow \infty} W_1(\mu_k, \mu) = 0. \quad (69)$$

We will next show that

$$\lim_{k \rightarrow \infty} W_1(f(\mu_k), f(\mu)) = 0. \quad (70)$$

First, we consider the case when $\kappa(\mu) > 0$. In this case, also $\kappa(\mu_k) > 0$ when n is large enough. Then, we can use the fact that $(x, a) \rightarrow R_a(x)$ is C^1 -smooth in the domain $(x, a) \in [-3, 3] \times (0, 1]$, i.e., when a is strictly positive. This implies that the limit (70) is valid when $\kappa(\mu) > 0$.

Second, we consider the case when $\kappa(\mu) = 0$. Then, $\mu([- \frac{3}{2} - \frac{1}{10}, \frac{3}{2} + \frac{1}{10}]) = 0$ and $f(\mu) = \mu$. For all $\epsilon > 0$ there is $n_\epsilon > 0$ such that for $n \geq n_\epsilon$ it holds that $W_1(\mu_n, \mu) < \epsilon$ and $\mu_k([- \frac{3}{2}, \frac{3}{2}]) < \epsilon$.

We see that $R_{a(\mu)}(x)$ is the identity map for $x \in [-3, 3] \setminus [-\frac{3}{2}, \frac{3}{2}]$ and $R_{a(\kappa)}$ maps the interval $[-\frac{3}{2}, \frac{3}{2}]$ to itself. Thus, $n \geq n_\epsilon$, we have by (67),

$$\begin{aligned} W_1(f(\mu_k), f(\mu)) &\leq 3\left(\mu_k\left(\left[-\frac{3}{2}, \frac{3}{2}\right]\right) + \mu\left(\left[-\frac{3}{2}, \frac{3}{2}\right]\right)\right) + W_1(\mu_k, \mu) \\ &\leq 3\epsilon + W_1(\mu_k, \mu) \\ &\leq 4\epsilon. \end{aligned} \quad (71)$$

These show that the limit (70) is valid also when $\kappa(\mu) > 0$. This proves that the limit (70) is valid. Hence, f is continuous in 1-Wassestein metric. This proves the claim. \square

In the following, we use the 1-Wasserstein topology in the set $\mathcal{P}([-3, 3])$.

Lemma 6. *There are no continuous maps $G : \mathcal{P}([-3, 3]) \times [-3, 3] \rightarrow [-3, 3]$, such that*

$$f(\mu) = f_G(\mu). \quad (72)$$

Proof. For $\epsilon > 0$, let

$$\begin{aligned} \mu_\epsilon &= (1 - \epsilon)\delta_{x_0} + \epsilon\delta_{\sqrt{\epsilon}}, \\ \nu_\epsilon &= (1 - \epsilon)\delta_{x_0} + \epsilon\delta_{R_{1/\epsilon}(\sqrt{\epsilon})}, \end{aligned}$$

where $x_0 = 2$. We see that as $\epsilon \rightarrow 0$, we have

$$\lim_{\epsilon \rightarrow 0} W_1(\mu_\epsilon, \delta_{x_0}) = 0, \quad (73)$$

$$\lim_{\epsilon \rightarrow 0} W_1(\nu_\epsilon, \delta_{x_0}) = 0. \quad (74)$$

We have $\kappa(\mu_\epsilon) = \epsilon$ so that $a(\epsilon) = 1/\epsilon$ and thus we see that

$$f(\mu_\epsilon) = \nu_\epsilon. \quad (75)$$

Moreover,

$$R_{a(\mu_\epsilon)}(\sqrt{\epsilon}) = R_{1/\epsilon}(\sqrt{\epsilon}) \quad (76)$$

$$= \sqrt{\epsilon} + \frac{1}{10} \cos^2\left(\frac{1}{2}\pi\sqrt{\epsilon}\right) \cos\left(\frac{1}{\epsilon}\sqrt{\epsilon}\right) \quad (77)$$

$$= \sqrt{\epsilon} + \frac{1}{10} \cos^2\left(\frac{1}{2}\pi\sqrt{\epsilon}\right) \cos\left(\frac{1}{\sqrt{\epsilon}}\right). \quad (78)$$

Let us assume that there is a continuous map $G : \mathcal{P}([-3, 3]) \times [-3, 3] \rightarrow [-3, 3]$, where in the set $\mathcal{P}([-3, 3])$ we use the 1-Wasserstein topology such that

$$f(\mu) = f_G(\mu) = (G(\mu))\#\mu. \quad (79)$$

We observe that

$$f(\mu_\epsilon) = \nu_\epsilon \quad (80)$$

implies that when $0 < \epsilon < \frac{1}{2}$ we have $\mu_\epsilon \in \mathcal{M}_{fin,dif}^+([-3, 3])$ and

$$G(\nu_\epsilon, x)|_{x=2} = 2, \quad (81)$$

$$G(\nu_\epsilon, x)|_{x=\sqrt{\epsilon}} = R_{1/\epsilon}(\sqrt{\epsilon}). \quad (82)$$

Thus,

$$\limsup_{\epsilon \rightarrow 0+} G(\mu_\epsilon, x) \Big|_{x=\sqrt{\epsilon}} = \limsup_{\epsilon \rightarrow 0+} \sqrt{\epsilon} + \frac{1}{10} \cos^2\left(\frac{1}{2}\pi\sqrt{\epsilon}\right) \cos\left(\frac{1}{\sqrt{\epsilon}}\right) = +\frac{1}{10}, \quad (83)$$

$$\liminf_{\epsilon \rightarrow 0+} G(\mu_\epsilon, x) \Big|_{x=\sqrt{\epsilon}} = \liminf_{\epsilon \rightarrow 0+} \sqrt{\epsilon} + \frac{1}{10} \cos^2\left(\frac{1}{2}\pi\sqrt{\epsilon}\right) \cos\left(\frac{1}{\sqrt{\epsilon}}\right) = -\frac{1}{10}. \quad (84)$$

Formulas (83), (84), and (73) are in contradiction with the assumption that the map $G : \mathcal{P}([-3, 3]) \times [-3, 3] \rightarrow [-3, 3]$ is continuous. This proves the claim. \square

1512 The above lemmas yield Proposition 1. □
 1513

1514 To discuss the connection of the above counterexample with LLMs, we consider a sequence of
 1515 tokens $(x_1, x_2, \dots, x_n) \in \Omega^n$, where $\Omega \subset \mathbb{R}^d$, that are identified with discrete measures $\frac{1}{n} \sum_{i=1}^n \delta_{x_i}$
 1516 via the map ι given in formula (4). Below, as an interesting counterexample, we will construct a map
 1517 $f : \mathcal{M}_{fin}^+([-3, 3]) \rightarrow \mathcal{M}_{fin}^+([-3, 3])$ for which the corresponding map $F = \iota^{-1} \circ f \circ \iota$ maps a
 1518 sequence of tokens $X = (x_1, x_2, \dots, x_n) \in [-3, 3]^n \subset \mathbb{R}^n$ to a sequence

$$1519 \quad F(X) = (y_1(X, x_1), y_1(X, x_2), \dots, y_n(X, x_n)) \in [-3, 3]^n \subset \mathbb{R}^n.$$

1520
 1521 Let us consider an example where $d = 1$ and let $\Omega = [-3, 3]$ be the space where we consider the
 1522 tokens and $B_1 = [-1, 1]$ and $B_2 = [-2, 2]$ be balls (i.e. intervals) centered at zero.
 1523

1524 This map has the following property: Let $n > 1$ be very large and consider a sequence $X_n =$
 1525 (x_1, x_2, \dots, x_n) where

$$1526 \quad x_1, x_2, x_3 \in B_1, \quad x_4, x_5, x_6, x_7, \dots, x_n \in \Omega \setminus B_2$$

1527
 1528 that is, the first three tokens are in the smaller neighborhood of the point 0 and all other tokens are
 1529 outside the larger neighborhood of the point 0. Denote the image of this sequence of tokens in the
 1530 map F by

$$1531 \quad F(X_n) = F(x_1, x_2, \dots, x_n) = (y_1(X_n, x_1), y_2(X_n, x_2), \dots, y_n(X_n, x_n)).$$

1532
 1533 When n is large, the measure $\mu_X(B_2)$, of the set B_2 with respect to the measure $\mu_X = \frac{1}{n} \sum_{i=1}^n \delta_{x_i}$,
 1534 is small. More precisely, $\mu_X(B_2) = \frac{3}{n}$. Then, when f is the map constructed below in formulas
 1535 (63)-(65) below, the function

$$1536 \quad x_1 \rightarrow (y_1(X_n, x_1), y_2(X_n, x_2), y_3(X_n, x_3))$$

1537
 1538 converges to a discontinuous function as $n \rightarrow \infty$. This means that when the prompt becomes
 1539 sufficiently long, then the map F transforms some of the tokens in a possible unstable way. As a
 1540 possible playful example, two long, almost similar prompts, coded with map which assigns tokens
 1541 in \mathbb{R}^d for words, so that the names ‘Alice’ and ‘Elise’ are mapped to tokens that are very close to
 1542 each others, that is, $|\iota(\text{Alice}) - \iota(\text{Elise})|$ is small. We consider to very long prompts which are the
 1543 same except their first words (in this example, we use a long ‘Lorem ipsum’ text that is commonly
 1544 used in graphic design and publishing as a dummy or placeholder text). The prompts

$$1545 \quad X_n = (\text{Alice}, \text{is}, \text{studying}, \text{the}, \text{text}, \text{Lorem}, \text{ipsum}, \text{dolor}, \text{sit}, \text{amet}, \dots, \text{nibh}),$$

$$1546 \quad X'_n = (\text{Elise}, \text{is}, \text{studying}, \text{the}, \text{text}, \text{Lorem}, \text{ipsum}, \text{dolor}, \text{sit}, \text{amet}, \dots, \text{nibh}),$$

1547
 1548 could possibly be mapped in the composition of F and a permutation S (that changes the 1st and
 1549 the 3rd words)

$$1550 \quad (S \circ F)(X_n) = (\text{The}, \text{reader}, \text{LOVES}, \text{the}, \text{text}, \text{Lorem}, \text{ipsum}, \text{dolor}, \text{sit}, \text{amet}, \dots, \text{nibh}),$$

$$1551 \quad (S \circ F)(X'_n) = (\text{The}, \text{reader}, \text{HATES}, \text{the}, \text{text}, \text{Lorem}, \text{ipsum}, \text{dolor}, \text{sit}, \text{amet}, \dots, \text{nibh}).$$

1552
 1553
 1554
 1555
 1556
 1557
 1558
 1559
 1560
 1561
 1562
 1563
 1564
 1565