

# On the Universality of Invertible Neural Networks

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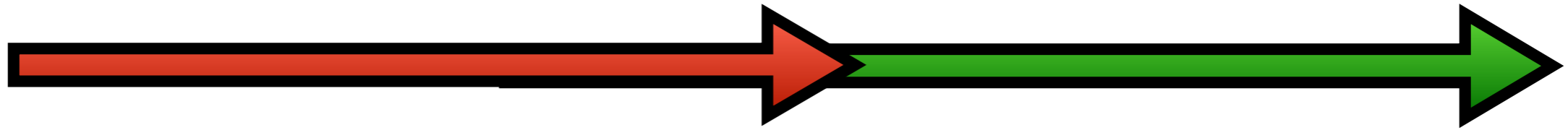


**Joint work with Koichi Tojo, Kenta Oono, Masahiro Ikeda, and Masashi Sugiyama.**

# Today's talk structure

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## 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:  
RIKEN JRA Program  
and Masason Foundation.



### Recent Research Interests:

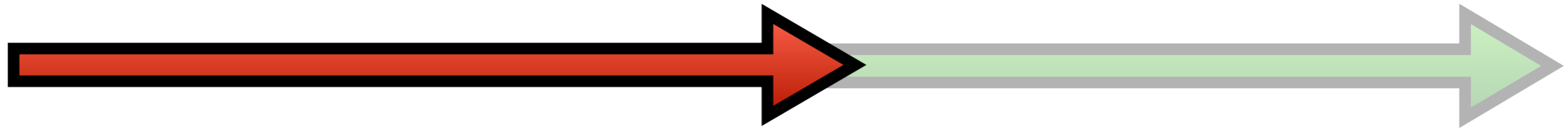
General methodology of machine learning.  
In particular: "Causality for machine learning"

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

# Today's talk structure

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## Part 1

Introduction.

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

## Part 2

Details of the theory.

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  $f$ )

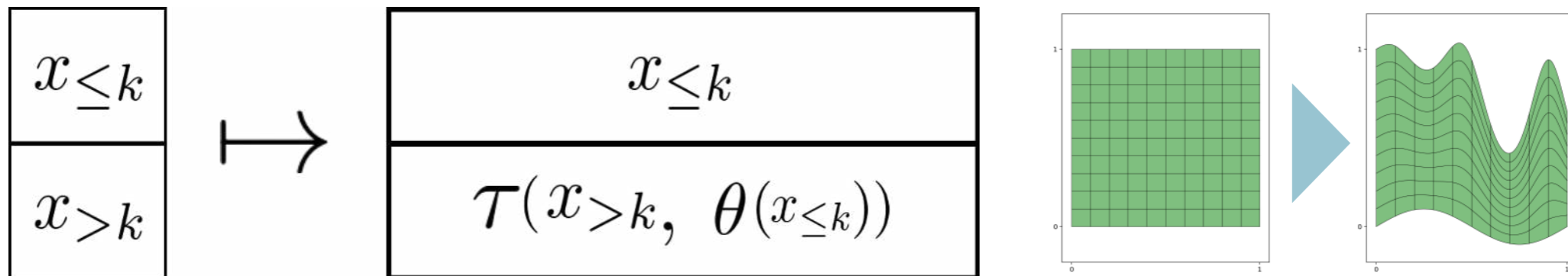
## Example (Designs of flow layers $\mathcal{G}$ )

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

# Example 1: Coupling Flows

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

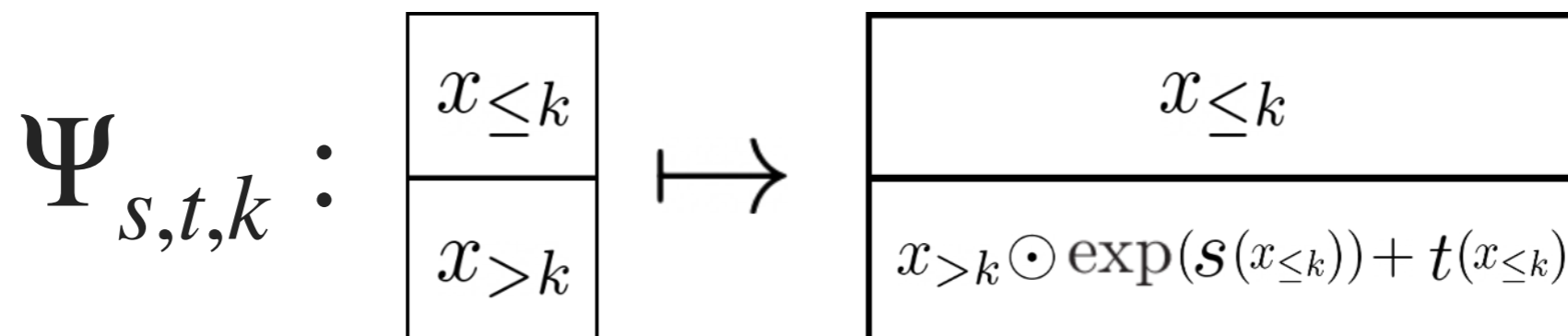


**Idea:** Keep some dimensions unchanged. (Strong constraint!)

**CF-INN** = Coupling-flow based INN.

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

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



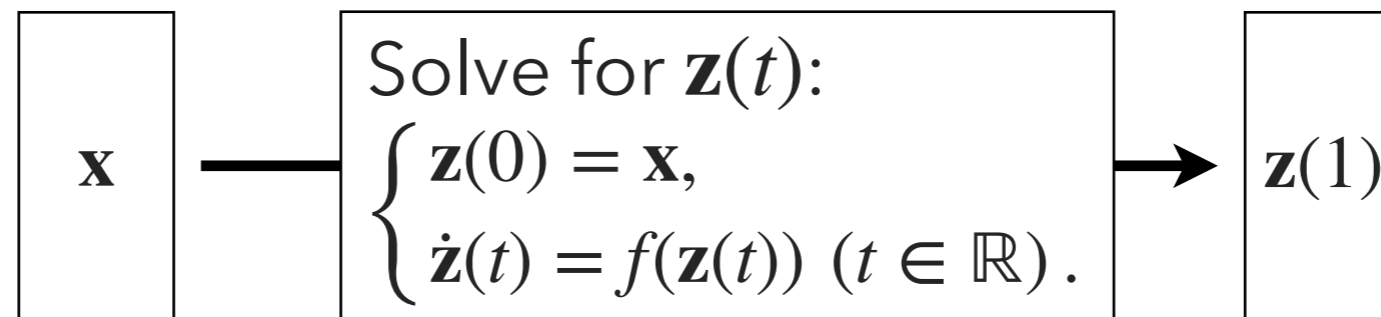
# Example 2: Neural Ordinary Differential Equations

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## 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:

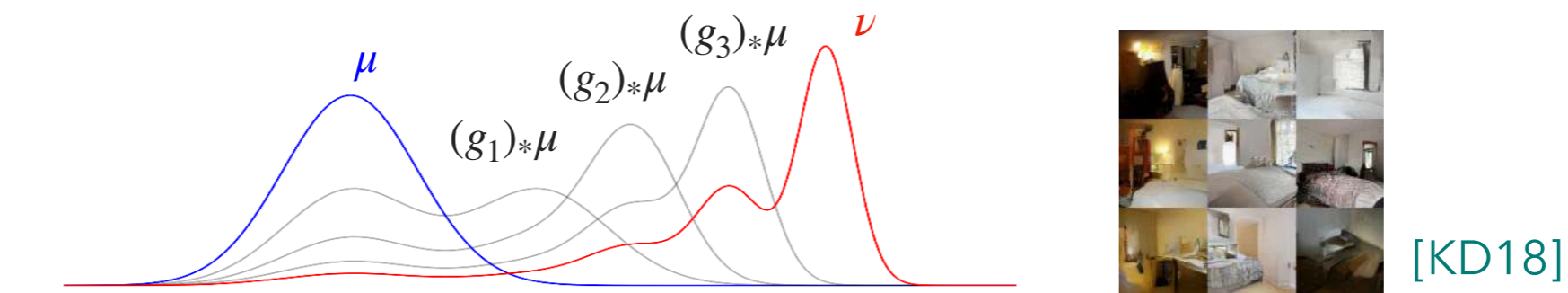
$$\text{NODEs}(\mathcal{H}) := \{\mathbf{x} \mapsto \mathbf{z}(1) \mid f \in \mathcal{H}\}$$

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

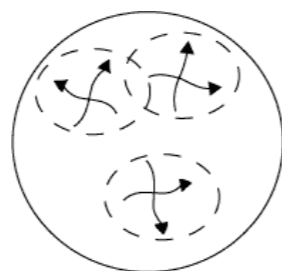
- ✓ **Explicit and efficient invertibility.**
- ✓ **Tractability** of Jacobian determinant (for nicely designed  $\mathcal{G}$ ).

## Usages of INNs

- Approximate distributions (normalizing flows).



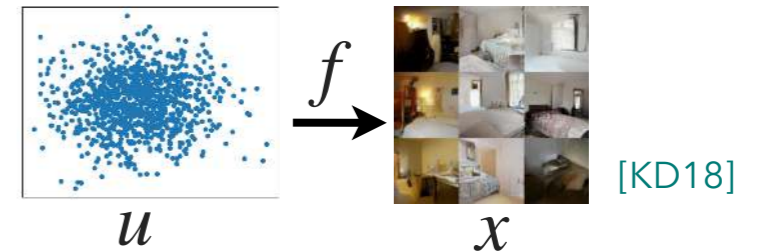
- Approximate invertible maps (feature extraction & manipulation).





# 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:

↓ easily invertible

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

↑ known

↑ 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  $f^{-1}$ .

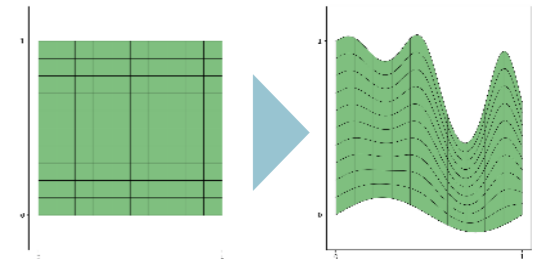
## Examples

- 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

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## 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"?

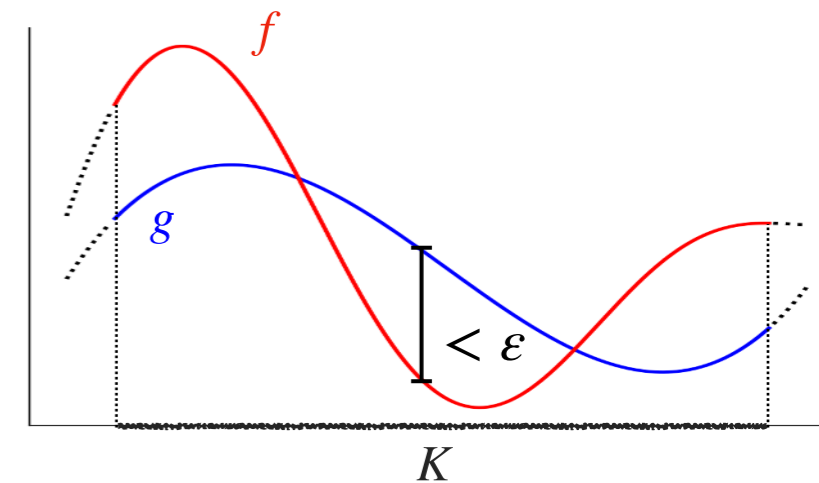
Here,

**"Representation power" = Universal approximation property.**

**Definition** (informal) [C89,HSW89]

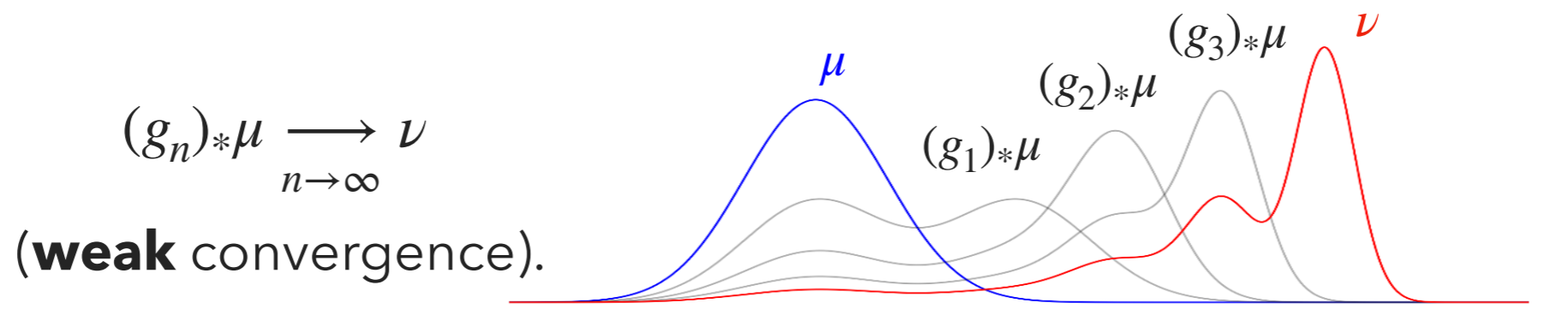
sup- ( $L^p$ -) **universal approximator**:

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.

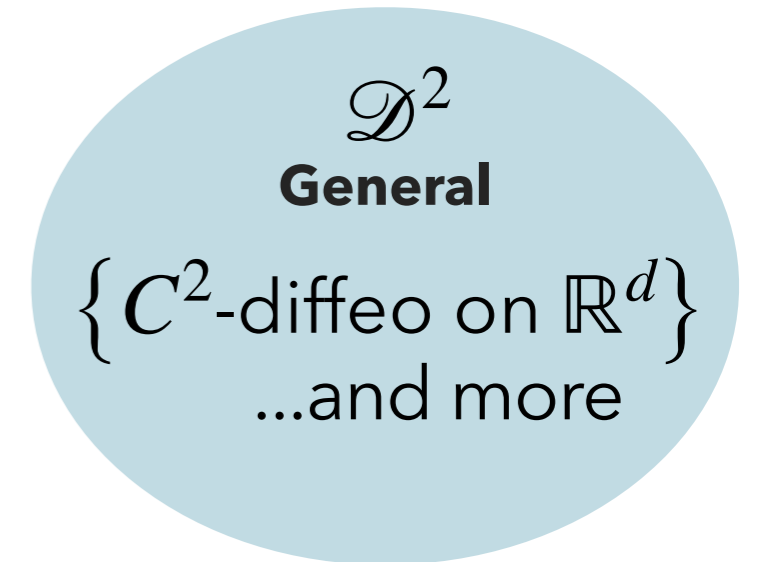


## Definition (Approximation target $\mathcal{D}^2$ )

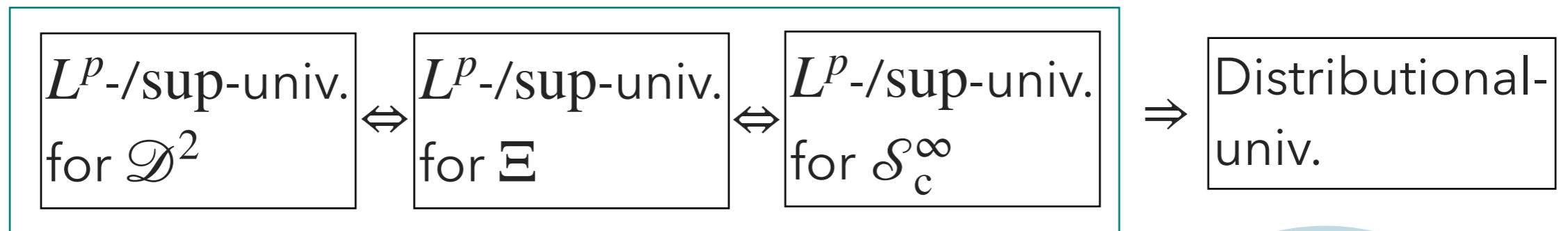
Fairly **large set** of smooth invertible maps.

$$\mathcal{D}^2 := \left\{ C^2\text{-diffeo of the form } f : U_f \rightarrow f(U_f) \right\}$$

$$(U_f \subset \mathbb{R}^d : \text{open } C^2\text{-diffeo to } \mathbb{R}^d)$$

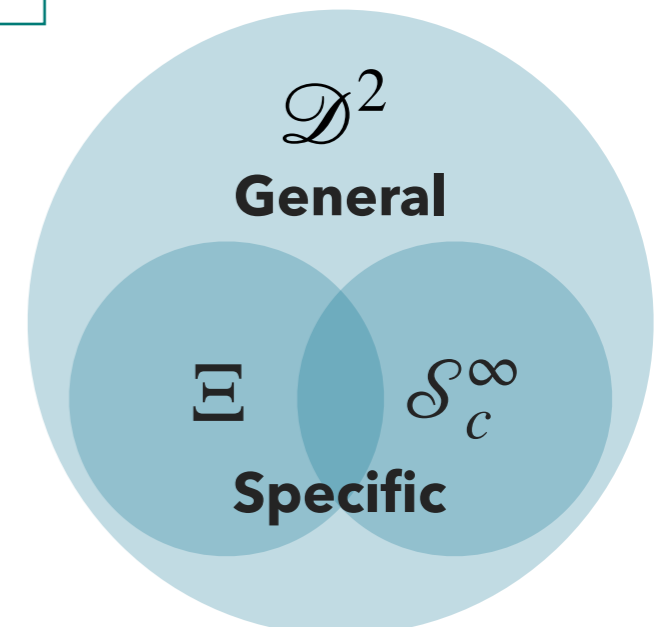


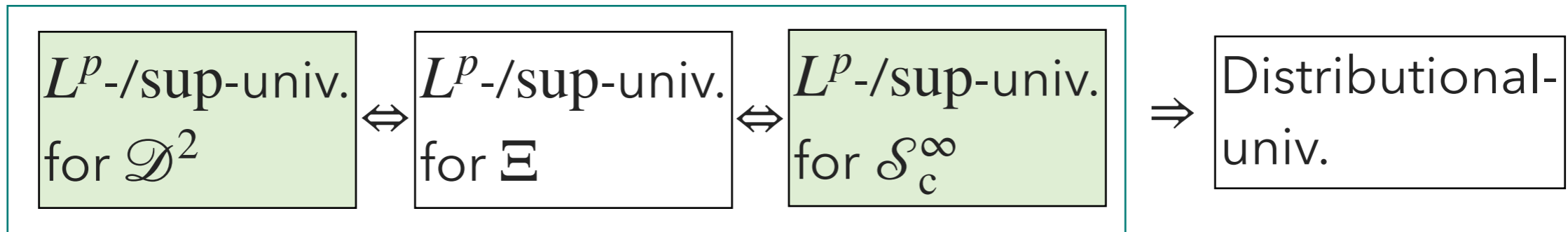
## Paper 1 Result (Theoretical Framework) (under mild regularity conditions)



$\Xi$  : "flow endpoints"

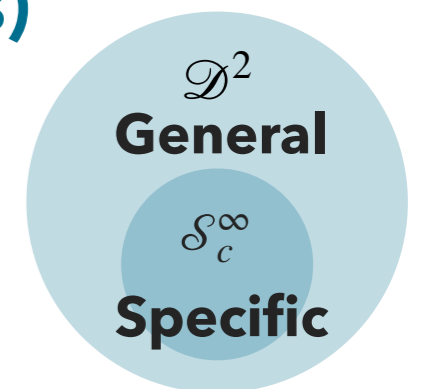
**Application of a structure theorem  
in differential geometry**





## Paper 1 Result (Examples of Universal Coupling Flows)

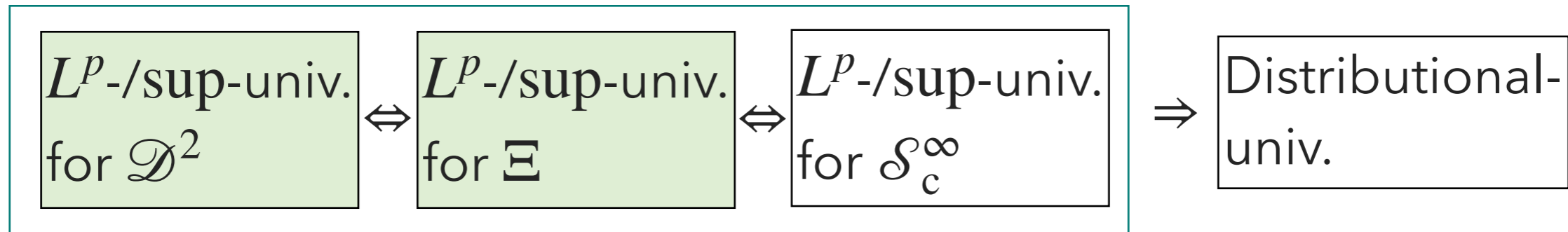
- **Sum-of-squares polynomial flow** (SoS-flow) [JSY19]
- **Deep sigmoidal flow** (DSF; aka. NAF) [HKLC18]



yield **sup-univ. INNs for  $\mathcal{S}_c^\infty$  (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  $\mathcal{S}_c^\infty$   
(and hence for  $\mathcal{D}^2$ , and also Dist-univ.).



## Paper 2 Result (Analysis of NODEs)

NODEs yield sup-univ. INNs for  $\Xi$   
(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.**

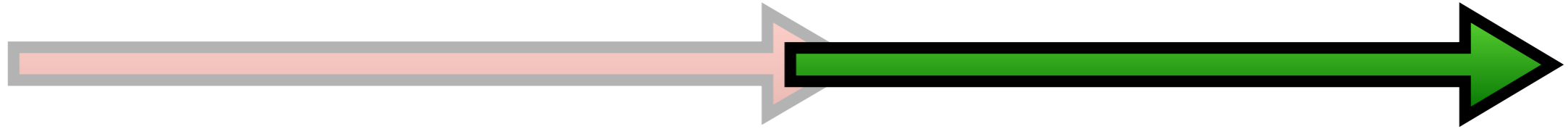
## Message

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

# Today's talk structure

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## Part 1

Introduction.

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

## Part 2

Details of the theory.

Theoretical preliminaries  
and proof machinery.

## Isao Ishikawa

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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** !

# $L^p$ -Universal approximators

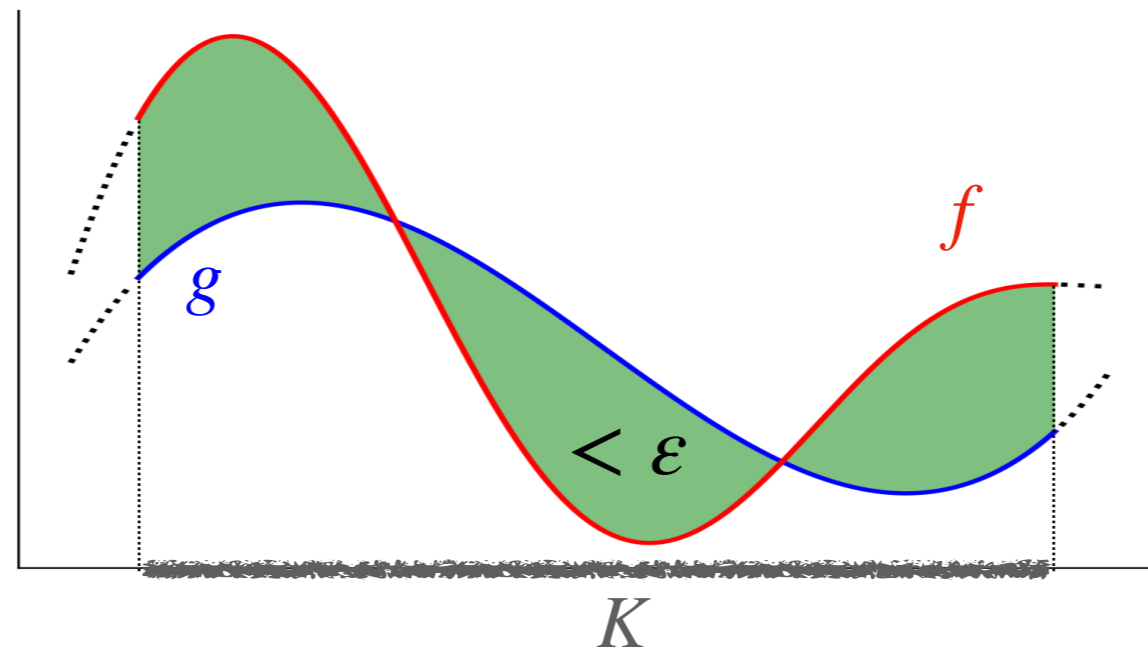
$\mathcal{M}$ : model, set of measurable bijection from  $\mathbb{R}^d$  to  $\mathbb{R}^d$  (e.g. INNs)

$\mathcal{F}$ : 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

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

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



# sup-Universal approximators

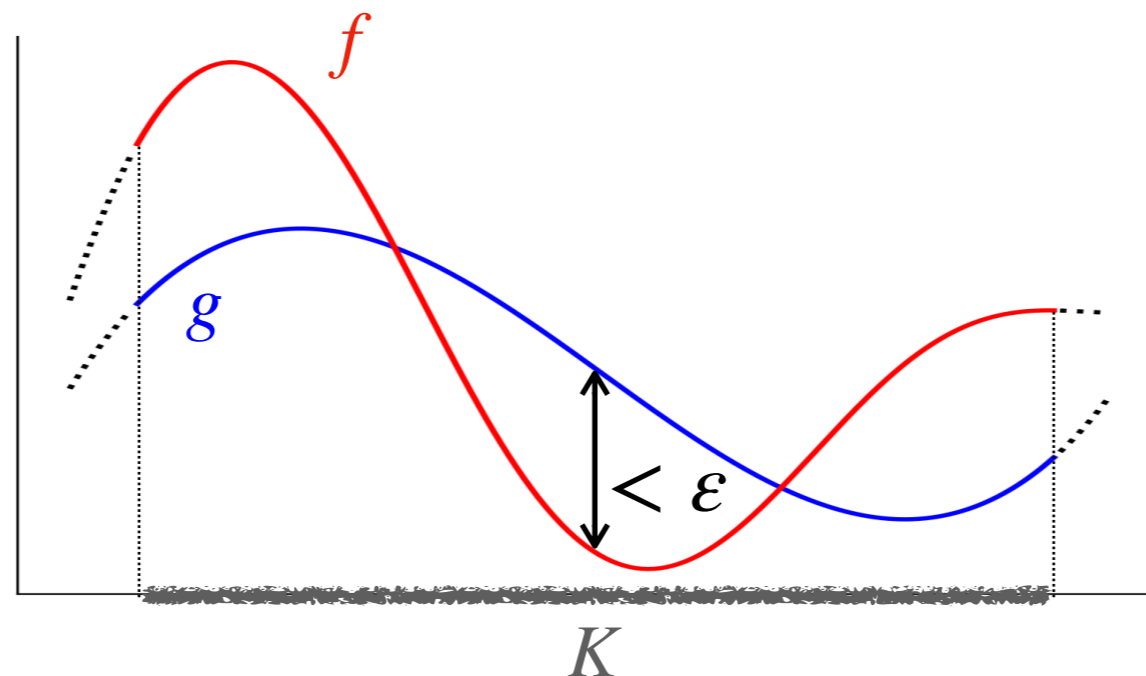
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$\mathcal{M}$  is an **sup-universal approximator** for  $\mathcal{F}$  if

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

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



## 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

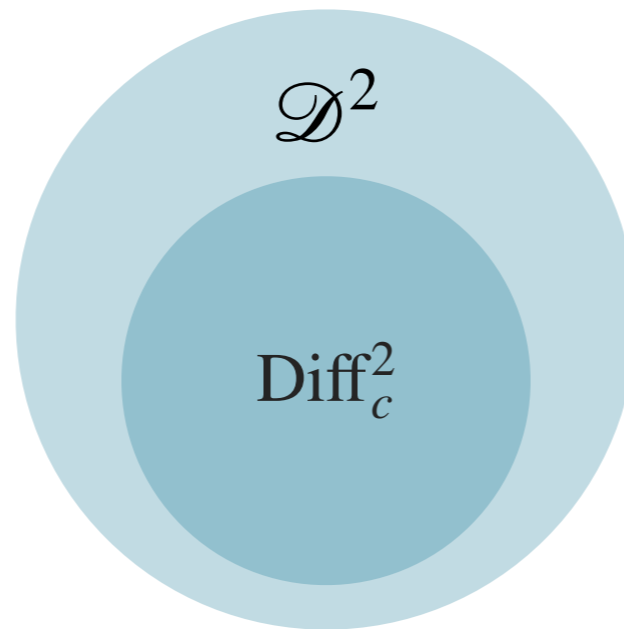
$$G_r \circ \dots \circ G_1 \approx F_r \circ \dots \circ F_1 \text{ (} L^p\text{-approximation on } K\text{)}$$

## 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)

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



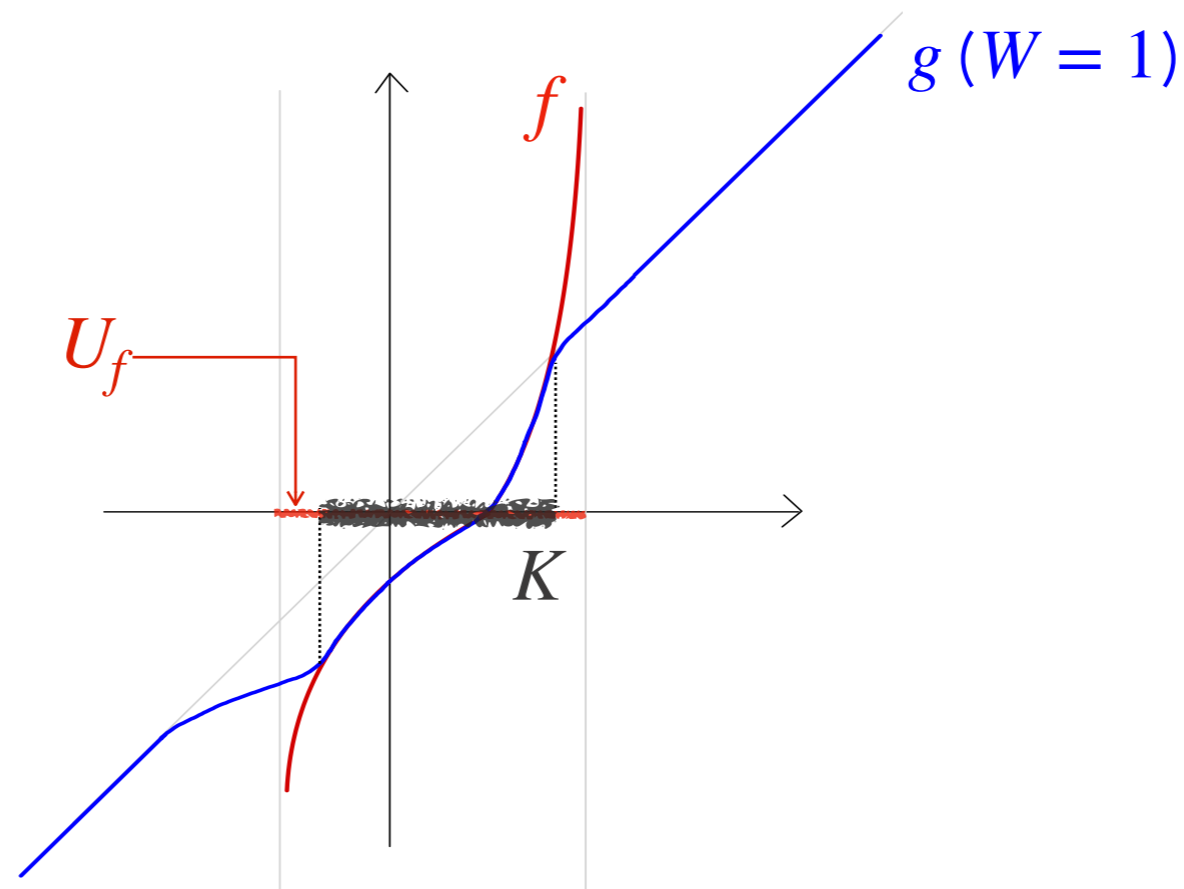
**Theorem** (Herman, Thurston, Epstein, and Mather)

$\text{Diff}_c^2$  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

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



# Flow endpoints

**Definition** (flow endpoints  $\Xi$ )

w.r.t. Whitney topology.  
↓

$g \in \text{Diff}_c^2$ : **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  $\phi(1) = g$

$\Xi := \{\text{flow endpoints}\}$

$$\forall s, t, s+t \in [0,1], \quad \phi(s+t) = \phi(s) \circ \phi(t)$$

**Proposition**

The set of finite compositions of flow endpoints (the group generated by  $\Xi$ ) is a **nontrivial normal subgroup** of  $\text{Diff}_c^2$ .

**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,

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



$L^p$ -/sup-univ.  
for  $\Xi$

$f \in \mathcal{D}^2$ : 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  $\Xi$

(and hence sup-univ. for  $\mathcal{D}^2$ . Also Dist-univ.).

# Proof outline of result in Paper 1

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



$L^p$ -/sup-univ.  
for  $\mathcal{S}_c^\infty$

$\mathcal{S}_c^\infty := \{ \tau : \text{compactly supported } \tau(\mathbf{x}, y) = (\mathbf{x}, u(\mathbf{x}, y)) \} \subset \text{Diff}_c^2$   
 $u : \mathbb{R}^{d-1} \rightarrow \mathbb{R}, (\mathbf{x}, y) \in \mathbb{R}^{d-1} \times \mathbb{R}$

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

$\parallel \ll$  Extend  $f|_K$

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

$\parallel \ll$  **structure theorem of diffeomorphism group**

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

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

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

**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

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

$\because g = \phi(1)$  ( $\phi : [0,1] \rightarrow \text{Diff}_c^2$ : "additive" and continuous)

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

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

## 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

$$\left( \frac{\partial g_{i+k-1}}{\partial x_{j+k-1}}(x) \right)_{i,j=1,\dots,d-k-1} dg = \begin{pmatrix} \dots & \text{invertible} \\ \dots & \dots \end{pmatrix}$$

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 in Paper 1

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



$L^p$ -/sup-univ.  
for  $\mathcal{S}_c^\infty$

$\mathcal{S}_c^\infty := \{ \tau : \text{compactly supported } \tau(\mathbf{x}, y) = (\mathbf{x}, u(\mathbf{x}, y)) \} \subset \text{Diff}_c^2$   
 $u : \mathbb{R}^{d-1} \rightarrow \mathbb{R}, (\mathbf{x}, y) \in \mathbb{R}^{d-1} \times \mathbb{R}$

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

$\parallel \ll$  Extend  $f|_K$

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

$\parallel \ll$  **structure theorem of diffeomorphism group**

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

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

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

**Decompose  $f|_K$  into simpler mappings**



# How the result can be used

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**You show**

sup-univ. for  $\mathcal{S}_c^\infty$



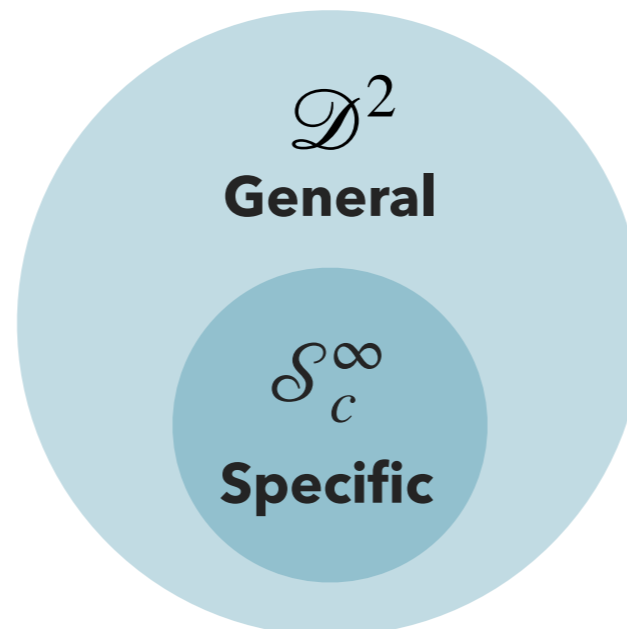
$L^p$ -univ. for  $\mathcal{S}_c^\infty$

**You get**

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



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



# Upgrade Existing Guarantees

Regrading guarantees for existing INN architectures:

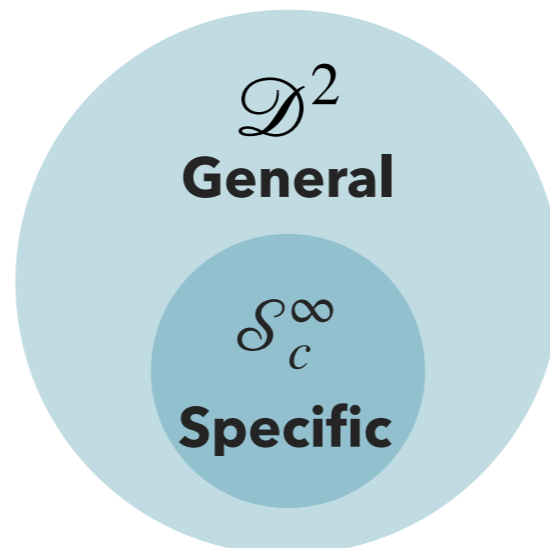
- **Sum-of-squares polynomial flow** (SoS-flow)
- **Deep sigmoidal flow** (DSF; aka. NAF)

Previously known/claimed [JSY19, HKLC18]:

sup-universality for  $\mathcal{S}_c^\infty$



sup-universality for  $\mathcal{D}^2$



**Definition** (distributional universal approximator)

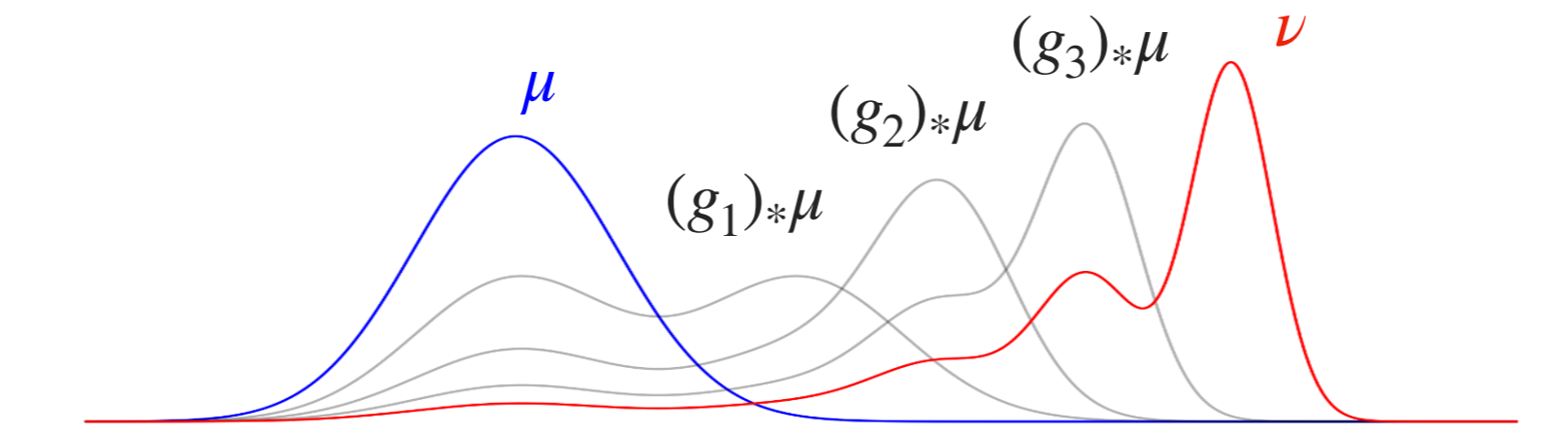
$\mathcal{M}$ : model, set of measurable bijection from  $\mathbb{R}^d$  to  $\mathbb{R}^d$  (e.g. INNs)

$\mathcal{P}$ : absolutely continuous probability measures

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

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

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



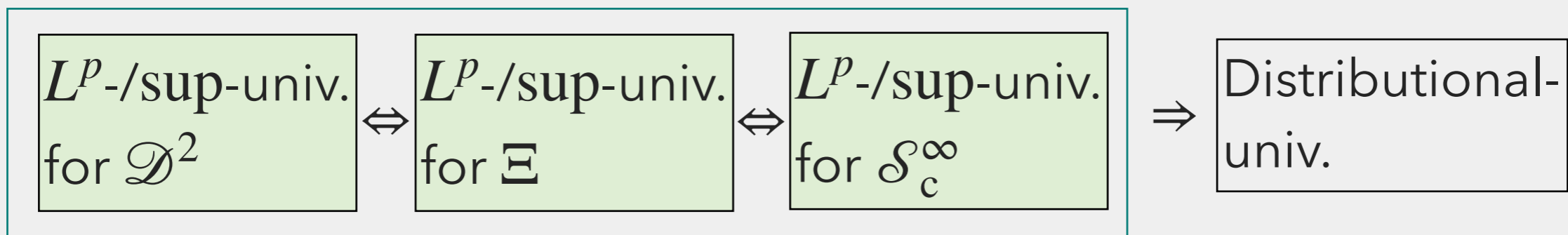
## Proposition

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  $\mathbb{R}^{d-1}$  (e.g., MLPs)

$\text{INN}_{\mathcal{H}\text{-ACF}}$  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

## Theorem

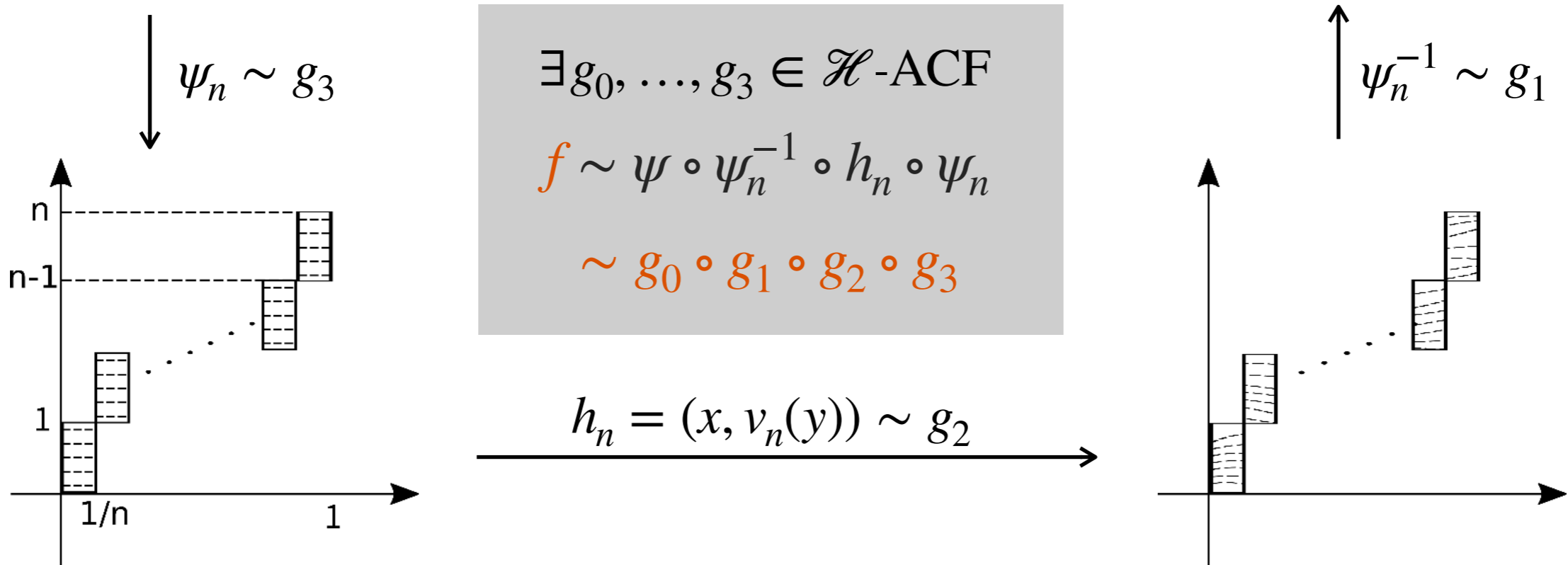
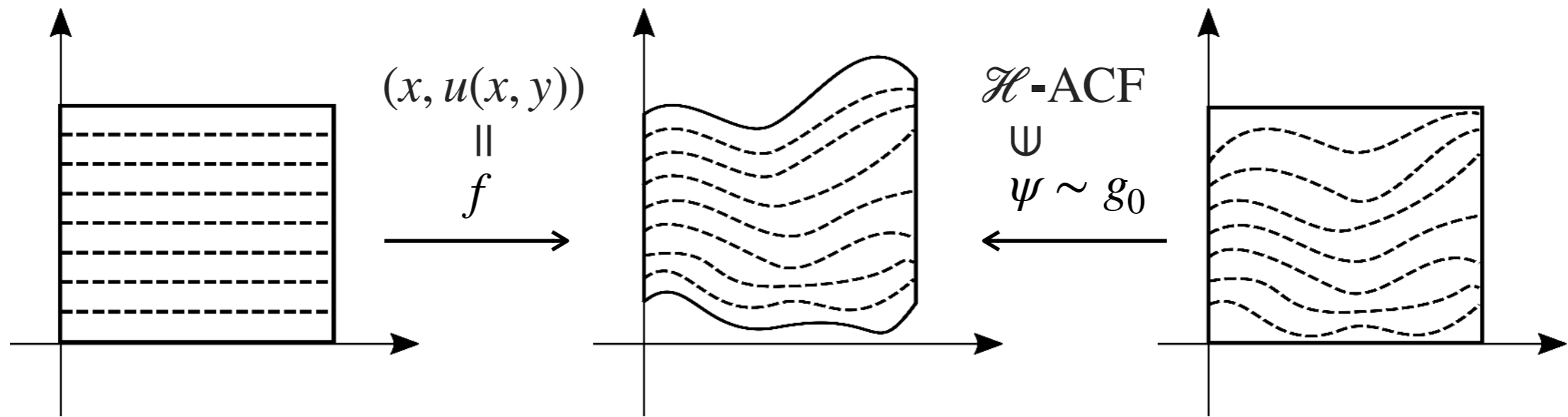
Assume  $\mathcal{H}$  arbitrarily approximates any element in  $C_c^\infty(\mathbb{R}^{d-1})$ , and is composed of piecewise  $C^1$ -functions (e.g. MLPs with ReLU activation, RKHS with Gaussian kernel, e.t.c).

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

# Universality of CF-INNs

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

For detail, look at our paper !



$$\exists g_0, \dots, g_3 \in \mathcal{H}\text{-ACF}$$

$$f \sim \psi \circ \psi_n^{-1} \circ h_n \circ \psi_n$$

$$\sim g_0 \circ g_1 \circ g_2 \circ g_3$$

$$\psi_n := \Psi_{d-1,1,t_n} \quad t_n := \sum_{k=0}^{n-1} k \mathbf{1}_{[k/n, (k+1)/n)} \quad v_n(y) = \begin{cases} u(k/n, y) + k & y \in [k, k+1), \\ y & \text{otherwise.} \end{cases}$$

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

$\Leftrightarrow$

$L^p$ -/sup-univ.  
for  $\Xi$

$\Leftrightarrow$

$L^p$ -/sup-univ.  
for  $\mathcal{S}_c^\infty$

$\Rightarrow$

Distributional-  
univ.

## Paper 1 Result (Affine Coupling Flows yield universal INNs)

Affine Coupling Flows yield  $L^p$ -univ. INNs for  $\mathcal{S}_c^\infty$   
(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.



## 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.

## Message

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

## 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>

# Appendix

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