Structure Preserving Deep Learning

Matthias J. Ehrhardt

Institute for Mathematical Innovation, University of Bath, UK

January 27, 2021

Joint work with:
M. Benning (Queen Mary, UK), C. Etmann, C.-B. Schönlieb, F. Sherry (all Cambridge, UK), E. Celledoni, B. Owren (both NTNU, Norway), R. McLachlan (Massey, New Zealand)

Outline

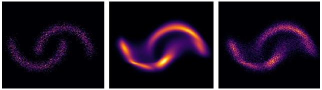
Towards deep learning with **guarantees**: stability, invertibility, equivariance, invariance, existence of solutions

Outline

Towards deep learning with **guarantees**: stability, invertibility, equivariance, invariance, existence of solutions

1) Deep learning and differential equations: Optimal control, stability and deep limits

2) Structure preserving deep neural networks: Equivariance and Invertibility



[1] Celledoni, MJE, Etmann, McLachlan, Owren, Schönlieb, Sherry, "Structure preserving deep learning," arxiv:2006.03364, 2020.

[2] Benning, Celledoni, MJE, Owren, and Schönlieb, "Deep learning as optimal control problems: models and numerical methods," J. Comput. Dyn. 6(2) 2019.

[3] Haber and Ruthotto, "Stable architectures for deep neural networks," Inverse Probl. 34(1) 2018.

Classification with Deep Learning

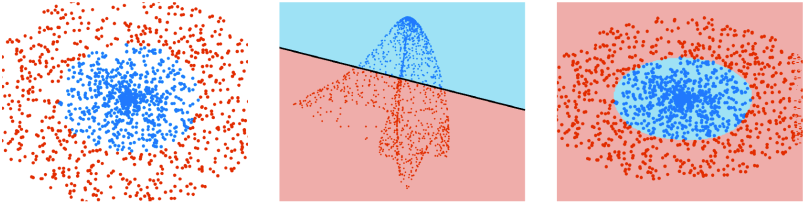
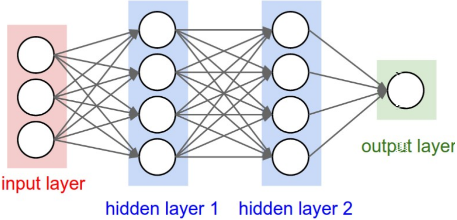


Figure courtesy of L. Ruthotto.

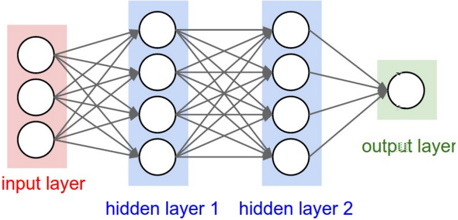
- *labeled training data* $(x_k, y_k)_{k=1,\ldots,K}$
- transform data with *hidden layers*
- perform *linear classification*
- *generalization* to unseen data

Deep Learning / Deep Neural Networks (DNN)



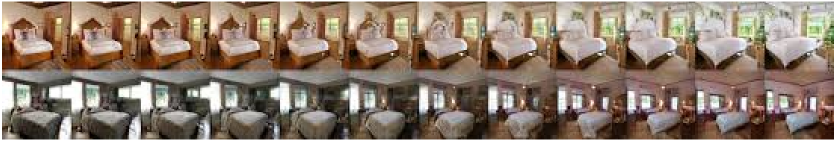
- *input layer*: given data, features, e.g. image of dog
- *hidden layers*: transform data
- *output layer* classification result, e.g. label "dog"
- invented in the 50's
- recent success by massive data and computing power
- applications: image classification, face recognition, self-driving cars, ...

Deep Learning / Deep Neural Networks (DNN)

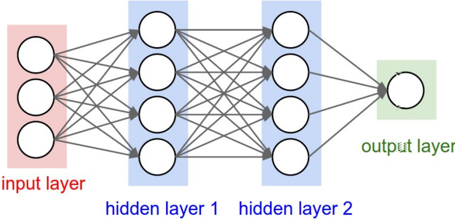


- *input layer*: given data, features, e.g. image of dog
- *hidden layers*: transform data
- *output layer* classification result, e.g. label "dog"

- invented in the 50's
- recent success by massive data and computing power
- applications: image classification, face recognition, self-driving cars, ...

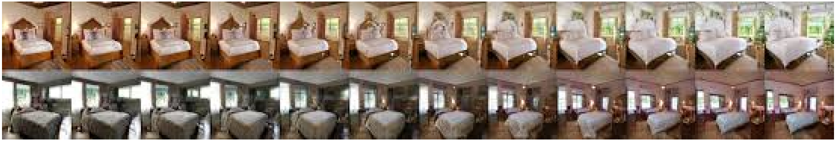


Deep Learning / Deep Neural Networks (DNN)

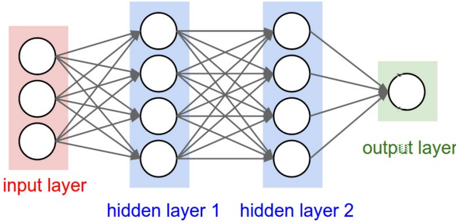


- *input layer*: given data, features, e.g. image of dog
- *hidden layers*: transform data
- *output layer* classification result, e.g. label "dog"

- invented in the 50's
- recent success by massive data and computing power
- applications: image classification, face recognition, self-driving cars, ...



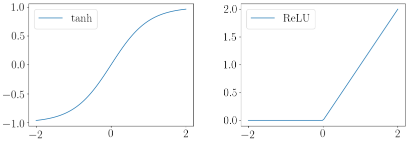
Mathematical Formulation of Deep Learning



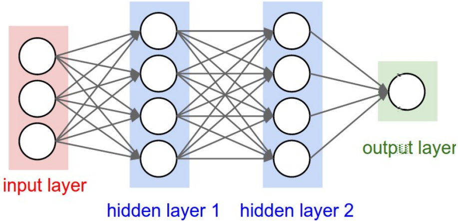
- *input layer*: $x^0 \in \mathbb{R}^n$
- *hidden layers* $\{x^k\}_{k=1,\dots,K}$, K *depth*/number of layers of DNN, *forward propagation*

$$x^{k+1} = \sigma(A^k x^k + b^k)$$

activation function: $\sigma : \mathbb{R} \to \mathbb{R}$ applied component-wise, e.g. $\sigma(x) = \tanh(x)$, ReLU: $\sigma(x) = \max(x, 0)$



Mathematical Formulation of Deep Learning

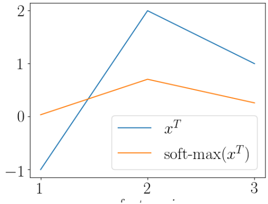


- *output layer* $y \in \mathbb{S}^{m-1}$, classification result, e.g. $m = 2$, $y = [1, 0]$ may correspond to "dog"

$$y = \tau(Wx^K + \omega)$$

$\tau : \mathbb{R}^m \to \mathbb{R}^m$, e.g. soft-max:

$$\tau(x)_i = \frac{\exp(x_i)}{\sum_j \exp(x_j)}$$



Supervised Learning with Deep Neural Networks

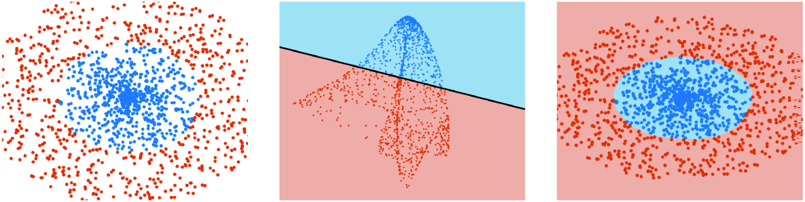


Figure courtesy of L. Ruthotto.

The Learning Problem

Given *training data* $(x_n, y_n)_{n=1,\dots,N}$ find $A = \{A^k\}_{k=1,\dots,K}$, $b = \{b^k\}_{k=1,\dots,K}$, W, ω that solve

$$\min_{A,b,W,\omega} \sum_{n=1}^{N} \|\tau(W x_n^K + \omega) - y_n\|^2 + R(A, b, W, \omega)$$

$$\text{s.t.} \quad x_n^{k+1} = \sigma(A^k x_n^k + b^k), \quad x_n^0 = x_n$$

- Quality of learning measured by *generalization*

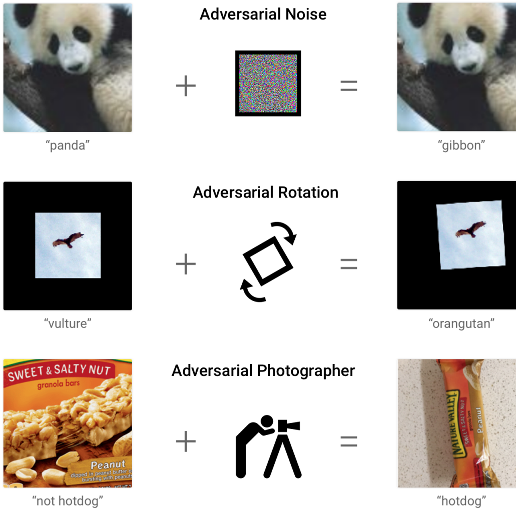
Word of warning

Deep learning is great, but ...

- need a lot of data
- difficult to train
- can be fooled
- ...

Deep learning needs ...

- mathematical guarantees
- explainable models
- ...



https://ai.googleblog.com/2018/09/introducing-unrestricted-adversarial.html

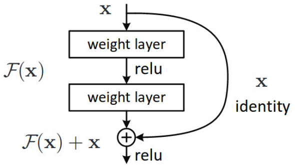
Deep Learning meets Optimal Control

Deep Residual Neural Networks (ResNet)

- "Standard" Neural Networks

$$x^{k+1} = \sigma(A^k x^k + b^k)$$

- Deep Residual Neural Networks (ResNet) He, Zhang, Ren, Sun 2015 ($>$ 68000 citations on GoogleScholar)



$$x^{k+1} = x^k + \Delta t\, \sigma(A^k x^k + b^k)$$

Linking ResNet with ODEs

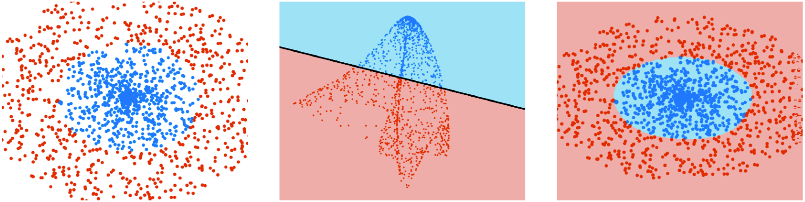
ResNet is Forward Euler discretization $\dot{x}(t) \approx \frac{x(t+\Delta t) - x(t)}{\Delta t}$ of

$$\dot{x}(t) = \sigma(A(t)x(t) + b(t)), \quad t \in [0, T]$$

with continuous-time mappings A, b. $x^k := x(k\Delta t)$ ...

Haber and Ruthotto 2018, Li et al. 2018, Benning et al. 2019, ...

Optimal Control meets for Deep Learning



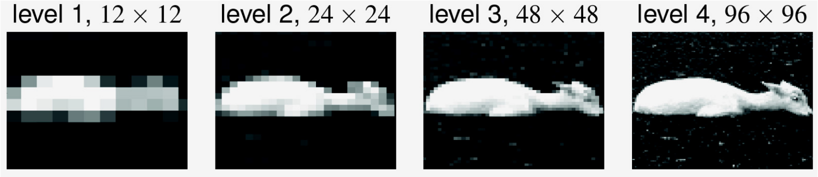
The Optimal Control Learning Problem

Given *training data* $(x_n, y_n)_{n=1,\dots,N}$ find $A : [0, T] \to \mathbb{R}^{M\times M}$, $b : [0, T] \to \mathbb{R}^{M}$, W, ω that solve

$$\min_{A,b,W,\omega} \sum_{n=1}^{N} \|\tau(W x_n(T) + \omega) - y_n\|^2 + R(A, b, W, \omega)$$

$$\text{s.t.} \quad \dot{x}_n = \sigma(A x_n + b), \quad x_n(0) = x_n$$

Potential advantages from Optimal Control / ODEs



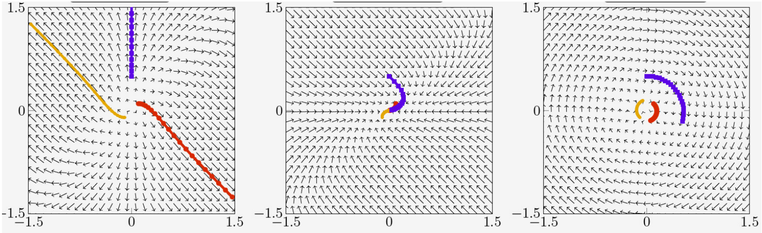
- Rich theory (see stability in a bit)
- New architectures
- New models, e.g. parametrization, regularization
- Advanced algorithms, e.g. Multi-resolution Learning
- ...

Utilize ODE knowledge

Stability and Generalization

- x_1 similar to x_2, then $x_1(T)$ should be similar to $x_2(T)$. Otherwise instability to small errors **prevents generalization**.
- Examples. $\sigma(y) = y, b = 0$

$$A_+ = \begin{pmatrix} 2 & -2 \\ 0 & 2 \end{pmatrix}, \quad A_- = \begin{pmatrix} -2 & 0 \\ 2 & -2 \end{pmatrix}, \quad A_0 = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$



Haber and Ruthotto 2018

Stability and Generalization

Theorem (very old)

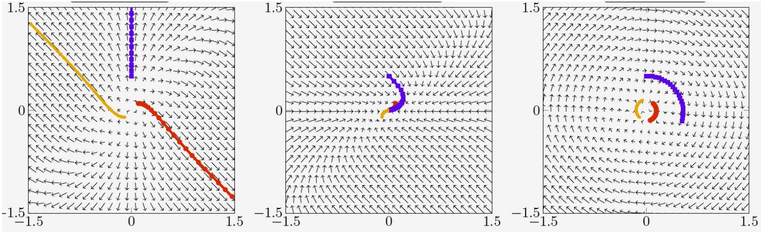
The **autonomous** *ODE* $\dot{x} = f(x)$ *is stable if the real parts of the eigenvalues of the Jacobian* Df *are non-positive.*

Corollary

Let $\dot{\sigma} \geq 0$*. Then forward propagation is* **stable** *if* $\mathrm{Re}(\lambda(A)) \leq 0$*.*

- Examples. $\sigma(y) = y, b = 0$

$$\lambda(A_+) = (2, 2), \quad \lambda(A_-) = (-2, -2), \quad \lambda(A_0) = (i, -i)$$

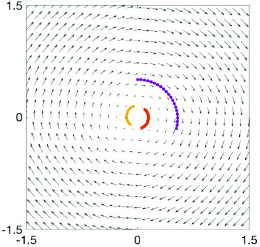


Haber and Ruthotto 2018

New **Unconditionally Stable** Architectures

- ResNet with **antisymmetric** transformation matrix

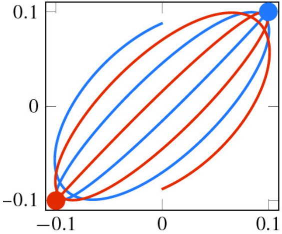
$$\dot{x} = \sigma\left((A - A^T)x + b\right)$$



- **Hamiltonian inspired Network**: ResNet with auxiliary variable and antisymmetric matrix

$$\begin{pmatrix}\dot{x}\\ \dot{z}\end{pmatrix} = \sigma\left(\begin{pmatrix}0 & A\\ -A^T & 0\end{pmatrix}\begin{pmatrix}x\\ z\end{pmatrix} + b\right)$$

$$x(0) = x_0, \quad z(0) = 0$$

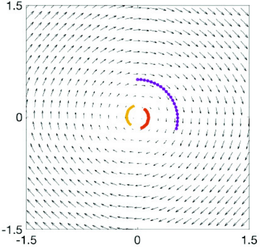


Haber and Ruthotto 2018

New **Unconditionally Stable** Architectures

- ResNet with **antisymmetric** transformation matrix

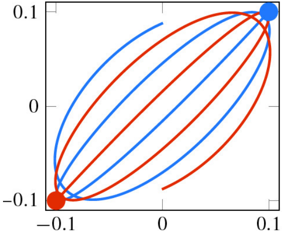
$$\dot{x} = \sigma\left((A - A^T)x + b\right)$$



- **Hamiltonian inspired Network**: ResNet with auxiliary variable and antisymmetric matrix

$$\begin{pmatrix}\dot{x}\\ \dot{z}\end{pmatrix} = \sigma\left(\begin{pmatrix}0 & A\\ -A^T & 0\end{pmatrix}\begin{pmatrix}x\\ z\end{pmatrix} + b\right)$$

$$x(0) = x_0, \quad z(0) = 0$$



Haber and Ruthotto 2018

Problem: this statement is **only true** for autonomous systems!

If the vector-field f depends on time, then similar statements are true but the theory is **rather weak**.

Revisiting Stability

Consider $\Phi_\theta(u) = u(T)$ with u solving $\dot{u}(t) = f(t, u(t)), t \in [0, T]$

What is a useful definition of **stability** for neural networks?

Definition (Stability 1: Lipschitz)

There exists $C > 0$ such that for all u, v we have

$$\|\Phi_\theta(u) - \Phi_\theta(v)\| \leq C\|u - v\| \tag{Lip}$$

Definition (Stability 2: Non-expansive)

For all u, v (Lip) holds with $C = 1$.

When is Φ_θ stable?

Recall $\Phi_\theta(u) = u(T)$ with u solving $\dot{u}(t) = f(t, u(t)), t \in [0, T]$

- Arguments based on **Lipschitz continuity** of f
  - If $f(t, \cdot)$ being L-Lipschitz, e.g. $f(t, u) = \sigma(A(t)u + b(t))$ with σ being S-Lipschitz and A continuous, then Def 1 holds with

$$C = \exp(T \cdot L) \quad (= \exp(T \cdot S \max_t \|A(t)\|)).$$

Celledoni et al. 2020, Zhang and Schaeffer 2020

When is Φ_θ stable?

Recall $\Phi_\theta(u) = u(T)$ with u solving $\dot{u}(t) = f(t, u(t)), t \in [0, T]$

- Arguments based on **Lipschitz continuity** of f
  - If $f(t, \cdot)$ being L-Lipschitz, e.g. $f(t, u) = \sigma(A(t)u + b(t))$ with σ being S-Lipschitz and A continuous, then Def 1 holds with

$$C = \exp(T \cdot L) \quad (= \exp(T \cdot S \max_t \|A(t)\|)).$$

Can't satisfy Def 2 since $C > 1$ for all non-trivial cases.

Celledoni et al. 2020, Zhang and Schaeffer 2020

When is Φ_θ stable?

Recall $\Phi_\theta(u) = u(T)$ with u solving $\dot{u}(t) = f(t, u(t)), t \in [0, T]$

- Arguments based on **Lipschitz continuity** of f
  - If $f(t, \cdot)$ being L-Lipschitz, e.g. $f(t, u) = \sigma(A(t)u + b(t))$ with σ being S-Lipschitz and A continuous, then Def 1 holds with

$$C = \exp(T \cdot L) \quad (= \exp(T \cdot S \max_t \|A(t)\|)).$$

Can't satisfy Def 2 since $C > 1$ for all non-trivial cases.

- Arguments based on **"one-sided" Lipschitz continuity** of f

$$\langle f(t, u_1) - f(t, u_2), u_1 - u_2 \rangle \leq \nu \|u_1 - u_2\|^2$$

  - If f is L-Lipschitz, then f is "one-sided" Lipschitz with $\nu = L$

$$\begin{aligned} \langle f(t, u_1) - f(t, u_2), u_1 - u_2 \rangle &\leq \|f(t, u_1) - f(t, u_2)\| \|u_1 - u_2\| \\ &\leq L \|u_1 - u_2\|^2 \end{aligned}$$

  - Then Ψ_θ is Lipschitz with $C = \exp(T \cdot \nu)$.

Celledoni et al. 2020, Zhang and Schaeffer 2020

When is Φ_θ stable?

Recall $\Phi_\theta(u) = u(T)$ with u solving $\dot{u}(t) = f(t, u(t)), t \in [0, T]$

- Arguments based on **Lipschitz continuity** of f
  - If $f(t, \cdot)$ being L-Lipschitz, e.g. $f(t, u) = \sigma(A(t)u + b(t))$ with σ being S-Lipschitz and A continuous, then Def 1 holds with

$$C = \exp(T \cdot L) \quad (= \exp(T \cdot S \max_t \|A(t)\|)).$$

Can't satisfy Def 2 since $C > 1$ for all non-trivial cases.

- Arguments based on **"one-sided" Lipschitz continuity** of f

$$\langle f(t, u_1) - f(t, u_2), u_1 - u_2 \rangle \leq \nu \|u_1 - u_2\|^2$$

  - If f is L-Lipschitz, then f is "one-sided" Lipschitz with $\nu = L$

$$\begin{aligned} \langle f(t, u_1) - f(t, u_2), u_1 - u_2 \rangle &\leq \|f(t, u_1) - f(t, u_2)\| \|u_1 - u_2\| \\ &\leq L \|u_1 - u_2\|^2 \end{aligned}$$

  - Then Ψ_θ is Lipschitz with $C = \exp(T \cdot \nu)$.
    Catch: ν can be non-positive, $\nu \leq 0$. Thus may satisfy Def 2

Celledoni et al. 2020, Zhang and Schaeffer 2020

Sufficient Conditions for Stability

Recall, $\Phi_\theta(u) = u(T)$ with u solving $\dot{u}(t) = f(t, u(t)), t \in [0, T]$
"one-sided" Lipschitz continuity of f

$$\langle f(t, u_1) - f(t, u_2), u_1 - u_2 \rangle \leq \nu \|u_1 - u_2\|^2 \tag{1}$$

Theorem

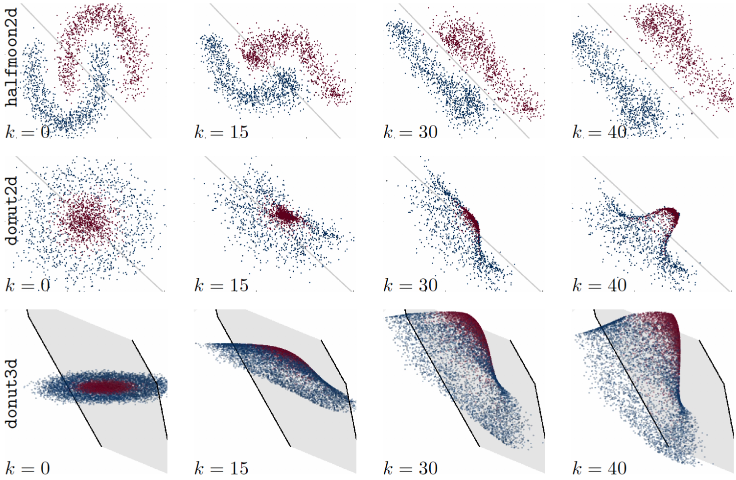
- *Let $V_t(u)$ be twice differentiable and convex. Then $f(t, u) = -\nabla V_t(u)$ satisfies the one-sided Lipschitz condition for some $\nu \leq 0$.*
- *Let $0 \leq \sigma' \leq 1$ almost everywhere. Then*

$$f(t, u) = -A^*(t)\sigma(A(t)u + b(t))$$

satisfies the one-sided Lipschitz condition with $-\mu_*^2 \leq \nu \leq 0$ where $\mu_* := \inf_t \mu(t)$ and $\mu(t)$ is the smallest singular value of $A(t)$.

Celledoni et al. 2020, Zhang and Schaeffer 2020

Examples: Forward propagation with ResNet



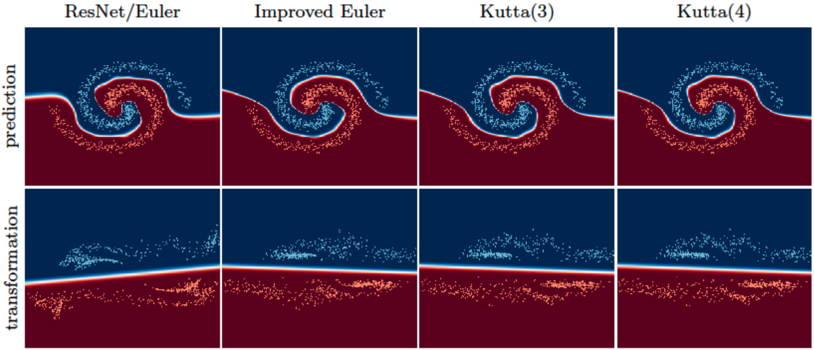
videos?

Celledoni et al. 2020

Examples: Different Runge-Kutta methods

$$\begin{array}{c|c} 0 & \\ \hline & 1 \end{array} \qquad \begin{array}{c|cc} 0 & & \\ 1 & 1 & \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array} \qquad \begin{array}{c|ccc} 0 & & & \\ \frac{1}{2} & \frac{1}{2} & & \\ 1 & -1 & 2 & \\ \hline & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \end{array} \qquad \begin{array}{c|cccc} 0 & & & & \\ \frac{1}{2} & \frac{1}{2} & & & \\ \frac{1}{2} & 0 & \frac{1}{2} & & \\ 1 & 0 & 0 & 1 & \\ \hline & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6} \end{array}$$

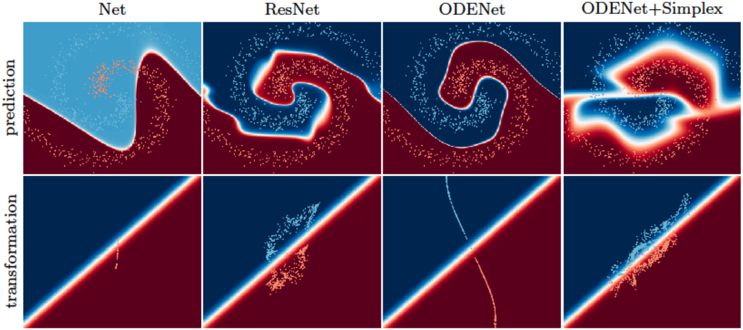
Table 1. Four explicit Runge–Kutta methods: ResNet/Euler, Improved Euler, Kutta(3) and Kutta(4).



Benning et al. 2019

Examples: Learn time steps

$x^{k+1} = x^k + \Delta t^k \sigma(A^k x^k + b^k)$
ODENet: Estimate $(\Delta t^k, A^k, b^k)$
Simplex constraint: $\Delta t^k \geq 0, \sum_k \Delta t^k = T$



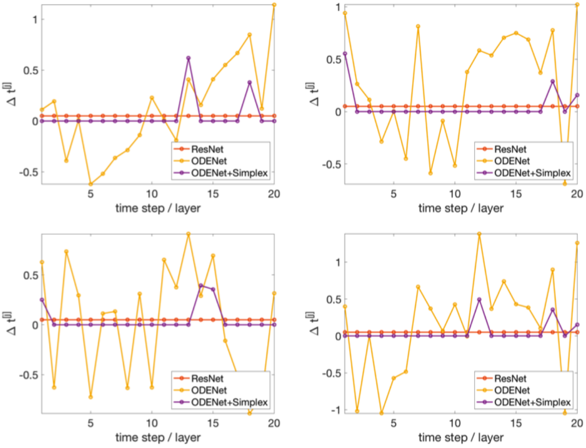
Benning et al. 2019

Examples: Learn time steps

$$x^{k+1} = x^k + \Delta t^k \sigma(A^k x^k + b^k)$$

ODENet: Estimate $(\Delta t^k, A^k, b^k)$

Simplex constraint: $\Delta t^k \geq 0, \sum_k \Delta t^k = T$



Benning et al. 2019

Deep Limits: Number of Layers $K \to \infty$ Thorpe and van Gennip 2018

Interpret discrete parameters as piecewise constant functions on $[0, T]$

Discrete Learning Problem

Find $\theta^K := (A^k, b^k)_{k=1,\dots,K}$ which minimize $E^K : L^2(\mu^K) \to \mathbb{R}$,
$E^K(\theta) = \sum_{k=1}^K \|x_n^K - y_n\|^2 + R^K(\theta)$ such that

$$x_n^{k+1} = x_n^k + \frac{T}{K}\sigma(A^k x_n^k + b^k), \quad x_n^0 = x_n$$

Continuous Learning Problem

Find $\theta^\infty := (A : [0, T] \to \mathbb{R}^{M\times M}, b : [0, T] \to \mathbb{R}^M)$ which minimize
$E^\infty : H^1 \to \mathbb{R}$, $E(\theta) = \sum_{k=1}^K \|x_n(T) - y_n\|^2 + R(\theta)$ such that

$$\dot{x}_n = \sigma(A x_n + b), \quad x_n(0) = x_n$$

Deep Limits: Number of Layers $K \to \infty$ Thorpe and van Gennip 2018

Interpret discrete parameters as piecewise constant functions on $[0, T]$

Discrete Learning Problem

Find $\theta^K := (A^k, b^k)_{k=1,\dots,K}$ which minimize $E^K : L^2(\mu^K) \to \mathbb{R}$,
$E^K(\theta) = \sum_{k=1}^K \|x_n^K - y_n\|^2 + R^K(\theta)$ such that

$$x_n^{k+1} = x_n^k + \frac{T}{K}\sigma(A^k x_n^k + b^k), \quad x_n^0 = x_n$$

Continuous Learning Problem

Find $\theta^\infty := (A : [0, T] \to \mathbb{R}^{M\times M}, b : [0, T] \to \mathbb{R}^M)$ which minimize
$E^\infty : H^1 \to \mathbb{R}$, $E(\theta) = \sum_{k=1}^K \|x_n(T) - y_n\|^2 + R(\theta)$ such that

$$\dot{x}_n = \sigma(A x_n + b), \quad x_n(0) = x_n$$

Theorem

*R^K, R suitable regularization and σ Lipschitz with $\sigma(0) = 0$.
Then 1) minimizers exist, 2) minimal values converge and 3) $\{\theta^K\}_{K\in\mathbb{N}} \subset L^2$ compact and* **any limit point is a minimizer** *of E.*

Enforcing Structure in Neural Networks

Invertible Neural Networks

Consider a neural network $\Psi : X \to X, \Psi(x) = (f_K \circ ... \circ f_1)(x)$
If f_i are **invertible**, then so is Ψ and $\Psi^{-1}(x) = (f_1^{-1} \circ ... \circ f_K^{-1})(x)$

Invertible Neural Networks

Consider a neural network $\Psi : X \to X, \Psi(x) = (f_K \circ ... \circ f_1)(x)$
If f_i are **invertible**, then so is Ψ and $\Psi^{-1}(x) = (f_1^{-1} \circ ... \circ f_K^{-1})(x)$

What are invertible networks **useful** for?

- **memory efficient backpropagation** (computing derivatives): can be implemented as $\mathcal{O}(1)$ rather than $\mathcal{O}(K)$

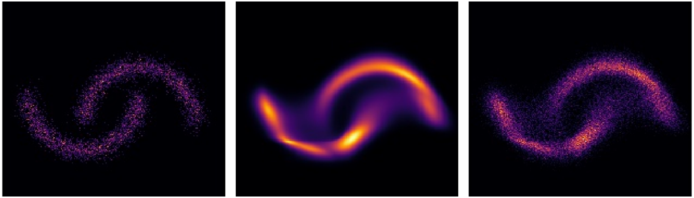
Invertible Neural Networks

Consider a neural network $\Psi : X \to X, \Psi(x) = (f_K \circ \ldots \circ f_1)(x)$
If f_i are **invertible**, then so is Ψ and $\Psi^{-1}(x) = (f_1^{-1} \circ \ldots \circ f_K^{-1})(x)$

What are invertible networks **useful** for?

- **memory efficient backpropagation** (computing derivatives): can be implemented as $\mathcal{O}(1)$ rather than $\mathcal{O}(K)$
- **generative modeling**: Usually learn Ψ_θ such that $x \sim (\Psi_\theta)_* \mu$ with PDF of μ being q. Easy to sample from $(\Psi_\theta)_* \mu$ but PDF unknown.
  If Ψ_θ is invertible, then $(\Psi_\theta)_* \mu$ has PDF

$$x \mapsto q(\Psi_\theta^{-1}(x)) |\det J\Psi_\theta^{-1}(x)|$$



Chen et al. 2019

Invertible Neural Networks

Types of invertible layers:

1) **Linear invertible layers**: LU factorization Kondor et al. 2018, pixel shuffle Dinh et al. 2014

Invertible Neural Networks

Types of invertible layers:

1) **Linear invertible layers**: LU factorization Kondor et al. 2018, pixel shuffle Dinh et al. 2014
2) **Coupling layers** Dinh et al. 2014, $x = (x_1, x_2)$

$$f(x_1, x_2) = (x_1, g_{h(x_1)}(x_2))$$

If g_a is invertible for any a , so is f with inverse

$$f^{-1}(x_1, x_2) = (x_1, g^{-1}_{h(x_1)}(x_2))$$

Simplest example: "additive coupling layer" $\gamma_a(b) = b + a$ has inverse $\gamma_a^{-1}(b) = b - a$.
See Din et al. 2016 and Durkan et al. 2019 for more examples.

Invertible Neural Networks

Types of invertible layers:

1) **Linear invertible layers**: LU factorization Kondor et al. 2018, pixel shuffle Dinh et al. 2014
2) **Coupling layers** Dinh et al. 2014, $x = (x_1, x_2)$

$$f(x_1, x_2) = (x_1, g_{h(x_1)}(x_2))$$

If g_a is invertible for any a , so is f with inverse

$$f^{-1}(x_1, x_2) = (x_1, g^{-1}_{h(x_1)}(x_2))$$

Simplest example: "additive coupling layer" $\gamma_a(b) = b + a$ has inverse $\gamma_a^{-1}(b) = b - a$.
See Din et al. 2016 and Durkan et al. 2019 for more examples.

3) **Residual layers**: $f(x) = x + g(x)$
If g is Lipschitz with constant $L < 1$, then f is invertible.
Problem: $f^{-1}(x)$ is not easy to compute, e.g. use fixed point iteration, and $L < 1$ hard to satisfy. See Behrmann et al. 2019 for more details.

Invertible Neural Networks

Types of invertible layers:

1) **Linear invertible layers**: LU factorization Kondor et al. 2018, pixel shuffle Dinh et al. 2014
2) **Coupling layers** Dinh et al. 2014, $x = (x_1, x_2)$

$$f(x_1, x_2) = (x_1, g_{h(x_1)}(x_2))$$

If g_a is invertible for any a , so is f with inverse

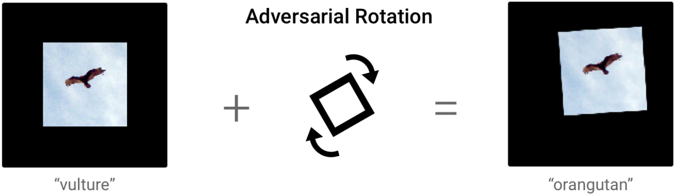
$$f^{-1}(x_1, x_2) = (x_1, g^{-1}_{h(x_1)}(x_2))$$

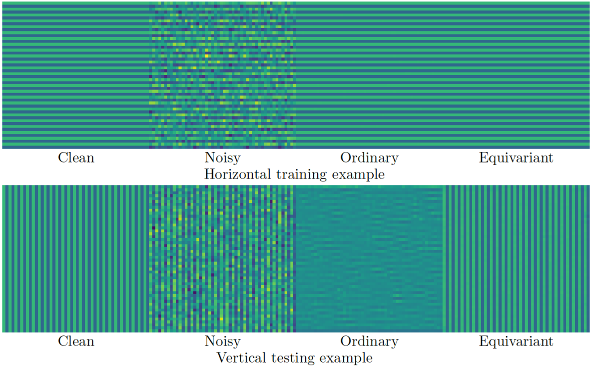
Simplest example: "additive coupling layer" $\gamma_a(b) = b + a$ has inverse $\gamma_a^{-1}(b) = b - a$.
See Din et al. 2016 and Durkan et al. 2019 for more examples.

3) **Residual layers**: $f(x) = x + g(x)$
If g is Lipschitz with constant $L < 1$, then f is invertible.
Problem: $f^{-1}(x)$ is not easy to compute, e.g. use fixed point iteration, and $L < 1$ hard to satisfy. See Behrmann et al. 2019 for more details.

Important: inverse must be "easy" to compute.

Equivariance and invariance





Sherry et al. 2021

Equivariance and invariance Cohen and Welling 2016, Cohen et al. 2019

Definition (Group equivariance and invariance)

Group G "acts" on spaces X and Y. For any $g \in G$ denote "action" g on $x \in X$ and $y \in Y$ by T_g^X and T_g^Y, respectively. We call a function $\Psi : X \to Y$ G-equivariant if for all $g \in G$ we have

$$\Psi \circ T_g^X = T_g^Y \circ \Psi$$

If Ψ is G-equivariant and G acts trivially on Y, then we call Ψ G-invariant. I.e. for all $x \in X$ and $g \in G$ $\Psi(T_g^X x) = \Psi(x)$.

Equivalence and invariance Cohen and Welling 2016, Cohen et al. 2019

Definition (Group equivariance and invariance)

Group G "acts" on spaces X and Y. For any $g \in G$ denote "action" g on $x \in X$ and $y \in Y$ by T_g^X and T_g^Y, respectively. We call a function $\Psi : X \to Y$ G-equivariant if for all $g \in G$ we have

$$\Psi \circ T_g^X = T_g^Y \circ \Psi$$

If Ψ is G-equivariant and G acts trivially on Y, then we call Ψ G-invariant. I.e. for all $x \in X$ and $g \in G$ $\Psi(T_g^X x) = \Psi(x)$.

Key property: If $\Psi_1 : X \to Y$ and $\Psi_2 : Y \to Z$ are G-equivariant (with the same action on Y), then $\Psi_2 \circ \Psi_1$ is G-equivariant, too!

Equivariance and invariance Cohen and Welling 2016, Cohen et al. 2019

Definition (Group equivariance and invariance)

Group G "acts" on spaces X and Y. For any $g \in G$ denote "action" g on $x \in X$ and $y \in Y$ by T_g^X and T_g^Y, respectively. We call a function $\Psi : X \to Y$ G-equivariant if for all $g \in G$ we have

$$\Psi \circ T_g^X = T_g^Y \circ \Psi$$

If Ψ is G-equivariant and G acts trivially on Y, then we call Ψ G-invariant. I.e. for all $x \in X$ and $g \in G$ $\Psi(T_g^X x) = \Psi(x)$.

Key property: If $\Psi_1 : X \to Y$ and $\Psi_2 : Y \to Z$ are G-equivariant (with the same action on Y), then $\Psi_2 \circ \Psi_1$ is G-equivariant, too!

Examples of interesting groups:

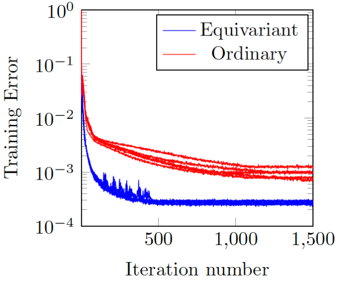
- translations
- rotations
- scaling

Application to inverse problems: Sherry et al. 2021 coming out soon!

Equivariance and invariance

Advantages of equivariance for neural networks:

- no need for data augmentation
- fewer parameters
- trains faster
- mathematical guarantees
- ...



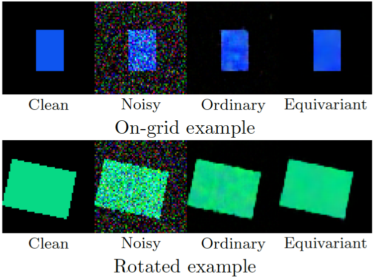


Figure: Celledoni et al. 2020

Cohen and Welling 2016, Cohen et al. 2019, Worall et al. 2017 ...

Conclusions

- **Connections** of deep learning to ODEs, optimal control, group theory ...
- **New architectures with mathematical guarantees**: stable, invertible, equivariant ...
- Direct benefit for applictions: **faster to train**, **less data**, ...

Open problems

E. Celledoni et al., "Structure preserving deep learning," arxiv:2006.03364, 2020.

- **discretization**
- **manifolds**
- **sampling complexity**
- ...