

On the Universality of Invertible Neural Networks

Takeshi Teshima^{1 2}, Isao Ishikawa^{3 2}

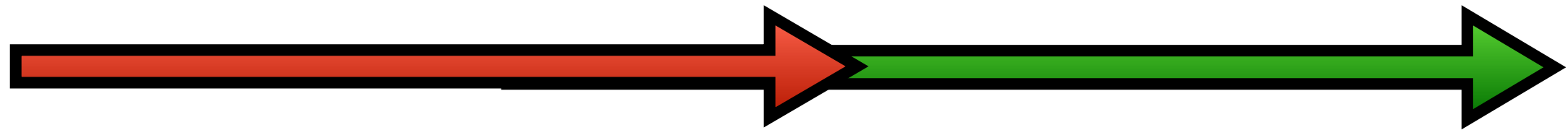
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Joint work with Koichi Tojo, Kenta Oono, Masahiro Ikeda, and Masashi Sugiyama.

Today's talk structure

2



Part 1

Introduction.

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

Part 2

Details of the theory.

Theoretical preliminaries
and proof machinery.

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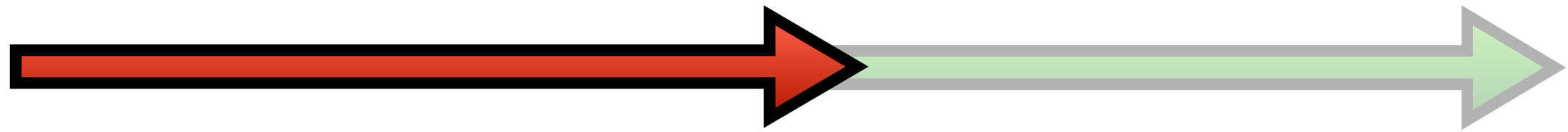
Recent Research Interests:

General methodology of machine learning.
In particular: "Causality for machine learning"

- Causal mechanism transfer \leftarrow I used INNs in this work
- Causal data augmentation

Today's talk structure

4



Part 1

Introduction.

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

Part 2

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Theoretical preliminaries
and proof machinery.

Goal

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

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

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

$$f = g_1 \circ W_1 \circ \dots \circ g_k \circ W_k \quad (g_i \in \mathcal{G}, W_i \in \text{Aff})$$

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

(\mathcal{G} is often rather simple \rightarrow Composed to model complex f)

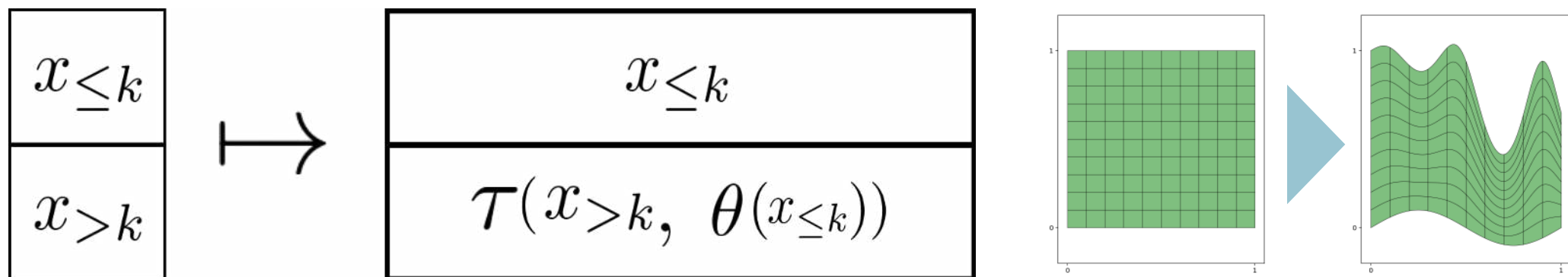
Example (Designs of flow layers \mathcal{G})

- Coupling-based flow layers [DKB14, PNRML19, KPB19]
- Neural ordinary differential equations [CRBD18]

Example1: Coupling Flows

6

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

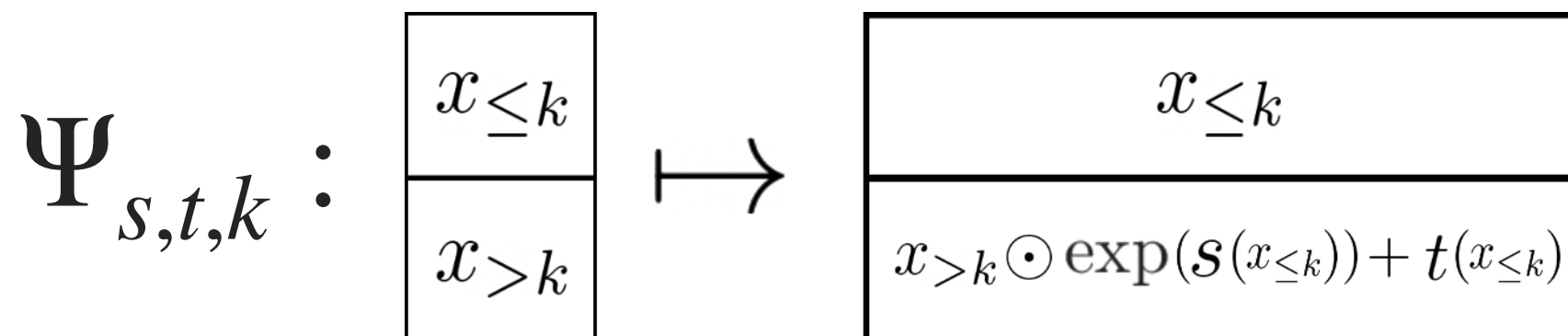


Idea: Keep some dimensions unchanged. (Strong constraint!)

CF-INN = Coupling-flow based INN.

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

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



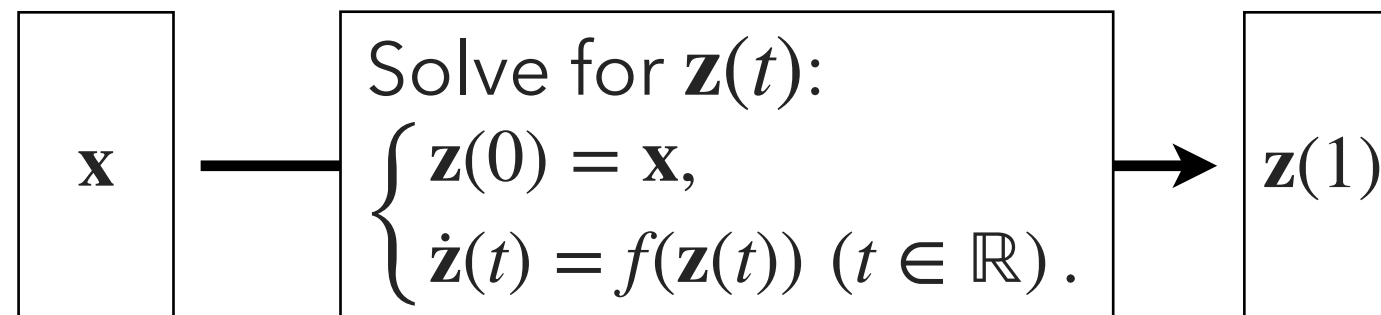
Example 2: Neural Ordinary Differential Equations

7

NODE layer

$$\text{Lip}(\mathbb{R}^d) := \{f: \mathbb{R}^d \rightarrow \mathbb{R}^d \mid f \text{ is Lipschitz}\}$$

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



NODE layers [CRBD18]

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

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

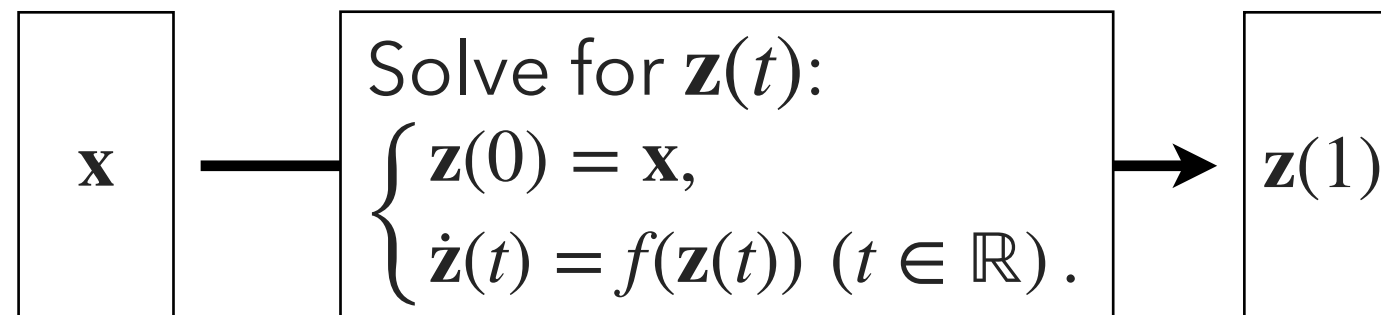
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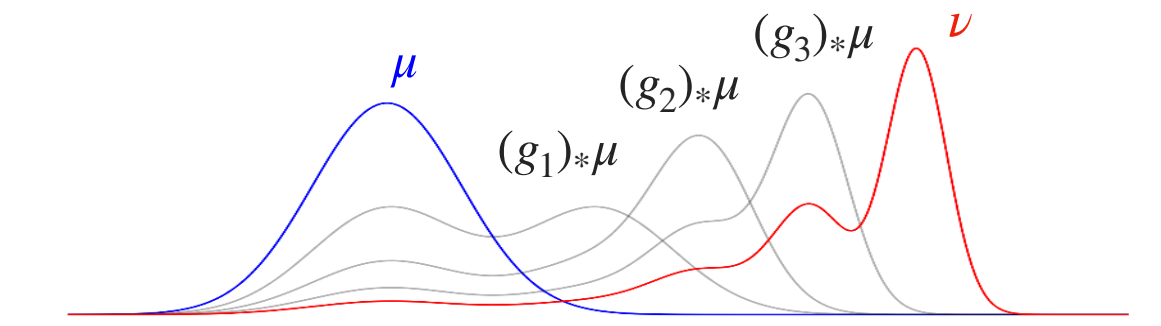
$$\text{NODEs}(\mathcal{H}) := \{\mathbf{x} \mapsto \mathbf{z}(1) \mid f \in \mathcal{H}\}$$

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

- ✓ **Explicit and efficient invertibility.**
- ✓ **Tractability** of Jacobian determinant (for nicely designed \mathcal{G}).

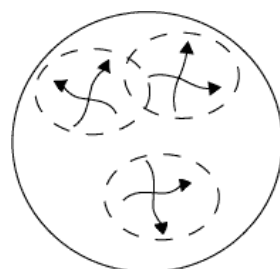
Usages of INNs

- Approximate distributions (normalizing flows).



[KD18]

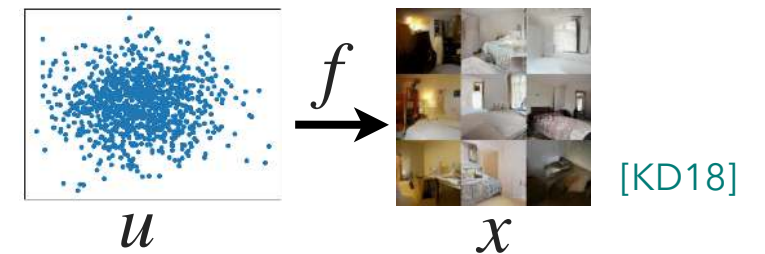
- Approximate invertible maps (feature extraction & manipulation).



[DSB17]

Application 1: Distribution Modeling 9

Normalizing Flows



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

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

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!)

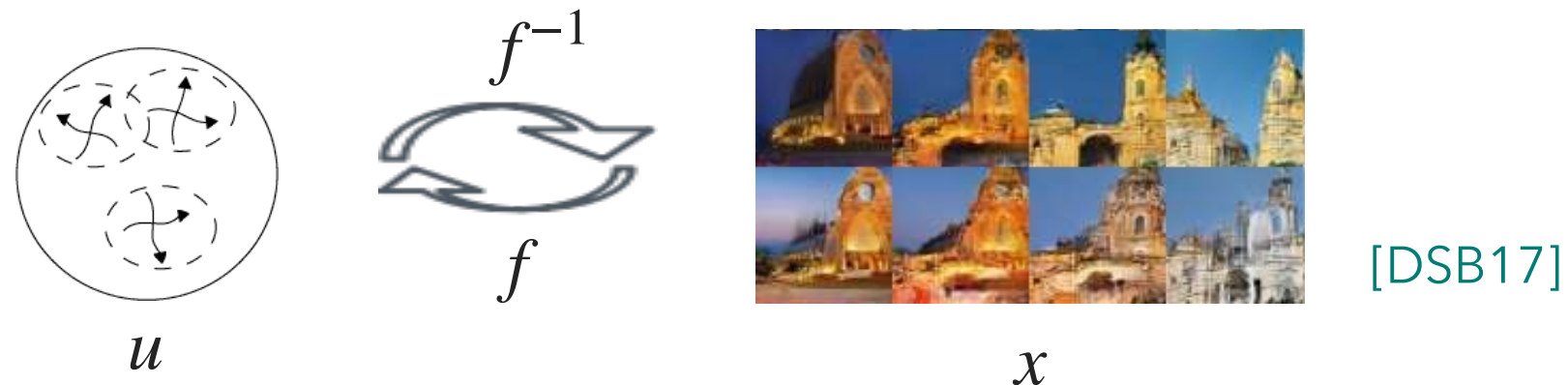
By change of variables formula:

$$\log p_x(x) = \log p_u(f^{-1}(x)) + \log \left| \det J_{f^{-1}}(x) \right| \quad (J_{f^{-1}}: \text{Jacobian of } f^{-1})$$

\downarrow easily invertible

\uparrow known \uparrow tractable

Feature Extraction & Manipulation



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} .

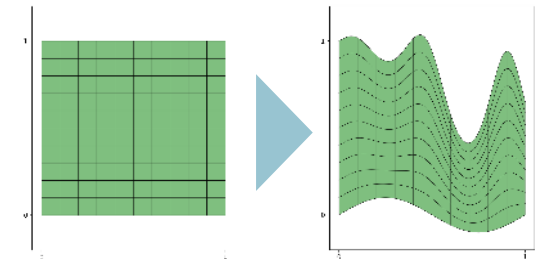
Examples

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

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

BUT...

\mathcal{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 \rightarrow restricted representation power?)

This talk is based on the following papers 12

Paper 1: Coupling-based invertible neural networks are universal diffeomorphism approximators (NeurIPS 2020) [TIT+20] 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]

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

What is "representation power"?

13

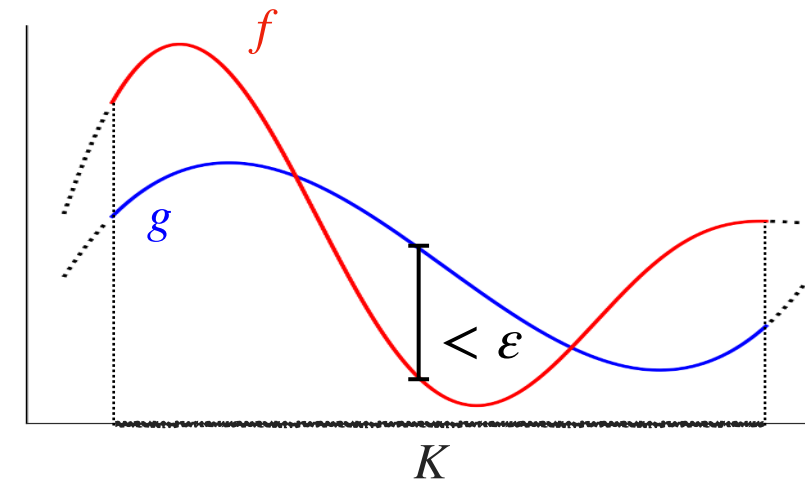
Here,

"Representation power" = Universal approximation property.

Definition (informal) [C89,HSW89]

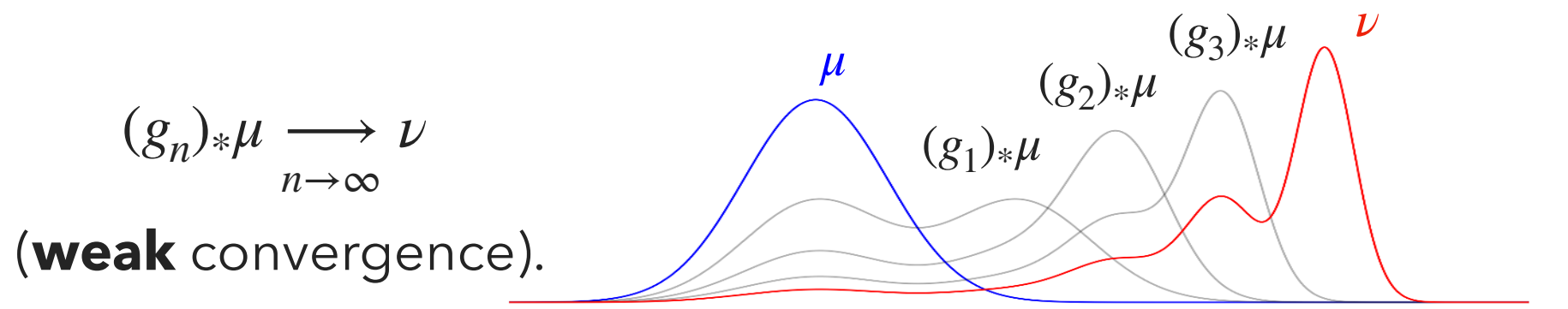
sup- (L^p -) universal approximator:

the model can approximate any target function w.r.t. sup- (L^p -) norm on a compact set.



Definition (informal)

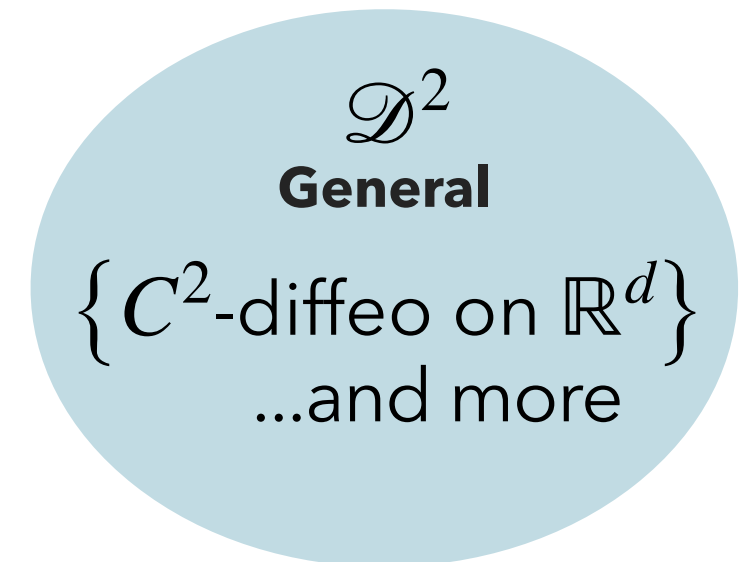
A model is a **distributional universal approximator** if it can transform one distribution arbitrarily close to any distribution.



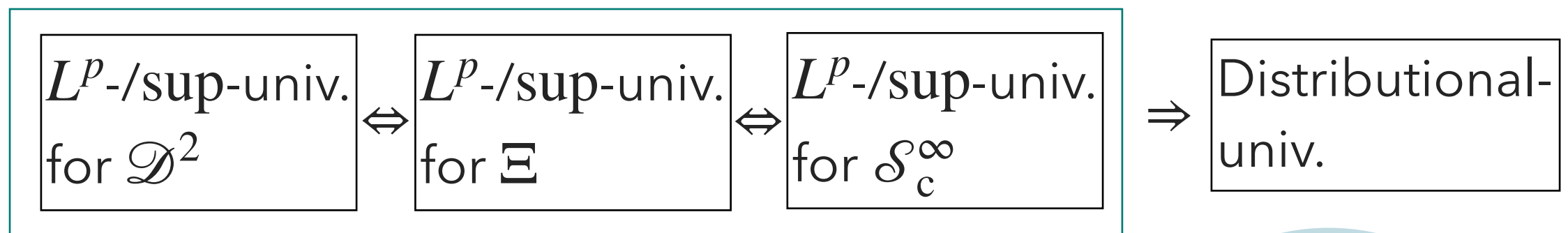
Definition (Approximation target \mathcal{D}^2)

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

$$\mathcal{D}^2 := \{C^2\text{-diffeo of the form } f : U_f \rightarrow f(U_f)\} \\ (U_f \subset \mathbb{R}^d : \text{open } C^2\text{-diffeo to } \mathbb{R}^d)$$

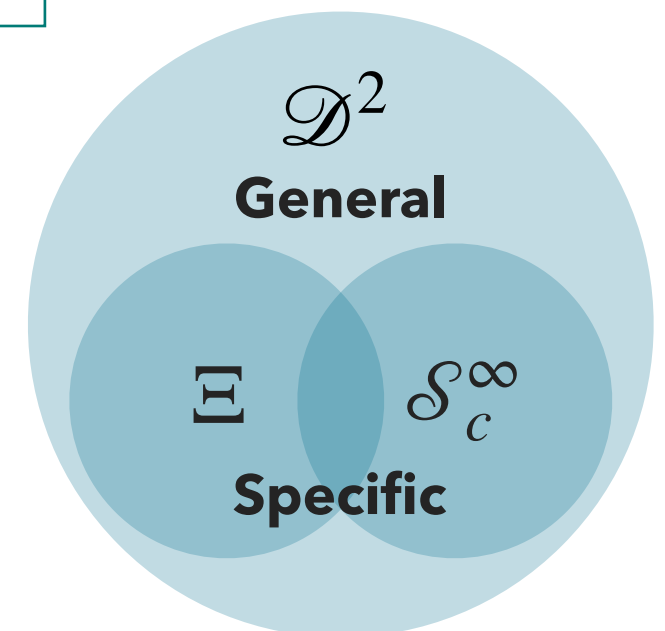


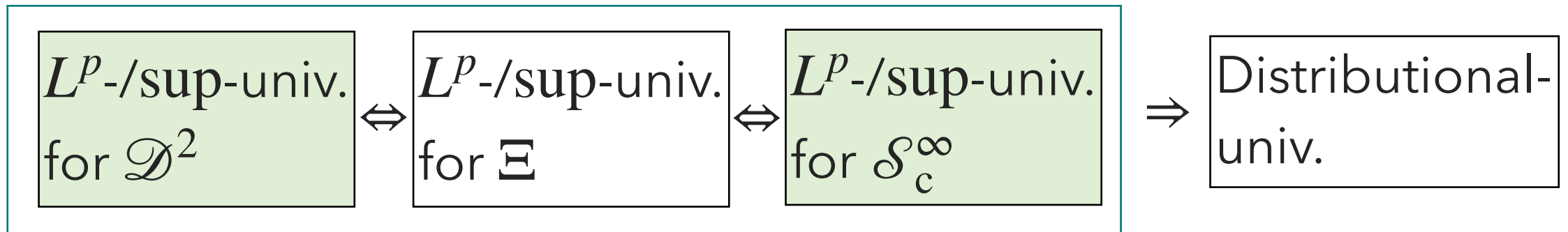
Paper 1 Result (Theoretical Framework) (under mild regularity conditions)



Ξ : "flow endpoints"

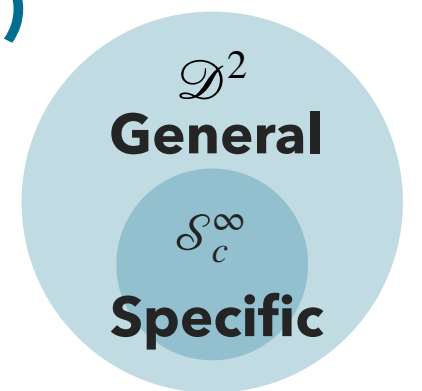
**Application of a structure theorem
in differential geometry**





Paper 1 Result (Examples of Universal Coupling Flows)

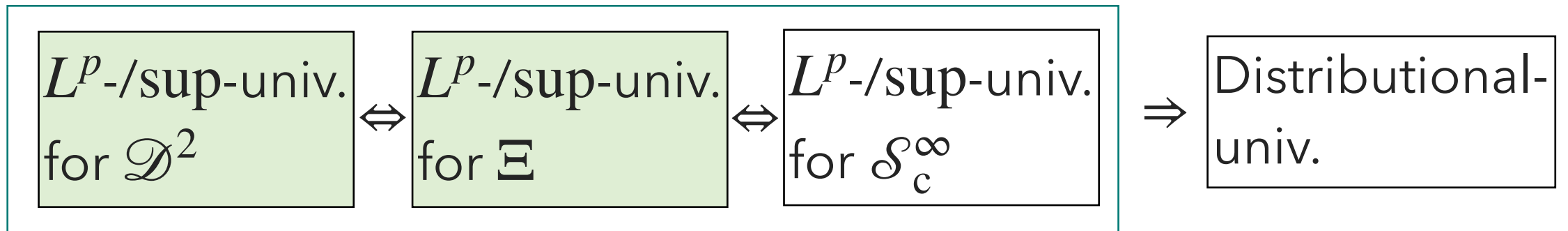
- **Sum-of-squares polynomial flow** (SoS-flow) [JSY19]
- **Deep sigmoidal flow** (DSF; aka. NAF) [HKLC18]



yield **sup-univ. INNs for \mathcal{S}_c^∞** (and hence for \mathcal{D}^2 , and also **Dist-univ.**).
(stronger than in [JSY19, HKLC18]).

Paper 1 Result (Affine Coupling Flows yield universal INNs)

Affine Coupling Flows yield L^p -univ. INNs for \mathcal{S}_c^∞
(and hence for \mathcal{D}^2 , and also Dist-univ.).



Paper 2 Result (Analysis of NODEs)

NODEs yield sup-univ. INNs for Ξ
(and hence sup-univ. for \mathcal{D}^2 . Also Dist-univ.).

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? 

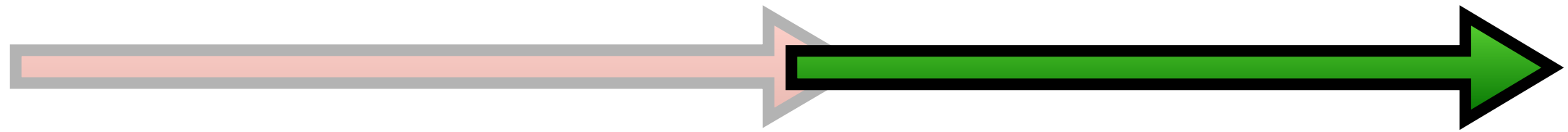
**"Coupling-based INNs (CF-INNs)" and
"NODE-based INNs (NODE-INNs)" are
"universal function approximators"
despite their special architectures.**

Message

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

Today's talk structure

18



Part 1

Introduction.

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

Part 2

Details of the theory.

Theoretical preliminaries
and proof machinery.

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Supported by CREST JPMJCR1913



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

1. Idea of proof
2. Notion of universalities
3. Machinery for proof
 - i) Compatibility of approximation and composition
 - ii) Structure theorem of diffeomorphism group
4. Proof outline of universality of NODE
5. Proof of results in paper 1

Difficulty

- We cannot use **techniques of functional analysis!**
 - INNs and \mathcal{D}^2 are **not** linear spaces

Recall : $\mathcal{D}^2 := \{C^2\text{-diffeo of the form } f : U_f \rightarrow f(U_f)\}$
($U_f \subset \mathbb{R}^d$: open C^2 -diffeo to \mathbb{R}^d)
 - Existing methods do not work....(e.g. Hahn-Banach theorem, Fourier transform, Stone-Weierstrass theorem, e.t.c)

Idea

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

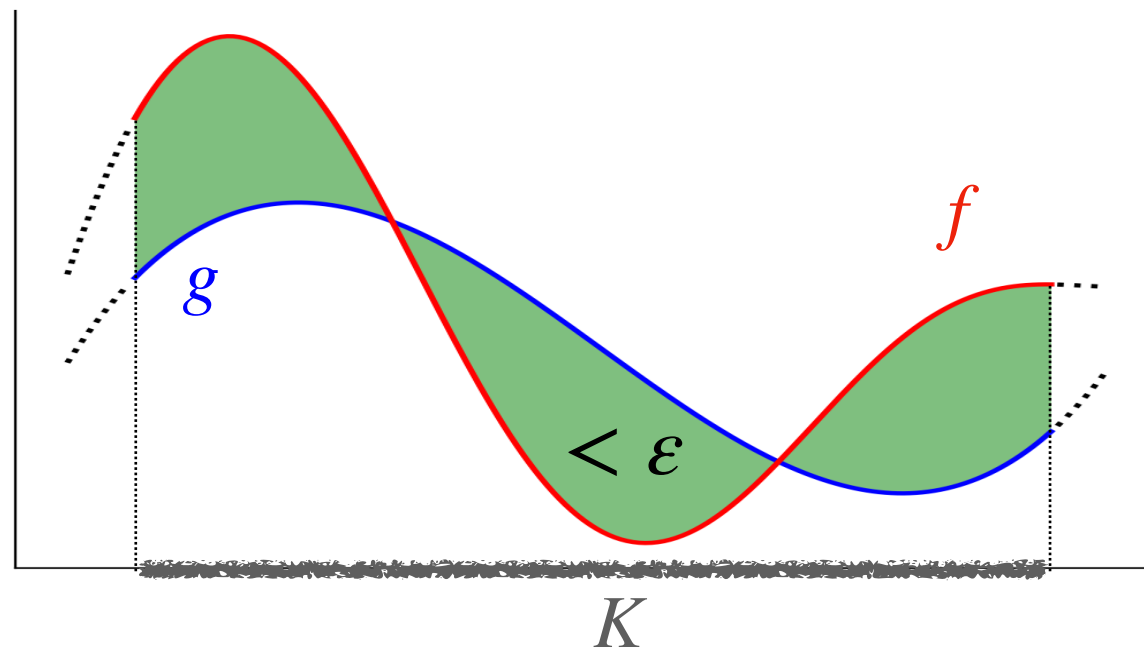
\mathcal{M} : model (e.g. set of INNs)

\mathcal{F} : target functions $f: U_f \rightarrow f(U_f)$ (e.g. \mathcal{D}^2)

\mathcal{M} is an **L^p -universal approximator** for \mathcal{F} if

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

$$\int_K |f(x) - g(x)|^p dx < \varepsilon$$



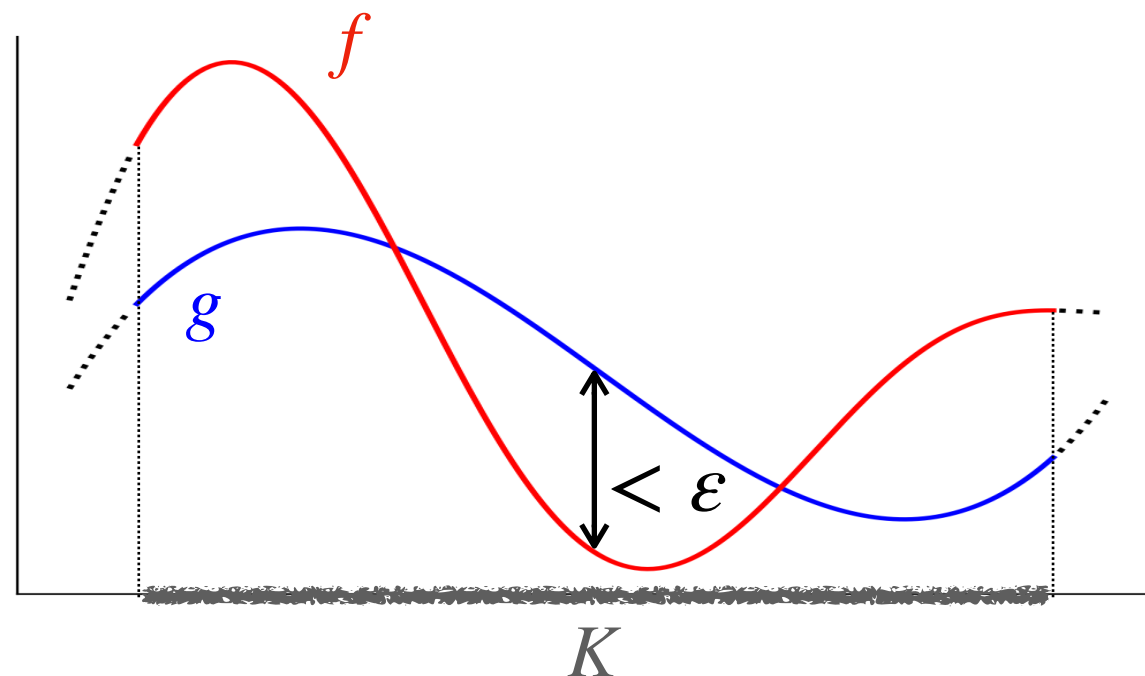
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$$\sup_{x \in K} |f(x) - g(x)| < \varepsilon$$



Proposition

A model \mathcal{M} is a **sup**-universal approximator for a target \mathcal{F}



A model \mathcal{M} is an **L^p** -universal approximator a target \mathcal{F}

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

Proposition

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

F_1, \dots, F_r : **linearly increasing** piecewise C^1 -diffeomorphisms

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

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

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

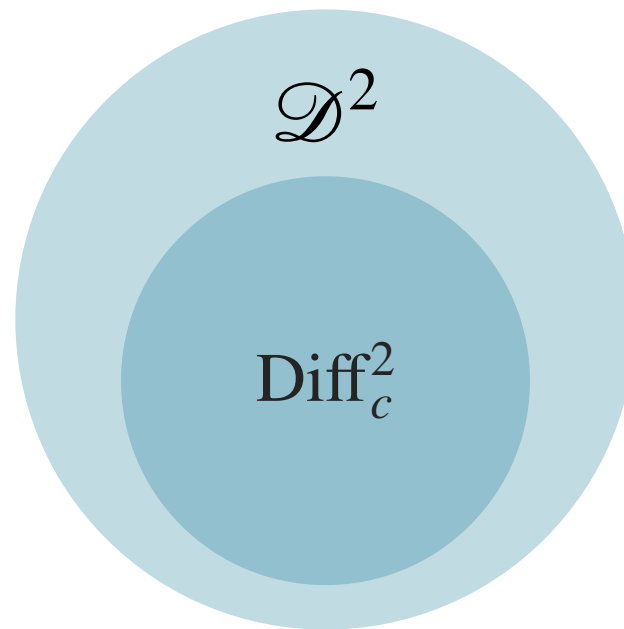
$$G_r \circ \dots \circ G_1 \approx F_r \circ \dots \circ F_1 \text{ (} L^p\text{-approximation on } K\text{)}$$

Remark

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

Definition (compactly supported diffeomorphisms)

Diff_c^2 : the set of C^2 -diffeomorphisms $f: \mathbb{R}^d \rightarrow \mathbb{R}^d$ such that $f(x) = x$ outside a compact subset ($U_f = \mathbb{R}^d$).



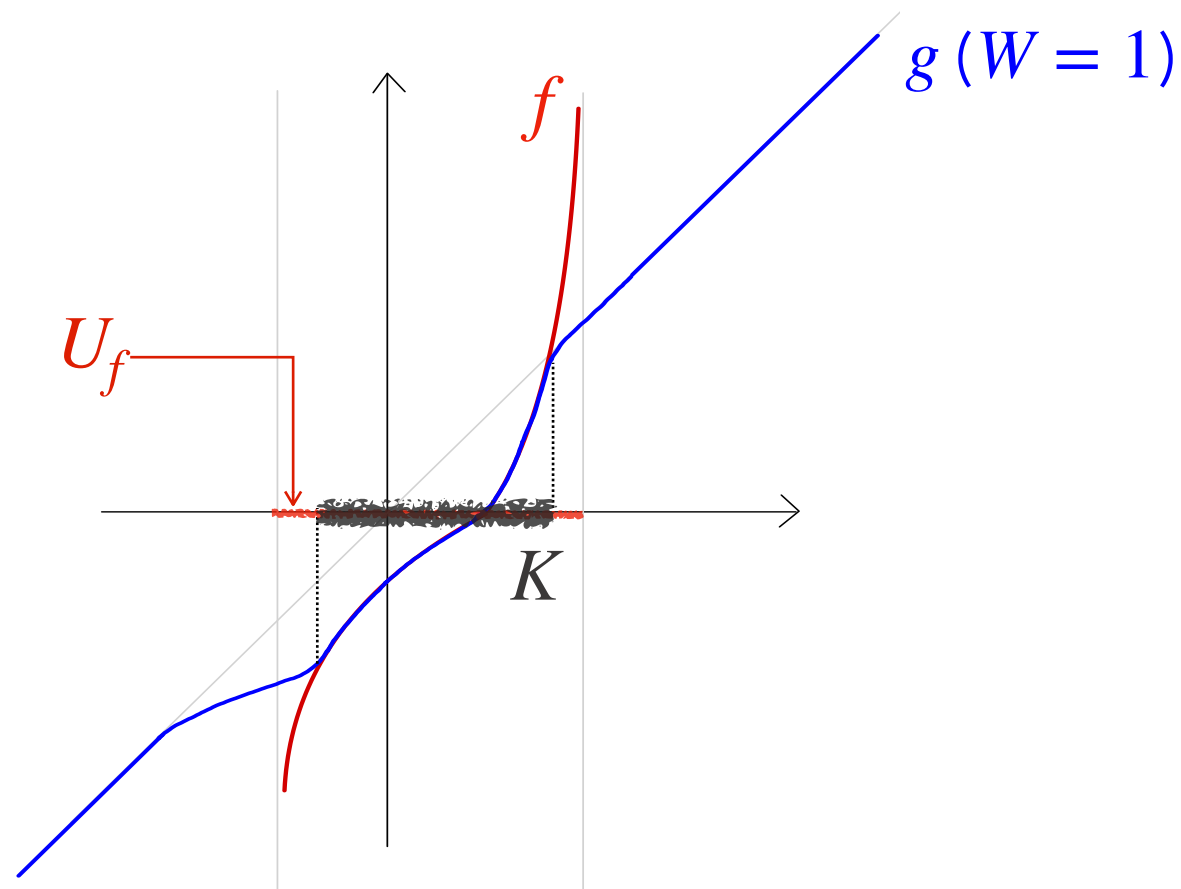
Theorem (Herman, Thurston, Epstein, and Mather)

Diff_c^2 is a **simple group** (does not have any proper normal subgroup except $\{\text{Id}\}$)

Proposition

For $f \in \mathcal{D}^2$ ($f: U_f \rightarrow \mathbb{R}^d$) and compact subset $K \subset U_f$, there exist an affine transform $W \in \text{Aff}$ and $g \in \text{Diff}_c^2$ such that

$$f|_K = W \circ g|_K.$$



Definition (flow endpoints Ξ)

$g \in \text{Diff}_c^2$: **flow endpoint** if there exists a **continuous** and **"additive"** map $\phi : [0,1] \rightarrow \text{Diff}_c^2$ such that $\phi(0) = \text{Id}$ and $\phi(1) = g$.

Proposition

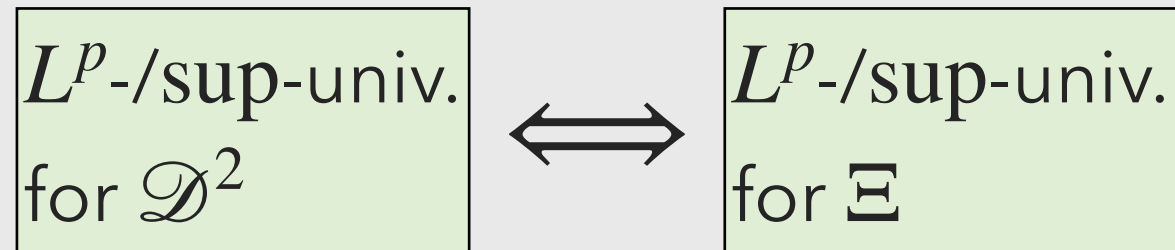
The set of finite compositions of flow endpoints (the group generated by Ξ) is a **nontrivial normal subgroup** of Diff_c^2 .

Corollary

For $g \in \text{Diff}_c^2$, there exist **finite** flow endpoints $g_1, \dots, g_m \in \Xi$ such that

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

In particular,



$f \in \mathcal{D}^2$: target, $K \subset U_f$: compact

$$f|_K \parallel \ll \text{Extend } f|_K$$

$\exists W \circ h$ (Aff & compactly supported C^2 -diffeomorphism)

$$\parallel \ll \text{structure theorem of diffeomorphism group}$$

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

\rightsquigarrow

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

Paper 2 Result (Analysis of NODEs)

NODEs yield sup-univ. INNs for Ξ
(and hence sup-univ. for \mathcal{D}^2 . Also Dist-univ.).

Proof outline of result 1

30

L^p -/sup-univ.
for \mathcal{D}^2



L^p -/sup-univ.
for \mathcal{S}_c^∞

$\mathcal{S}_c^\infty := \{ \tau : \text{compactly supported } \tau(\mathbf{x}, y) = (\mathbf{x}, u(\mathbf{x}, y)) \}$

$f|_K$

$f \in \mathcal{D}^2$: target, $K \subset U_f$: compact

$\parallel \ll \text{Extend } f|_K$

$\exists W \circ h$ (Aff & compactly supported C^2 -diffeomorphism)

$\parallel \ll \text{structure theorem of diffeomorphism group}$

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

\parallel

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

\parallel

$\tau_1 \circ \sigma_1 \circ \dots$ (**permutations & \mathcal{S}_c^∞**)

Decompose $f|_K$ into simpler mappings

Definition (nearly-Id elements)

$g \in \text{Diff}_c^2$: **nearly-Id element** if $\|dg(x) - I\| < 1$ for $x \in \mathbb{R}^d$

Proposition

For a flow endpoint $g \in \text{Diff}_c^2$, there exist nearly-Id elements $g_1, \dots, g_m \in \text{Diff}_c^2$ such that

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

Proposition

For a nearly-Id element $g \in \text{Diff}_c^2$, there exist $\tau_1, \dots, \tau_d \in \mathcal{S}_c^2$ and $\sigma_1, \dots, \sigma_d \in \mathfrak{S}_d$ such that

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

Lemma for this proposition

For $g = (g_i)_{i=1}^d \in \text{Diff}_c^2$, if for any $k = 1, \dots, d$, the submatrix of its jacobian

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

is invertible for all x , then there exist $\tau_1, \dots, \tau_d \in \mathcal{S}_c^2$ and $\sigma_1, \dots, \sigma_d \in \mathfrak{S}_d$ such that

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

Proof outline of result 1

33

L^p -/sup-univ.
for \mathcal{D}^2



L^p -/sup-univ.
for \mathcal{S}_c^∞

$\mathcal{S}_c^\infty := \{ \tau : \text{compactly supported } \tau(\mathbf{x}, y) = (\mathbf{x}, u(\mathbf{x}, y)) \}$

$f|_K$

$f \in \mathcal{D}^2$: target, $K \subset U_f$: compact

$\parallel \ll \text{Extend } f|_K$

$\exists W \circ h$ (Aff & compactly supported C^2 -diffeomorphism)

$\parallel \ll \text{structure theorem of diffeomorphism group}$

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

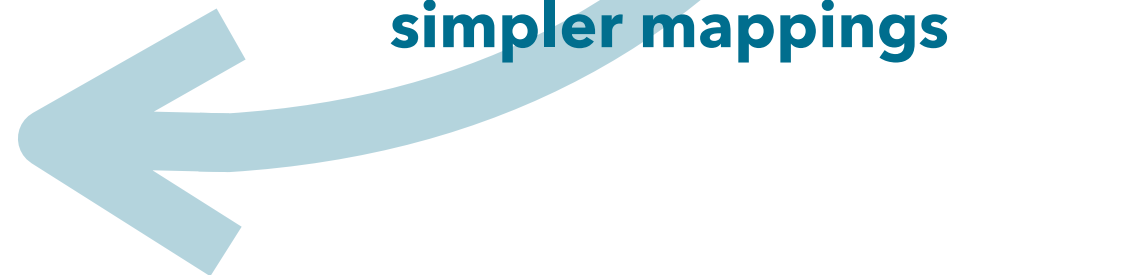
\parallel

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

\parallel

$\tau_1 \circ \sigma_1 \circ \dots$ (**permutations & \mathcal{S}_c^∞**)

Decompose $f|_K$ into simpler mappings



How the result can be used

34

You show

sup-univ. for \mathcal{S}_c^∞



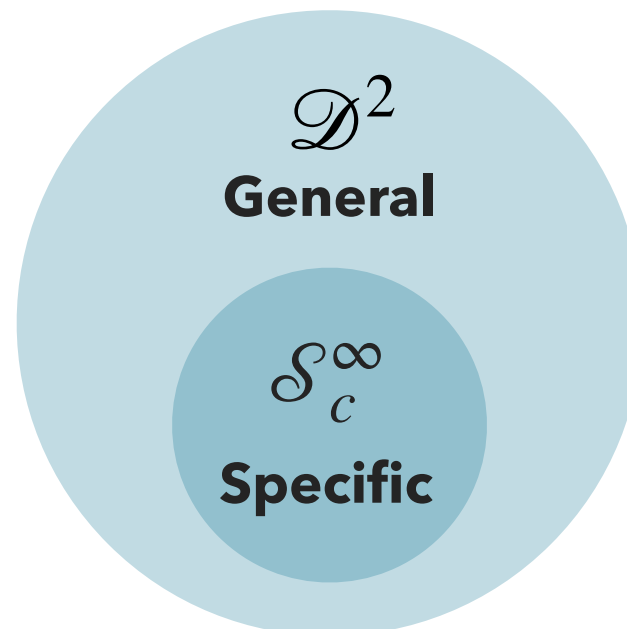
L^p -univ. for \mathcal{S}_c^∞

You get

sup-univ. for \mathcal{D}^2



L^p -univ. for \mathcal{D}^2



Upgrade Existing Guarantees

35

Regrading guarantees for existing INN architectures:

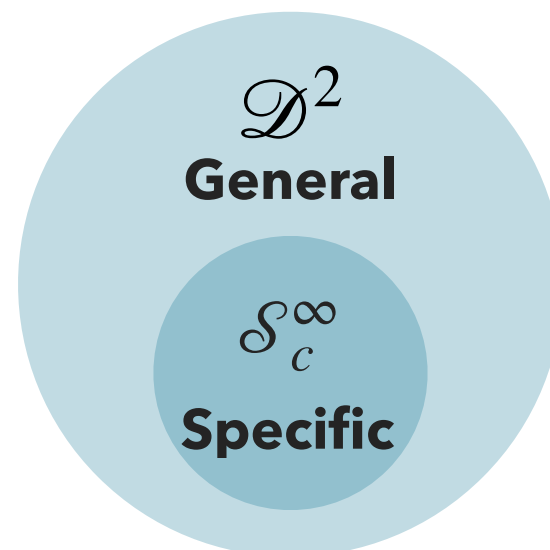
- **Sum-of-squares polynomial flow** (SoS-flow)
- **Deep sigmoidal flow** (DSF; aka. NAF)

Previously known/claimed [JSY19, HKLC18]:

sup-universality for \mathcal{S}_c^∞



sup-universality for \mathcal{D}^2



Definition (distributional universal approximator)

\mathcal{M} : set of measurable bijection from \mathbb{R}^d to \mathbb{R}^d (e.g. $\text{INN}_{\mathcal{G}}$)

\mathcal{P} : absolutely continuous probability measures

\mathcal{M} is a **distributional universal approximator** if

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

$$(g_n)_* \mu \xrightarrow[n \rightarrow \infty]{} \nu \quad (\textbf{weak convergence}).$$

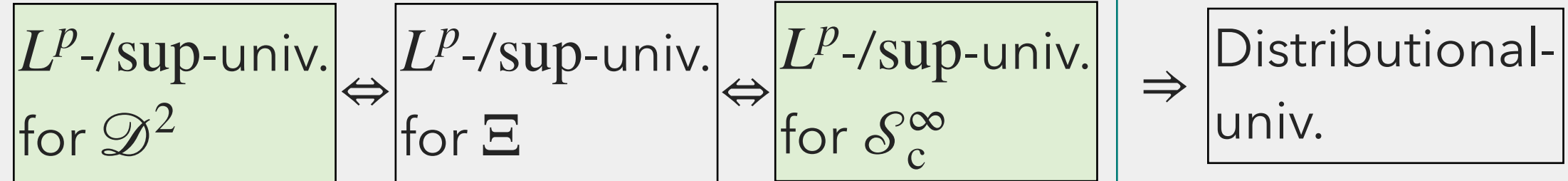
Proposition

A model \mathcal{M} is a L^p -universal approximator for a target \mathcal{D}^2



A model \mathcal{M} is a **distributional** universal approximator

In summary, we obtain



\mathcal{H} : functions on \mathbb{R}^{d-1}

$\text{INN}_{\mathcal{H}\text{-ACF}}$ is an INN with the flow layers composed of

$$\Psi_{d-1,s,t}(\mathbf{x}, y) := (\mathbf{x}, e^{s(\mathbf{x})}y + t(\mathbf{x}))$$

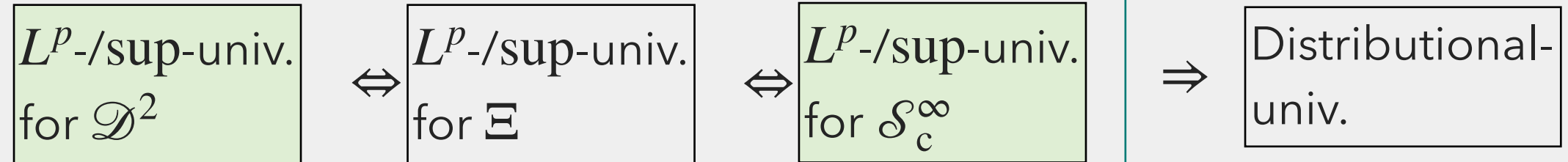
$$(\mathbf{x}, y) \in \mathbb{R}^{d-1} \times \mathbb{R}, s, t \in \mathcal{H}$$

One of the simplest CF-INN

Lemma

Assume \mathcal{H} arbitrarily approximates any element in $C_c^\infty(\mathbb{R}^{d-1})$, and is composed of piecewise C^1 -functions (e.g. MLPs with ReLU activation, RKHS with Gaussian kernel, e.t.c).

Then, $\text{INN}_{\mathcal{H}\text{-ACF}}$ is an L^p -universal approximator for \mathcal{S}_c^∞



Paper 1 Result (Affine Coupling Flows yield universal INNs)

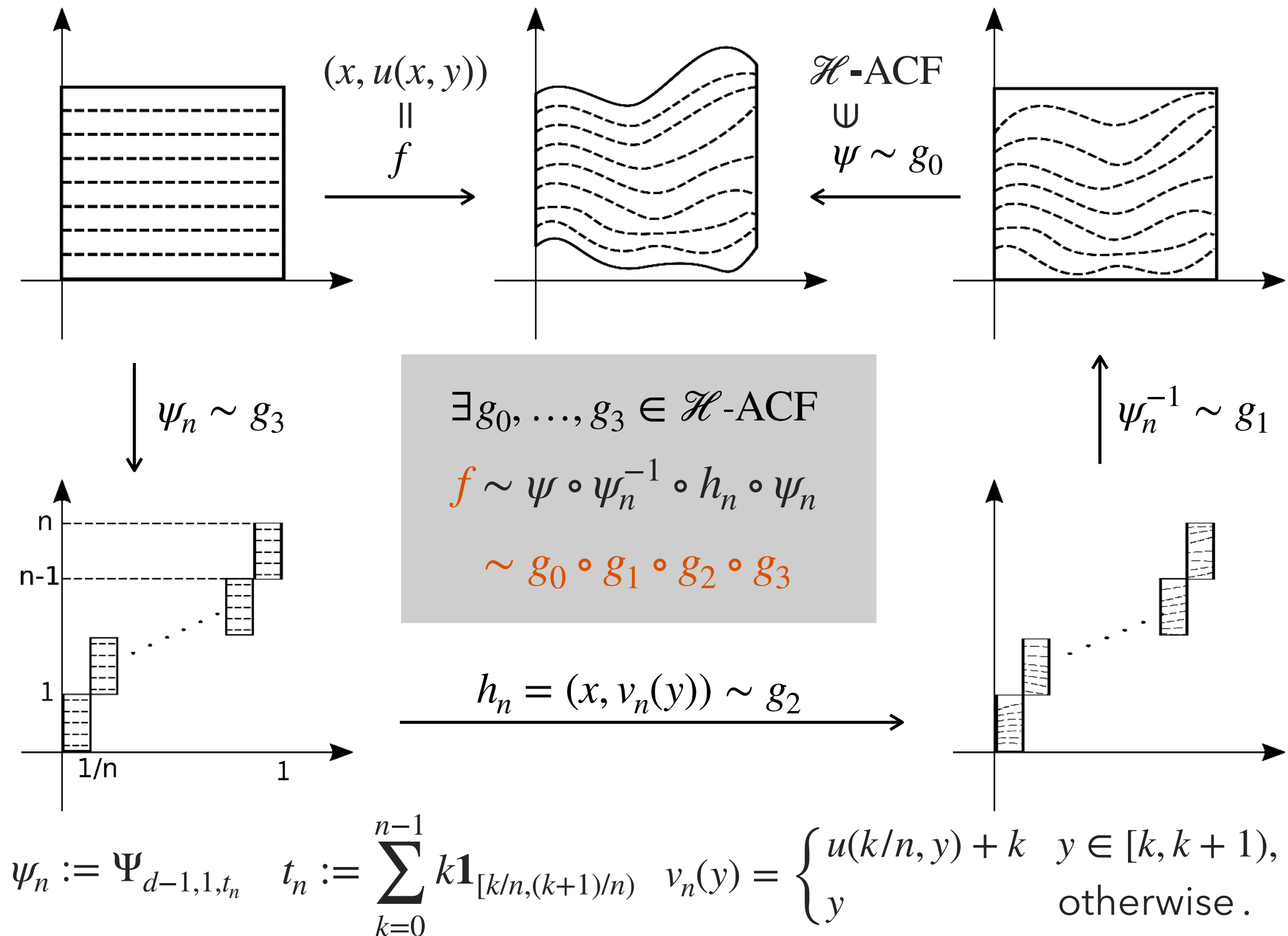
Affine Coupling Flows yield L^p -univ. INNs for \mathcal{S}_c^∞ (and hence for \mathcal{D}^2 , and also Dist-univ.).

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.

- We may assume $K = [0,1]^2$

For detail, look at our paper !



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 sup-universal approximator.

Future work

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

Our papers are available at

[1] <https://papers.nips.cc/paper/2020/hash/2290a7385ed77cc5592dc2153229f082-Abstract.html>

[2] <http://arxiv.org/abs/2012.02414>

Message

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

Appendix

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