可逆ニューラルネットのSobolev空間における普遍性について

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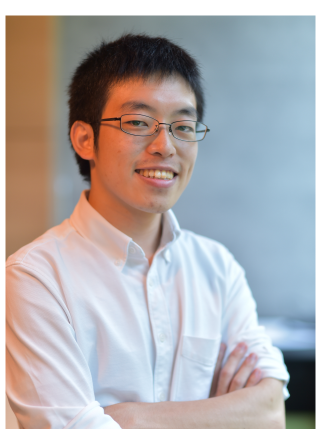

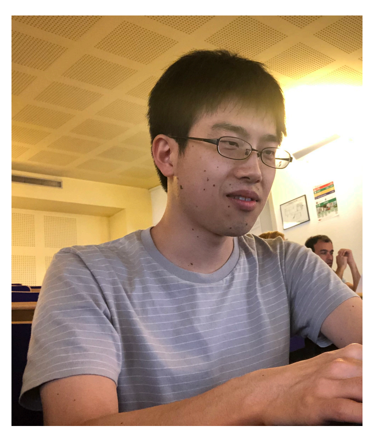


Joint work with Koichi Tojo, Kenta Oono, Masahiro Ikeda, and Masashi Sugiyama.

Self-introduction

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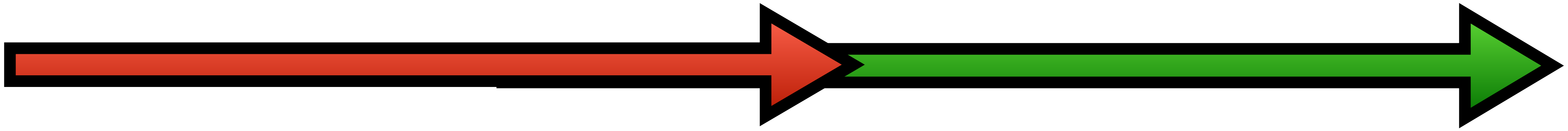
Recent Research Interests:

Mathematical analysis of theoretical backgrounds of machine learning and data analysis

- Analysis of representation power of neural networks
- Data analysis via Koopman operator

Today's talk structure



Part 1

Introduction.

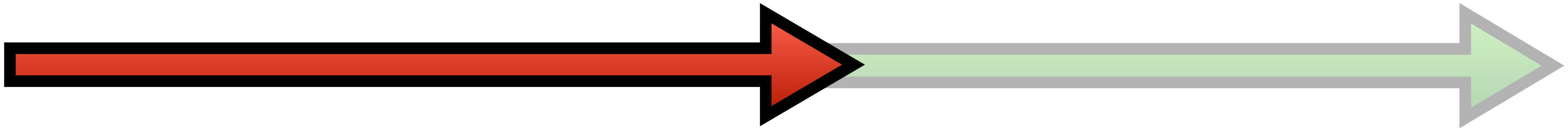
Overview of what we did and why it's important.

Part 2

Details of the theory.

Theoretical preliminaries and proof machinery.

Today's talk structure



Part 1

Introduction.

Overview of what we did and why it's important.

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Theoretical preliminaries and proof machinery.

Invertible Neural Networks (INNs)

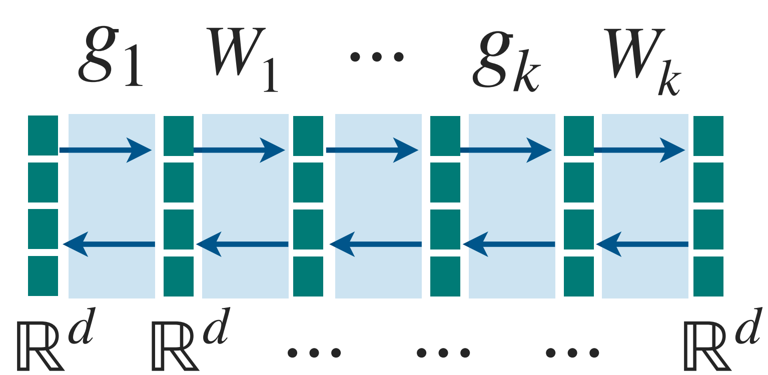
Goal

Understand theoretical props of **invertible neural networks (INNs)**.

Invertible Neural Networks (INNs) generated by $\mathscr{G}$

Compositions of **flow maps/layers** $\mathscr{G}$ and **affine transforms** Aff.

$$f = W_1 \circ g_1 \circ \cdots \circ W_k \circ g_k \qquad (g_i \in \mathscr{G}, W_i \in \mathrm{Aff})$$



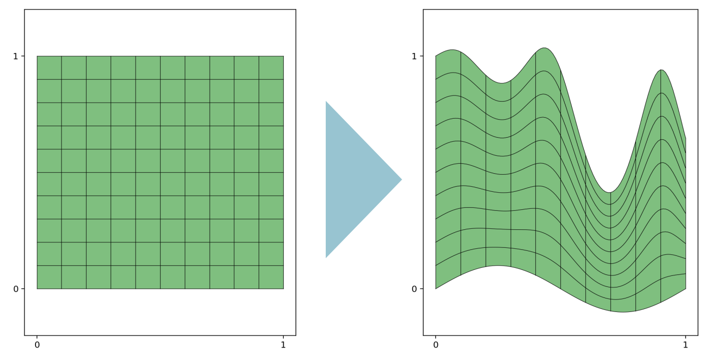
$\mathscr{G}$ is parametrized ("trainable") but **designed to be invertible**.

($\mathscr{G}$ is often rather simple → Composed to model complex f)

Example1: Coupling Flows

Coupling flows (CFs) [DKB14, PNRML19, KPB19]

$$\begin{bmatrix} x_{\le k} \\ x_{>k} \end{bmatrix} \mapsto \begin{bmatrix} x_{\le k} \\ \tau(x_{>k},\ \theta(x_{\le k})) \end{bmatrix}$$



Idea: Keep some dimensions unchanged. (Strong constraint!)

CF-INN = Coupling-flow based INN.

Affine-coupling flows (ACFs) [DKB14,DSB17,KD18]

One of the simplest CFs using **coordinate-wise affine transformation**:

$$\Psi_{s,t,k} : \begin{bmatrix} x_{\le k} \\ x_{>k} \end{bmatrix} \mapsto \begin{bmatrix} x_{\le k} \\ x_{>k} \odot \exp(s(x_{\le k})) + t(x_{\le k}) \end{bmatrix}$$

Example 2: Neural Ordinary Differential Equations

NODE layer

$$\mathrm{Lip}(\mathbb{R}^d) := \{f\colon \mathbb{R}^d \to \mathbb{R}^d \mid f \ \textbf{ is Lipschitz}\}$$

For each $f \in \mathrm{Lip}(\mathbb{R}^d)$, we define an invertible map $\mathbf{x} \mapsto \mathbf{z}(1)$ via an initial value problem [DJ76]

$$\boxed{\mathbf{x}} \longrightarrow \boxed{\text{Solve for } \mathbf{z}(t)\text{:} \ \begin{cases} \mathbf{z}(0) = \mathbf{x}, \\ \dot{\mathbf{z}}(t) = f(\mathbf{z}(t)) \ \ (t \in \mathbb{R}) \,. \end{cases}} \longrightarrow \boxed{\mathbf{z}(1)}$$

NODE layers [CRBD18]

Then, for $\mathscr{H} \subset \mathrm{Lip}(\mathbb{R}^d)$, consider the set of NODEs:

$$\mathrm{NODEs}(\mathscr{H}) := \{\mathbf{x} \mapsto \mathbf{z}(1) \mid f \in \mathscr{H}\}$$

Applications of INNs

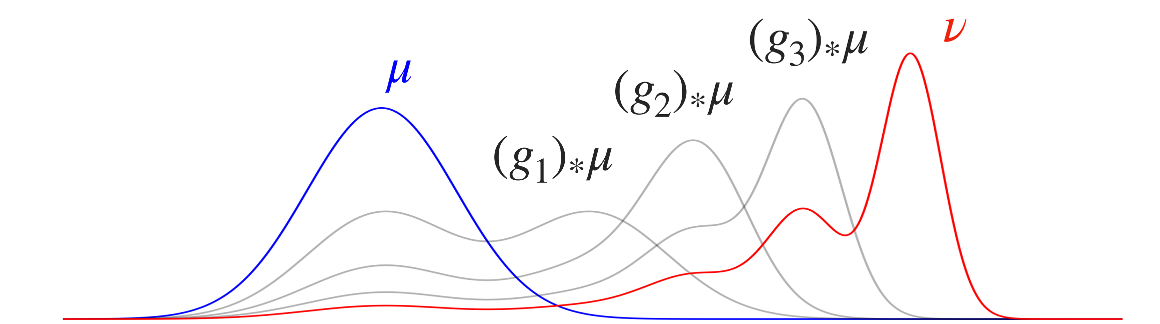
Useful properties of INNs (for nicely designed $\mathscr{G}$)

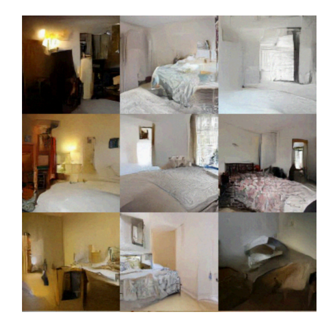
✓ **Explicit** and **efficient invertibility**.

✓ **Tractability** of Jacobian determinant (for nicely designed $\mathscr{G}$).

Usages of INNs

- Approximate distributions (normalizing flows).



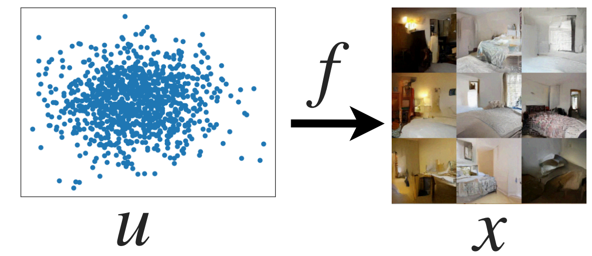


[KD18]

- Approximate invertible maps (feature extraction & manipulation).

[DSB17]

Application 1: Distribution Modeling



[KD18]

Normalizing Flows

Express x as a transformation f of a real vector u sampled from p_u:

$$x = f(u) \quad \text{where} \quad u \sim p_u$$

Examples

- Generative modeling [DSB17,KD18,OLB+18,KLSKY19,ZMWN19]
- Probabilistic inference [BM19,WSB19,LW17,AKRK19]
- Semi-supervised learning [IKFW20]

Training by Maximum Likelihood (Invertibility+Tractable Jacobian!)

By change of variables formula:

↓ easily invertible

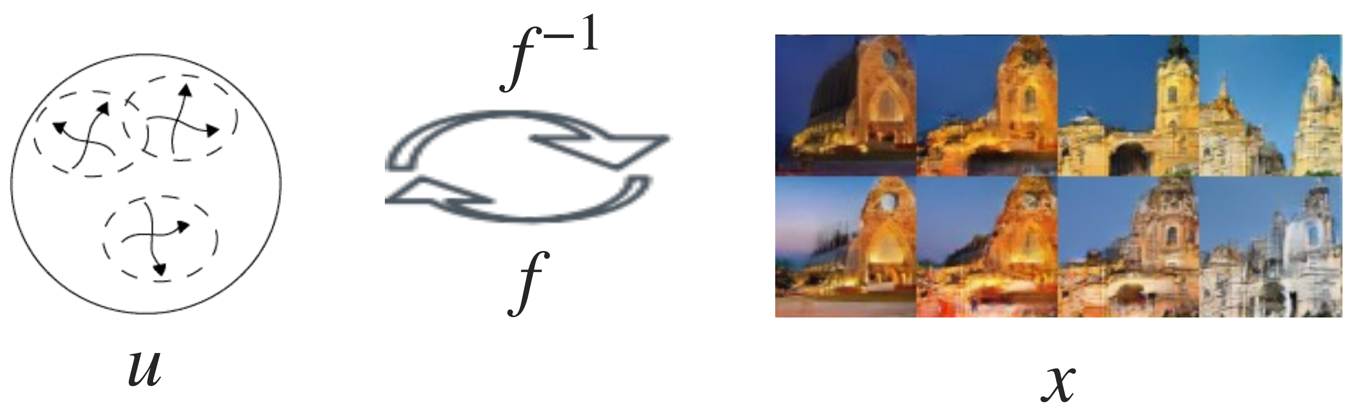
$$\boxed{\log p_x(x) = \log p_u(f^{-1}(x)) + \log \left| \det J_{f^{-1}}(x) \right|}$$

($J_{f^{-1}}$: Jacobian of f^{-1})

↑ known ↑ tractable

Application 2: Function Modeling

Feature Extraction & Manipulation



[DSB17]

1. Extract latent representation u from x by f.
2. Modify u in the latent space (e.g., interpolation).
3. Map back to the data space by f^{-1}.

Examples

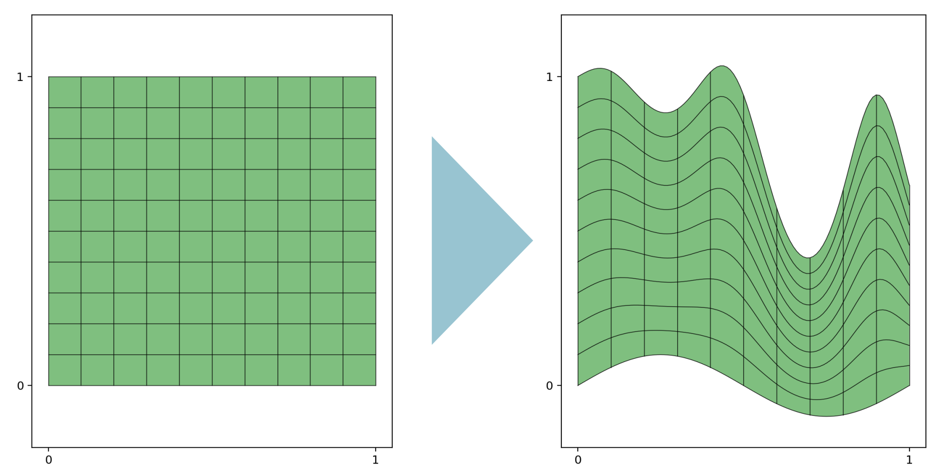
- Generative modeling [DSB17,KD18,OLB+18,KLSKY19,ZMWN19]
- Semi-supervised learning [IKFW20]
- Transfer learning [TSS20]

How flexible are INNs?

INN f is used for **distribution modeling** (application 1) and **invertible function modeling** (application 2).

BUT...

$\mathscr{G}$ relies on special designs to maintain good properties.
(e.g., CF layers keep some dimensions unchanged)



Complications

- The layers have clever specific designs (e.g., ACFs).
- Function composition is the only way to build complex models.
  (Operations such as addition or multiplications are not allowed.)

Research question

Can these INNs have sufficient representation power?

(Restricted function form → restricted representation power?)

This talk is based on the following paper

arXiv: **2204.07415**
based on the following paper

Paper 1: Coupling-based invertible neural networks are universal diffeomorphism approximators (NeurIPS 2020) [TIT+20] NEURAL INFORMATION PROCESSING SYSTEMS **Oral paper!**

- Proposed **a general theoretical framework** to analyze the representation power (universalities) of invertible models.
- Analyzed **CF-INNs** (**ACFs** and more advanced ones).

Paper 2: Universal Approximation Property of Neural Ordinary Differential Equations (NeurIPS 2020 DiffGeo4DL Workshop) [TTI+20] NEURAL INFORMATION PROCESSING SYSTEMS

- Analyzed **NODEs**, building on the general framework.
- (with minor modification to the general framework)

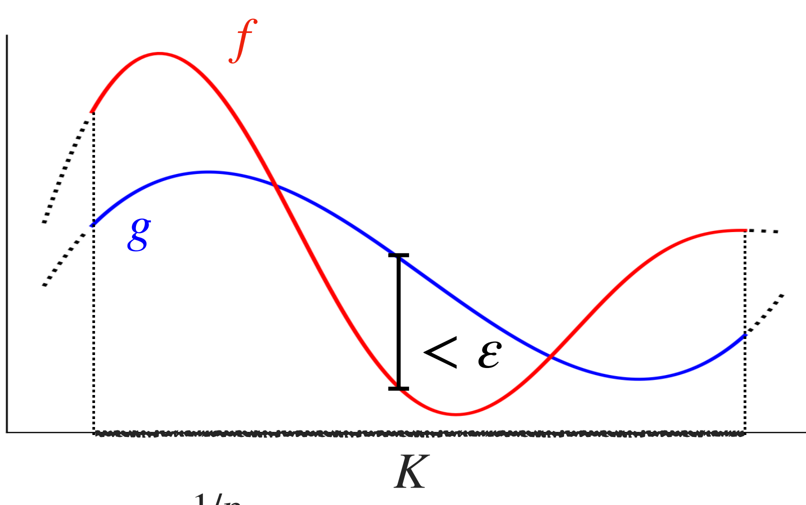
What is "representation power"?

Here,

"Representation power" = Universal approximation property.

Definition (informal) [C89,HSW89]

$W^{r,p}$**-universal approximator**:
the model can approximate any target function w.r.t. $W^{r,p}$-norm on a compact set.



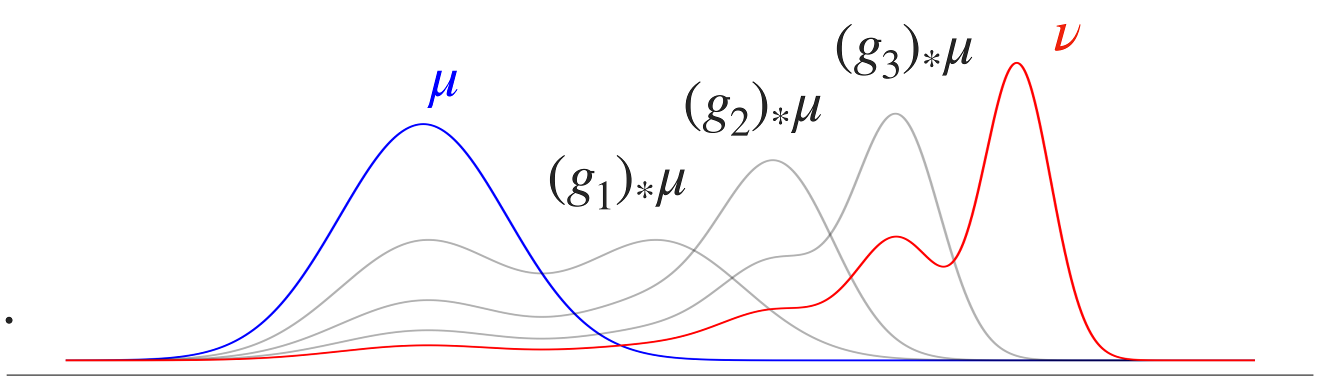
$$W^{r,p}\text{-norm} : \|f-g\|_{r,p,K} = \sum_{|\alpha|\le r}\left(\int_K \|\partial^\alpha (f-g)(x)\|^p dx\right)^{1/p}$$

Definition (informal)

A model is a **distributional universal approximator** if it can transform one distribution arbitrarily close to any distribution.

$$(g_n)_*\mu \xrightarrow[n\to\infty]{} \nu$$

(convergence).



Target Class

Definition (Approximation target $\mathscr{D}^r$)

Fairly **large set** of smooth invertible maps.

$$\mathscr{D}^r := \left\{ C^r\text{-diffeo of the form } f : U_f \to f(U_f) \right\}$$
$$(U_f \subset \mathbb{R}^d : \text{open } C^r\text{-diffeomorphic to } \mathbb{R}^d)$$

$\mathscr{D}^r$

General

$\left\{ C^\infty\text{-diffeo on } \mathbb{R}^d \right\}$

...and more

Main Result

Theorem (Theoretical Framework)

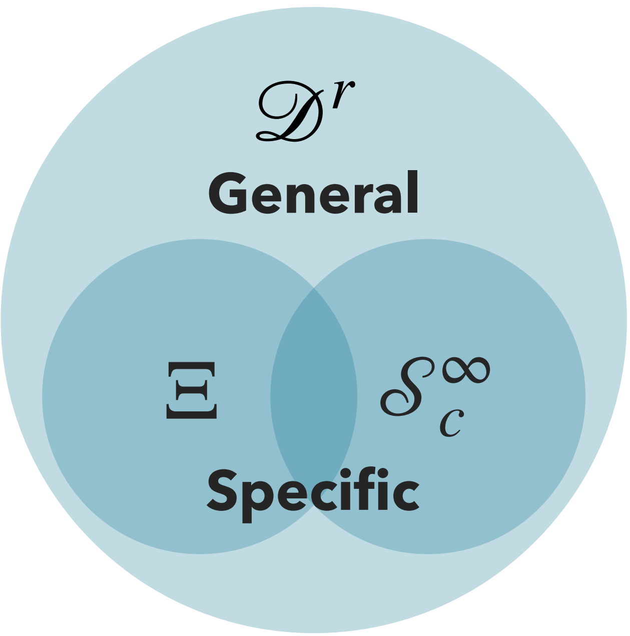
(under mild regularity conditions)

$$\boxed{\boxed{\begin{array}{l}W^{r,p}\text{-univ.}\\ \text{for } \mathscr{D}^2\end{array}} \Leftrightarrow \boxed{\begin{array}{l}W^{r,p}\text{-univ.}\\ \text{for } \Xi\end{array}} \Leftrightarrow \boxed{\begin{array}{l}W^{r,p}\text{-univ.}\\ \text{for } \mathscr{S}^\infty_{\mathrm{c}}\end{array}}} \Rightarrow \boxed{\begin{array}{l}\text{Dist. univ.}\\ \text{weak top. if } r = 0\\ \text{total var. top. if } r \geq 1\end{array}}$$

Ξ : "flow endpoints"

$$\mathscr{S}^\infty_c := \left\{\tau : \text{コンパクト台微分同相 } \tau(\mathbf{x}, y) = (\mathbf{x}, u(\mathbf{x}, y))\right\}$$

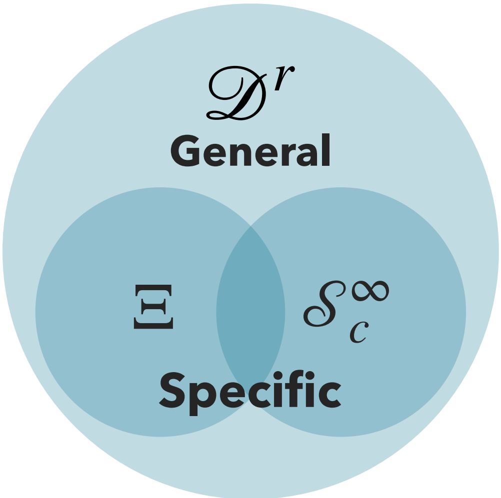
$$u : \mathbb{R}^{d-1} \times \mathbb{R} \to \mathbb{R}, \quad (\mathbf{x}, y) \in \mathbb{R}^{d-1} \times \mathbb{R}$$



Corollaries

$W^{r,p}$-univ. for $\mathscr{D}^2$ $\Leftrightarrow$ $W^{r,p}$-univ. for Ξ $\Leftrightarrow$ $W^{r,p}$-univ. for $\mathscr{S}_{\mathrm{c}}^{\infty}$ $\Rightarrow$ Dist. univ. weak top if $r = 0$ total var top if $r \geq 1$

Examples of Universal Coupling Flows



- **Sum-of-squares polynomial flow** (SoS-flow) [JSY19]
- **Deep sigmoidal flow** (DSF; aka. NAF) [HKLC18]

yield $W^{r,\infty}$**-univ. INNs for** $\mathscr{S}_{\mathrm{c}}^{\infty}$ **(and hence for** $\mathscr{D}^r$**, and also dist-univ.)**.

(stronger than in [JSY19, HKLC18]).

Affine Coupling Flows yield universal INNs

Affine Coupling Flows yield L^p-univ. INNs for $\mathscr{S}_{\mathrm{c}}^{\infty}$ (and hence for $\mathscr{D}^0$, and also dist-univ.).

Corollaries

$W^{r,p}$-univ. for $\mathscr{D}^2$ $\Leftrightarrow$ $W^{r,p}$-univ. for Ξ $\Leftrightarrow$ $W^{r,p}$-univ. for $\mathscr{S}_c^\infty$ $\Rightarrow$ Dist. univ.
weak top if $r = 0$
total var top if $r \geq 1$

Universality of NODEs

NODEs yield $W^{r,\infty}$-univ. INNs for Ξ
(and hence $\sup$-univ. for $\mathscr{D}^r$. Also Dist-univ.).

Overview and Recap

What did we do?

Theoretically investigated:
Are our INNs expressive enough?

INNs = Invertible neural networks

Why important?

Models without a representation power guarantee are hard to rely on.

What is the result?

"Coupling-based INNs (CF-INNs)" and "NODE-based INNs (NODE-INNs)" are "universal function approximators" despite their special architectures.

Message

CF-INNs and NODE-INNs can be relied on in modeling invertible functions and probability distributions.

Today's talk structure

Part 1

Introduction.

Overview of what we did and why it's important.

Part 2

Details of the theory.

Theoretical preliminaries and proof machinery.

Idea of Proof

We assume $d \geq 7$

Difficulty

- We cannot use **techniques of functional analysis**!
  - INNs and $\mathscr{D}^r$ are **not** linear spaces

$(r \geq 0)$

Recall : $\mathscr{D}^r := \left\{ C^r\text{-diffeo of the form } f : U_f \to f(U_f) \right\}$

$(U_f \subset \mathbb{R}^d$: open C^r-diffeo to $\mathbb{R}^d)$

  - Existing methods do not work....(e.g. Hahn-Banach theorem, Fourier transform, Stone-Weirestrass theorem, e.t.c)

Idea

- Utilize a concrete structure of the **diffeomorphism group** !

$W^{r,p}$-Universal approximators

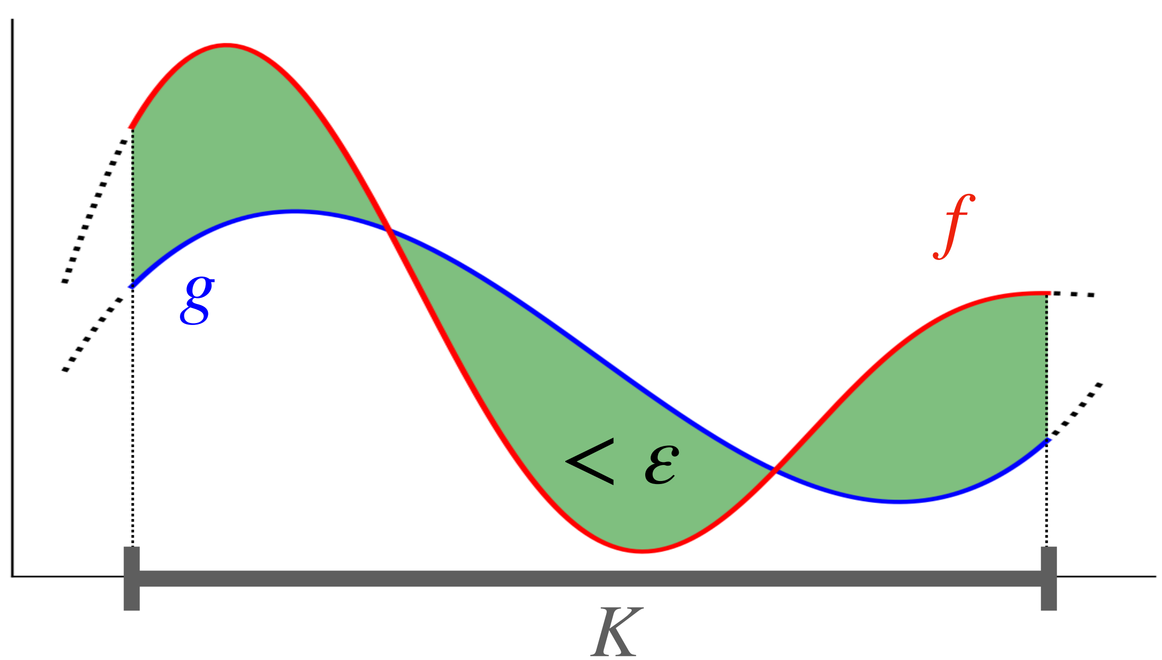
$\mathscr{M}$: model, set of measurable bijection from $\mathbb{R}^d$ to $\mathbb{R}^d$ (e.g. INNs)

$\mathscr{F}$: target functions $f: U_f \to f(U_f)$ (e.g. $\mathscr{D}^r$)

$\mathscr{M}$ is an $W^{r,p}$-**universal approximator** for $\mathscr{F}$ **if**

$\forall f \in \mathscr{F}$, $\forall \varepsilon > 0$, $\forall K \subset U_f$: compact , $\exists g \in \mathscr{M}$

$$\|f - g\|_{r,p,K} := \sum_{|\alpha| \le r} \left(\int_K \|\partial^\alpha (f - g)(x)\|^p dx \right)^{1/p} < \varepsilon$$



Relation of universalities

Proposition

For $\infty \geq r > r'$,

A model $\mathscr{M}$ is a $W^{r,p}$-universal approximator for a target $\mathscr{F}$

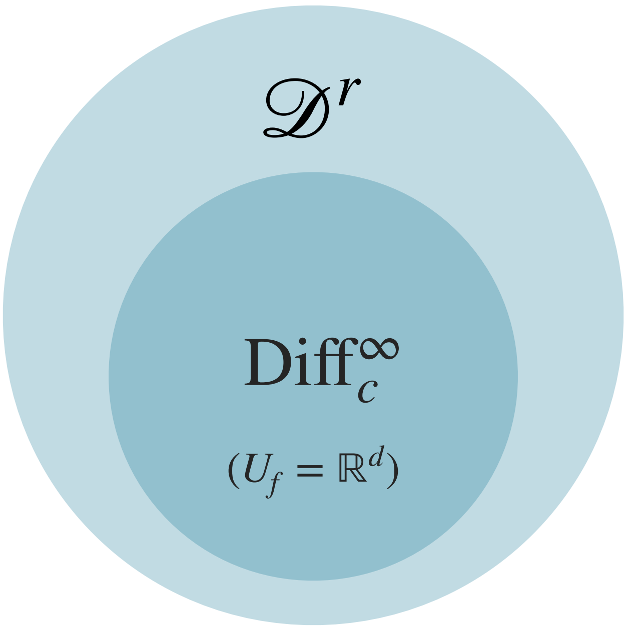
$$\Downarrow$$

A model $\mathscr{M}$ is an $W^{r',p}$-universal approximator a target $\mathscr{F}$

A structure theorem of diffeomorphism groups

Definition (compactly supported diffeomorphisms)

Diff_c^∞: the set of C^∞-diffeomorphisms $f : \mathbb{R}^d \to \mathbb{R}^d$ such that $f(x) = x$ outside a compact subset



Theorem (Herman, Thurston, Epstein, and Mather)

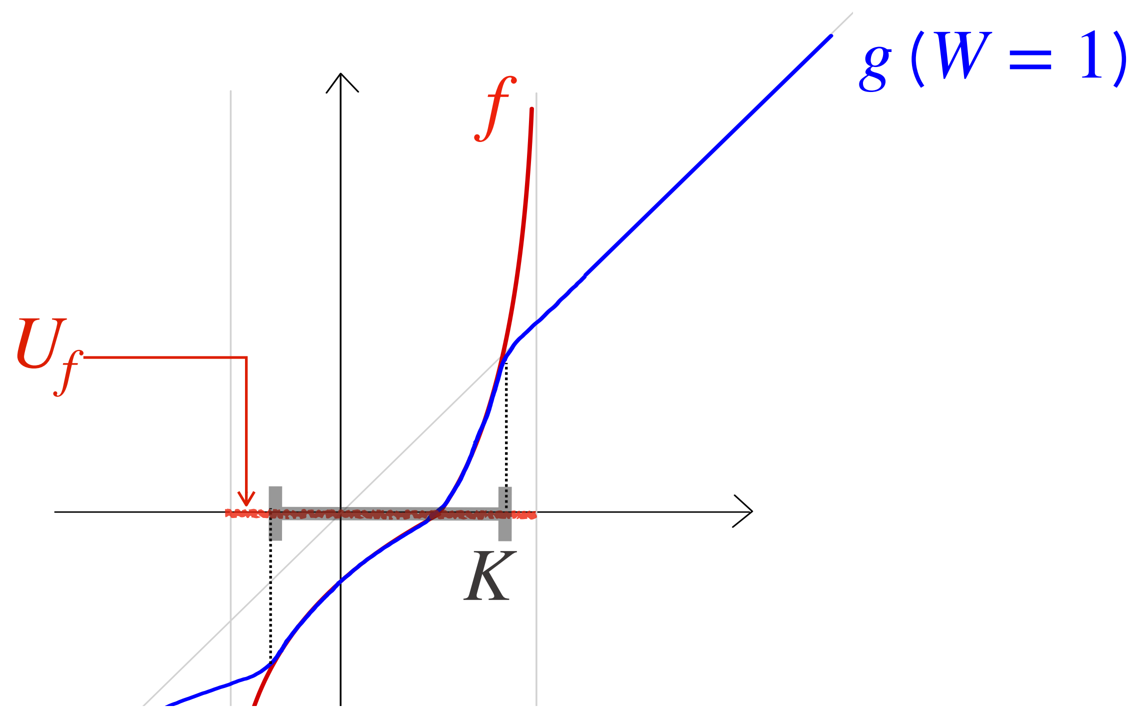
Diff_c^∞ is a **simple group** (does not have any proper normal subgroup except $\{\mathrm{Id}\}$)

Extension of $\mathscr{D}^r$

Proposition

For $f \in \mathscr{D}^r$ $(f : U_f \to \mathbb{R}^d)$ and compact subset $K \subset U_f$ (assume $d \geq 7$ if $(p, r) = (\infty, r)$), there exist an affine transform $W \in \mathrm{Aff}$ and $g \in \mathrm{Diff}_c^\infty$ such that

$$f|_K \sim W \circ g|_K \text{ (with any precision in } W^{r,p}\text{-norm)}$$



Remark

If $(p, r) = (\infty, 0)$, we use Annulus Theorem by Kirby (1969, $d \geq 5$) and an approximation theorem by Cornell (1963) (Cornell's result needs the condition $d \geq 7$).

Flow endpoints

Definition (flow endpoints Ξ)

$g \in \mathrm{Diff}_c^\infty$: **flow endpoint if** there exists a **continuous** and **"additive"** map $\phi : [0,1] \to \mathrm{Diff}_c^\infty$ such that $\phi(0) = \mathrm{Id}$ and $\phi(1) = g$

$\Xi :=$ {flow endpoints}

Proposition

The set of finite compositions of flow endpoints (the group generated by Ξ) is a **nontrivial normal subgroup** of Diff_c^∞.

Corollary

For $g \in \mathrm{Diff}_c^\infty$, there exist **finite** flow endpoints $g_1, \ldots, g_m \in \Xi$ such that

$$g = g_1 \circ \cdots \circ g_m.$$

In particular,

$$\boxed{W^{r,p}\text{-univ. for } \mathscr{D}^r} \iff \boxed{W^{r,p}\text{-univ. for } \Xi}$$

Universality of NODE

$f \in \mathscr{D}^r$: target, $K \subset U_f$: compact

$f|_K$

$\wr$ « approximate $f|_K$

$\exists W \circ h$ (Aff & compactly supported C^∞-diffeomorphism)

$\|$ « **structure theorem of diffeomorphism group**

$\exists h_1 \circ h_2 \circ \cdots$ (**flow endpoints**)

$\wr\wr$

element of $\mathrm{NODEs}(\mathscr{H})$ $\quad$ $\mathrm{NODEs}(\mathscr{H}) := \{\mathbf{x} \mapsto \mathbf{z}(1) \mid f \in \mathscr{H}\}$

Paper 2 Result (Analysis of NODEs)

NODEs yield $W^{r,\infty}$-univ. INNs for Ξ

(and hence $W^{r,\infty}$-univ. for $\mathscr{D}^r$. Also Dist-univ. for tot. var.).

Proof outline of result in Paper 1

$W^{r,p}$-univ. for $\mathscr{D}^r$ $\Longleftrightarrow$ $W^{r,p}$-univ. for $\mathscr{S}_c^\infty$

$\mathscr{S}_c^\infty := \{\tau :$ compactly supported $\tau(\mathbf{x}, y) = (\mathbf{x}, u(\mathbf{x}, y))\} \subset \mathrm{Diff}_c^\infty$

$u : \mathbb{R}^{d-1} \to \mathbb{R}, \quad (\mathbf{x}, y) \in \mathbb{R}^{d-1} \times \mathbb{R}$

$f|_K$ $\qquad f \in \mathscr{D}^r$: target, $K \subset U_f$: compact

$\wr$ « approximate $f|_K$

$\exists W \circ h$ (Aff & compactly supported C^∞-diffeomorphism)

$\|$ « **structure theorem of diffeomorphism group**

$\exists h_1 \circ h_2 \circ \cdots$ (**flow endpoints** Ξ)

$\|$

$\exists g_1 \circ g_2 \circ \cdots$ (nearly Ids)

$\|$

$\sigma_1 \circ \tau_1 \circ \cdots$ (**permutations &** $\mathscr{S}_c^\infty$)

Decompose $f|_K$ into simpler mappings

Nearly Id

Definition (nearly-Id elements)

$g \in \mathrm{Diff}_c^\infty$: **nearly-$\mathrm{Id}$ element if** $\|dg(x) - I\| < 1$ for $x \in \mathbb{R}^d$

Proposition

For a flow endpoint $g \in \mathrm{Diff}_c^\infty$, there exist nearly-$\mathrm{Id}$ elements $g_1, \ldots, g_m \in \mathrm{Diff}_c^\infty$ such that

$$g = g_1 \circ \cdots \circ g_m.$$

$\because$ $g = \phi(1)$ ($\phi : [0,1] \to \mathrm{Diff}_c^\infty$: "additive" and continuous)

Then, $g = \phi(1/m)^m$ and $\phi(1/m) \to \mathrm{Id}$ as $m \to \infty$

Thus, we define $g_1 = g_2 = \ldots = g_m = \phi(1/m)$ for sufficiently large m ∎

Decomposition of nearly Id's

Proposition

For a nearly-Id element $g \in \mathrm{Diff}_c^\infty$, there exist $\tau_1, \ldots, \tau_d \in \mathcal{S}_c^\infty$ and $\sigma_1, \ldots, \sigma_d \in \mathfrak{S}_d$ such that

$$g = \sigma_1 \circ \tau_1 \circ \cdots \circ \sigma_m \circ \tau_m.$$

Lemma for this proposition

For $g = (g_i)_{i=1}^d \in \mathrm{Diff}_c^\infty$, if for any $k = 1, \ldots, d$, the submatrix of its jacobian

$$\left(\frac{\partial g_{i+k-1}}{\partial x_{j+k-1}}(x) \right)_{i,j=1,\ldots,d-k-1}$$

is invertible for all x, then there exit $\tau_1, \ldots, \tau_d \in \mathcal{S}_c^\infty$ and $\sigma_1, \ldots, \sigma_d \in \mathfrak{S}_d$ such that

$$g = \sigma_1 \circ \tau_1 \circ \cdots \circ \sigma_m \circ \tau_m.$$

Compatibility of approximations and compositions

- Is a composition of approximations an approximation of the composition ?
- We may reduce the problem to approximations of small constituents

Proposition

$\mathscr{M}$: a set of piecewise C^1-diffeomorphisms

$F_1, \ldots, F_r$: **linearly increasing** piecewise C^1-diffeomorphims

Assume $\exists H_i \in \mathscr{M}$ such that

$$H_i \approx F_i \text{ (L^p-approximation on any compact sets)}$$

Then, for compact set $K \subset \mathbb{R}^d$, there exist $G_1, \ldots, G_r \in \mathscr{M}$ such that

$$G_r \circ \cdots \circ G_1 \approx F_r \circ \cdots \circ F_1 \text{ (L^p-approximation on K)}$$

Remark

If $\mathscr{M}$ is composed of **locally bounded** maps and F_i's are **continuous**, we have a similar proposition for $\sup$-universal approximators.

Proof outline of Main result

$W^{r,p}$-univ. for $\mathscr{D}^r$ $\iff$ $W^{r,p}$-univ. for $\mathscr{S}_c^\infty$

$\mathscr{S}_c^\infty := \{\tau :$ compactly supported $\tau(\mathbf{x}, y) = (\mathbf{x}, u(\mathbf{x}, y))\} \subset \mathrm{Diff}_c^\infty$

$u : \mathbb{R}^{d-1} \to \mathbb{R}, \quad (\mathbf{x}, y) \in \mathbb{R}^{d-1} \times \mathbb{R}$

$f|_K$ $\qquad f \in \mathscr{D}^r$: target, $K \subset U_f$: compact

$\wr$ « approximate $f|_K$

$\exists W \circ h$ (Aff & compactly supported C^∞-diffeomorphism)

$\|$ « **structure theorem of diffeomorphism group**

$\exists h_1 \circ h_2 \circ \cdots$ (**flow endpoints** Ξ)

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$\exists g_1 \circ g_2 \circ \cdots$ (nearly Ids)

$\|$

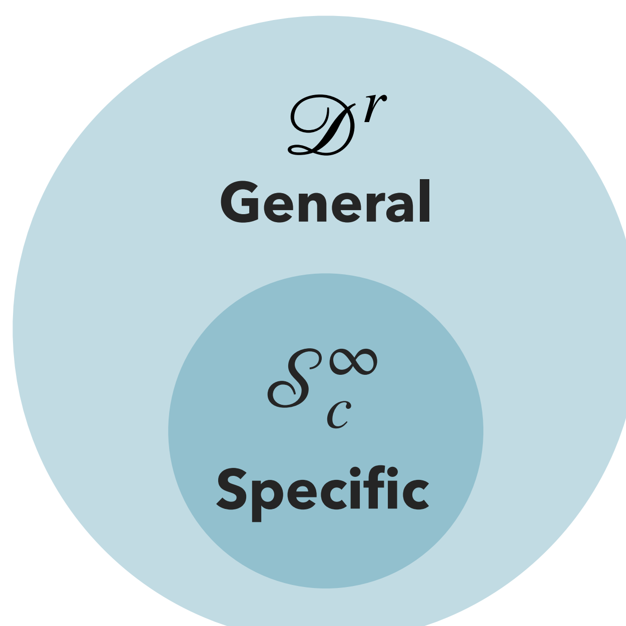
$\sigma_1 \circ \tau_1 \circ \cdots$ (**permutations &** $\mathscr{S}_c^\infty$)

Decompose $f|_K$ into simpler mappings

How the result can be used

You show		**You get**

$$
\begin{tikzcd}
W^{r,\infty}\text{-univ. for } \mathscr{S}_c^\infty \arrow[r, Rightarrow] \arrow[d, Rightarrow] & W^{r,\infty}\text{-univ. for } \mathscr{D}^r \arrow[d, Rightarrow] \\
W^{r,p}\text{-univ. for } \mathscr{S}_c^\infty \arrow[r, Rightarrow] & W^{r,p}\text{-univ. for } \mathscr{D}^r
\end{tikzcd}
$$



Upgrade Existing Guarantees

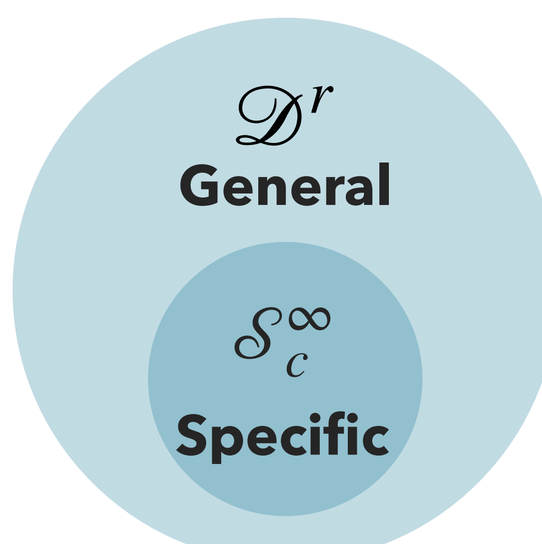
Regrading guarantees for existing INN architectures:

- **Sum-of-squares polynomial flow** (SoS-flow)
- **Deep sigmoidal flow** (DSF; aka. NAF)

Previously known/claimed [JSY19, HKLC18]:

L^∞-universality for $\mathscr{S}_c^\infty$

$W^{r,p}$-universality for $\mathscr{D}^r$ for $r \geq 0$



Distributional universal approximators

Definition (distributional universal approximator)

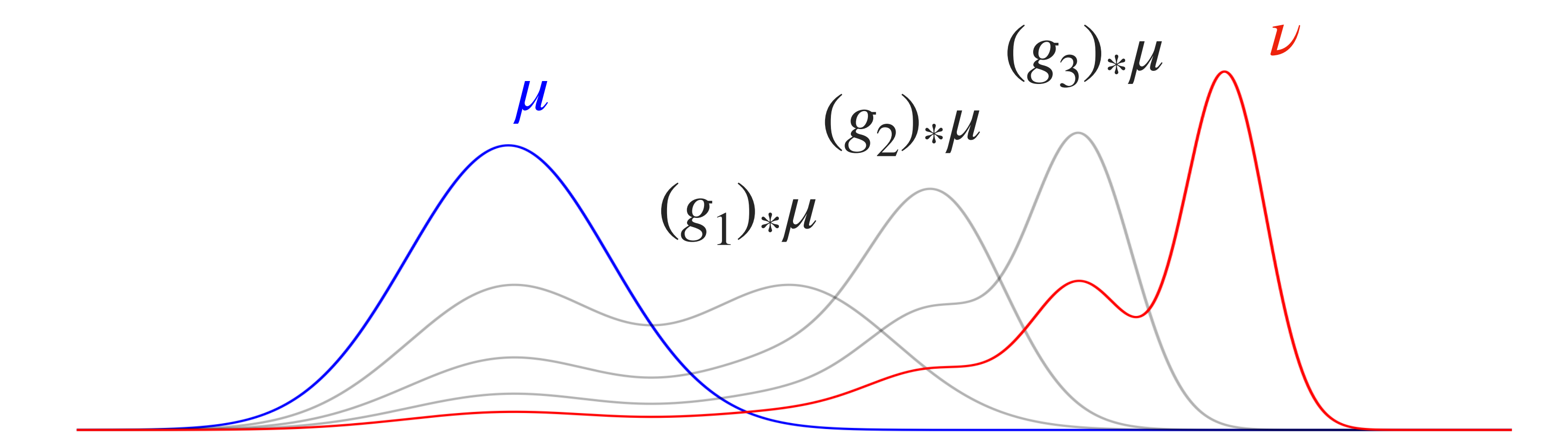
$\mathscr{M}$: model, set of measurable bijection from $\mathbb{R}^d$ to $\mathbb{R}^d$ (e.g. INNs)

$\mathscr{P}$: absolutely continuous probability measures with a topology

$\mathscr{M}$ is a **distributional universal approximator** w.r.t. the topology of $\mathscr{P}$ **if**

$\forall \mu, \nu \in \mathscr{P}, \ \exists \{g_n\}_{n=1}^{\infty} \subset \mathscr{M}$

$$(g_n)_* \mu \xrightarrow[n \to \infty]{} \nu \quad \text{(convergence in } \mathscr{P}\text{)}.$$



Relation of universalities

Proposition

A model $\mathscr{M}$ is a $W^{r,p}$-universal approximator for a target $\mathscr{D}^r$

$$\Downarrow$$

A model $\mathscr{M}$ is a distributional universal approximator w.r.t

- weak topology if $r = 0$
- total variation topology if $r > 0$

In summary, we obtain

$W^{r,p}$-univ. for $\mathscr{D}^2$ $\Leftrightarrow$ $W^{r,p}$-univ. for Ξ $\Leftrightarrow$ $W^{r,p}$-univ. for $\mathscr{S}_{\mathrm{c}}^{\infty}$ $\Rightarrow$ Dist. univ. weak top if $r = 0$ total var top if $r \geq 1$

Universality of CF-INNs

L^p-/sup-univ. for $\mathscr{D}^2$	$\Leftrightarrow$	L^p-/sup-univ. for Ξ	$\Leftrightarrow$	L^p-/sup-univ. for $\mathscr{S}^\infty_c$	$\Rightarrow$	Distributional-univ.

Affine Coupling Flows yield universal INNs

Affine Coupling Flows yield L^p-univ. INNs for $\mathscr{S}^\infty_c$
(and hence for $\mathscr{D}^0$, and also Dist-univ. w.r.t weak topology).

Remark

The representation power of invertible neural networks based on affine coupling flow is empirically known, and they were **conjectured** distributional universal approximator. We **affirmatively** answer this question.

Conclusion & Future Work

Conclusion

- Proposed a general theoretical framework to analyze the representation power (universalities) of invertible models.
- Guarantee the representation power of CF-INNs as an L^p-universal approximator.
- Guarantee the representation power of NODE-INNs as a $W^{r,\infty}$-universal approximator.

Future work

- Quantitative analysis: Estimate the number of layers required for the approximation given the smoothness of the target.

Message

CF-INNs and NODE-INNs can be relied on in modeling invertible functions and probability distributions.

Appendix

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