Usages of invertible neural networks

High-level summary

Research question

“How expressive are NODEs?”

NODE = Neural Ordinary Differential Equations [C89, KD18]

Why important?

• Strong (sup-norm) guarantee for a large class of invertible maps.
• cf. Previous result: Universality for $C^k(R^n, R^m)$ w.r.t. $L^p$-norm. [1122]

What is the result? ≡

Universality of NODE + Affine transform for a large class of diffeomorphisms w.r.t. sup-norm.

Usages of invertible neural networks

• Modelling distributions (a.k.a. normalizing flows).
• Modelling invertible maps (feature extraction & manipulation).

Message

NODE-based invertible neural networks have high representation power for approximating diffeomorphisms. They can be relied on in modeling invertible maps and distributions.

Preliminary: NODEs

NODE layer

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

For each $f \in \text{Lip}(R^d)$, we define an invertible map $x \mapsto z(1)$ via an initial value problem: [C89, KD18]

Definition (NODE layers)

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

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

Definition (Invertible neural networks based on $\mathcal{H}$-NODE)

$\text{INN}_{\mathcal{H}-\text{NODE}} := \{ W \circ \phi_1 \circ \cdots \circ \phi_1 \mid \phi_1, \ldots, \phi_1 \in \text{NODE}(\mathcal{H}), W \in \text{Aff}, k \in N \}$

Research question

Restricted functions $\rightarrow$ restricted representation power?

Preliminary: Universality

Definition (informal; Sec. 2.2) [C89]

sup-universal approximator: the model can approximate any target function w.r.t. sup-norm on a compact set.

Approximation target

Definition (approximation target $\mathcal{H}^2$; Sec. 3.1.)

$\mathcal{H}^2 \triangleq \{ f : \mathcal{U} \rightarrow f(\mathcal{U}) \mid f : C^2\text{-diffeo}, \mathcal{U} \subset R^d, \text{open} \supseteq R^d \}$

$\mathcal{H}^2$ is fairly large

Result: Universality of NODEs

Theorem (Sec. 3.2, Theorems 2, 3)

Assume $\mathcal{H}$ is a sup-universal approximator for $\text{Lip}(R^d)$.

$\text{INN}_{\mathcal{H}-\text{NODE}} \equiv$ a sup-universal approximator for $\mathcal{H}^2$.

Implication

High representation power of NODEs.

References

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