Deep learning and numerical analysis.

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Outline

- A numerical analysis view to deep learning
- Structure preservation
- Adversarial attacks - robust NNs
- Contractivity of ODEs and of numerical integrators
- Applications variational regularization in imaging
- B-stability and Conditional Stability on manifolds

Let $\mathcal{V}$ input space, $\mathcal{W}$ output space

$$\varphi : \mathcal{V} \to \mathcal{W}.$$

DNNs - **approximation theory**:

$$\varphi \approx \varphi_\theta$$

by a composition of L simpler maps (layers)

$$\varphi_\theta = \varphi_L \circ \varphi_{L-1} \circ \cdots \circ \varphi_1, \quad \varphi_\ell = \varphi_{\theta_\ell} \quad \varphi_{\theta_\ell} : \mathcal{V}_{\ell-1} \to \mathcal{V}_\ell$$

$\mathcal{V}_0 = \mathcal{V}$ and $\mathcal{V}_L = \mathcal{W}$, each φ_ℓ depends on a finite number of parameters θ_ℓ.

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Residual networks - **numerical ODEs**: $\mathcal{V}_{\ell-1} = \mathcal{V}_\ell = \mathcal{V}$ a compact subdomain of $\mathbb{R}^N$ and

$$\varphi_{\theta_\ell} = \mathrm{id} + hX_{\theta_\ell}, \quad X_{\theta_\ell} : x \mapsto \sigma(A_\ell x + b_\ell), \quad \theta_\ell := (A_\ell, b_\ell)$$

can be seen as the forward Euler discretization of the flow map of the ODE

$$\dot{y} = \sigma(A(t)y(t) + b(t)), \qquad y(0) = x, \qquad t \in [0, h]$$

(He et al. 2015, Haber and Ruthotto 2017, and E 2017).

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Learning - **variational methods**: optimising a cost function (distance) with respect to all the parameters

$$\min_{\varphi_\theta = \varphi_{\theta_L} \circ \cdots \circ \varphi_{\theta_1}} E(\varphi_\theta) = \min_{\{\theta_\ell\}_{\ell=1}^L} E(\varphi_{\theta_L} \circ \cdots \circ \varphi_{\theta_1})$$

is the **discretization of the optimal control problem**:

$$\inf_{A(t), b(t)} E(y(T)), \quad \text{subject to} \qquad \dot{y} = \sigma(Ay + b), \quad y(0) = x, \quad t \in [0, T].$$

Transitions in Runge–Kutta methods – Data Spiral

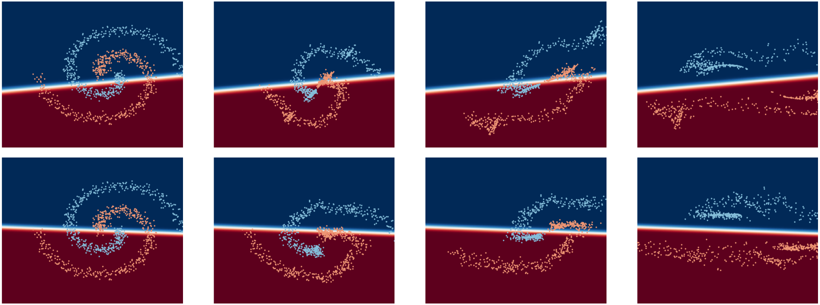

Figure: Snap shots of the transition from initial to final state through the network with the *Spiral* data set. Top, ResNet/Euler, and bottom, Runge-Kutta(4).

- The qualitative properties of the flow of the dynamical system are more important for the result than the extent to which the ODE flow is accurately reproduced.
- Can use the ODE as a means to construct neural networks with a prescribed structure.

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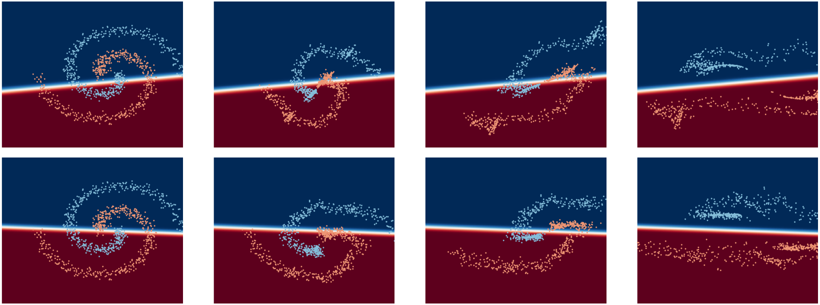

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Examples of structured NNs:

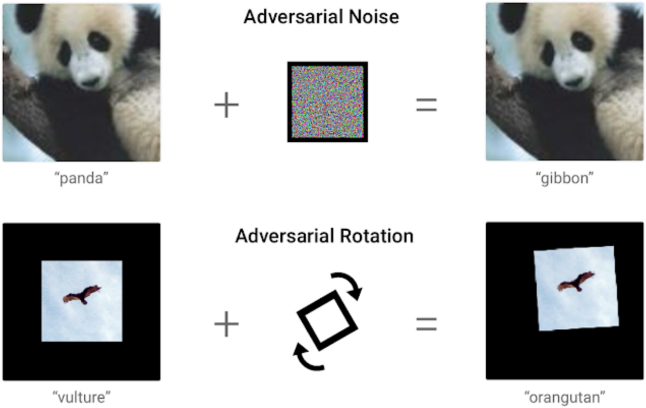
- 1-Lipshitz networks (adversarial attacks and image denoising).
- Symmetric neural networks (LLMs).
- Hamiltonian/Lagrangian neural networks (for learning dynamics from data).

-EC, Ehrhardt, Etmann, McLachlan, Owren, Schönlieb, Sherry, *Structure preserving deep learning*.

Lipschitz Networks

- Adversarial attacks
- Image denoising

(In)stability – adversarial attacks



https://ai.googleblog.com/2018/09/

Residual networks:

$$\varphi \approx \varphi_\theta = \varphi_{\theta_L} \circ \varphi_{\theta_{L-1}} \circ \cdots \circ \varphi_{\theta_1}, \qquad \varphi_{\theta_\ell} : \mathcal{V} \to \mathcal{V},$$

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forward Euler numerical integration of the ODE

$$\dot{y} = B(t)\sigma(A(t)y(t) + b(t)), \qquad y(0) = x, \qquad t \in [0, h].$$

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$$\dot{y} = B(t)\sigma(A(t)y(t) + b(t)), \qquad y(0) = x, \qquad t \in [0, h].$$

- We want to be able to guarantee that the layer φ_ℓ is a contractive map (when necessary), i.e.

  $$\|\varphi_\ell(y_2) - \varphi_\ell(y_1)\| < \|y_2 - y_1\|,$$

  so that we can compose contractive and non-contractive layers to construct a neural network with Lipschitz constant equal to 1.
- We can use known theory of numerical stability of contractive ODEs.

Contractivity of the underlying ODE

A vector field $X(t, y)$ is **contractive** in ℓ^2-norm if there is $\nu > 0$ such that for all y_1, y_2 and $t \in [0, T]$:

$$\langle X(t, y_2) - X(t, y_1), y_2 - y_1 \rangle \leq -\nu \|y_2 - y_1\|^2.$$

This implies that for any two integral curves $y(t)$ and $z(t)$

$$\|y(t) - z(t)\| \leq e^{-t\nu} \|y(0) - z(0)\|.$$

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The vector field

$$X(t,y(t)) = -A(t)^T \sigma(A(t)y(t) + b(t)),$$

with σ increasing function, $A \in \mathbb{R}^{n\times k}$, $b \in \mathbb{R}^n$, **is contractive**.

- EC, Ehrhardt, Etmann, McLachlan, Owren, Schönlieb, Sherry, *Structure preserving deep learning*, EJAM, 2021.

Contractivity of Runge-Kutta methods: B-stable numerical integration methods for ODEs

- B-stable Runge-Kutta methods (implicit) preserve **contractivity** independently on the step-size h. (Butcher 1975, Dahlquist 76, Burrage and Butcher 1979)
- Dekker and Verwer, Stability of Runge-Kutta methods for Stiff Nonlinear Differential Equations, 1984.

The **backward Euler method**

$$y_1 = y_0 + h\,X(t_1, y_1)$$

applied to contractive vector fields is non-expansive for all step-sizes $h > 0$.

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Proof: In ℓ_2-norm. Consider to initial values y_0 and x_0 and the Euler updates

$$y_0 = y_1 - hX(t_1, y_1)$$
$$x_0 = x_1 - hX(t_1, x_1)$$

then

$$y_0 - x_0 = y_1 - x_1 - h(X(t_1, y_1) - X(t_1, x_1))$$

taking the inner product of LHS and RHS with themselves we get

$$\|y_0 - x_0\|_2^2 = \|y_1 - x_1\|_2^2 - 2h\langle X(t_1, y_1) - X(t_1, x_1), y_1 - x_1\rangle + h^2\|X(t_1, y_1) - X(t_1, x_1))\|_2^2$$

using the contractivity condition we see that for all $h \geq 0$ the RHS is the sum of three positive terms and we have that $\|y_1 - x_1\|_2^2 \leq \|y_0 - x_0\|^2$, which means we have the non-expnsivity for all $h > 0$.

Contractivity of explicit Runge-Kutta methods: forward Euler

Theorem (Dahlquist and Jeltsch, 1979)
Suppose X satisfies the **cocoercivity condition**

$$\langle X(t,y_2) - X(t,y_1), y_2 - y_1 \rangle \leq -\bar{\nu} \| X(t,y_2) - X(t,y_1) \|^2, \quad \bar{\nu} \geq 0.$$

Then, if the stepsize h satisfies

$$h \leq 2\bar{\nu},$$

the **forward Euler method is non-expansive**.

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$$y_1 = y_0 + hX(t_0,y_0)$$
$$x_1 = x_0 + hX(t_0,x_0)$$

then

$$y_1-x_1 = y_0-x_0+h(X(t_0,y_0)-X(t_0,x_0))$$

taking the inner product with LHS with itself and RHS with itself we get

$$\|y_1-x_1\|_2^2 = \|y_0-x_0\|_2^2+2h\langle X(t_0,y_0)-X(t_0,x_0),y_0-x_0\rangle+h^2\|X(t_0,y_0)-X(t_0,x_0))\|_2^2$$

using the monotonicity condition and taking $h\leq 2\bar{\nu}$ we get

$$2\langle X(t_0,y_0)-X(t_0,x_0),y_0-x_0\rangle + h\|X(t_0,y_0)-X(t_0,x_0))\|_2^2\leq 0$$

and we get contractivity $\|y_1-x_1\|_2^2\leq\|y_0-x_0\|^2$.

Contractivity of explicit Runge-Kutta methods: forward Euler

Theorem (Dahlquist and Jeltsch, 1979 - Theory of circle contractivity)
Suppose X satisfies the **cocoercivity condition**

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Proposition
For σ non decreasing and L-Lipschitz, the vector field

$$X(t,y) = -A(t)^T \sigma(A(t)y + b),$$

with $A \in \mathbb{R}^{n\times k}$, $b \in \mathbb{R}^n$, satisfies the cocoercivity condition with $\bar{\nu} = \frac{1}{\|A\|^2 L}$.

Remark X is a gradient vector field:
$\dot{y} = -\nabla_y V, \qquad V(t,y(t)) = \langle \gamma\big(A(t)y(t) + b(t)\big), \mathbb{1} \rangle, \quad \gamma' = \sigma.$

- Sherry, EC, Ehrhardt, Murari, Owren and Schönlieb, *Designing Stable Neural Networks using Convex Analysis and ODEs*, 2023, arXiv:2306.17332

- Databases of images: using convolution neural networks
- Network:

$$\Psi = \varphi_1 \circ \psi_1 \circ \varphi_2 \circ \psi_2 \circ \cdots \circ \varphi_L \circ \psi_L$$

- Convenient to use orthogonal weights. $\|P\| = 1$, $\|Q\| = 1$, easier

$$\varphi_\ell(x) = x - h_1\, P^T \sigma(Px + p) \quad \text{contractive}$$
$$\psi_\ell(x) = x + h_2\, Q^T \sigma(Qx + q) \quad \text{expansive}$$
$$\sigma(x) = \max\left\{x, \frac{x}{2}\right\},\ P^T P = I,\ Q^T Q = I.$$

Robust classification of CIFAR10 and CIFAR100

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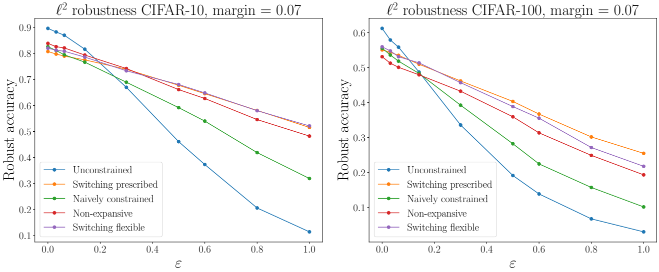
Using orthogonal convolutional NNs. by Wang et al., 2020. Adversarial examples using Foolbox.



EC, Murari, Owren, Schönlieb and Sherry, *Dynamical systems based neural networks*, 2023, SISC

- Extensions to graph neural networks in:
  - M Eliasof, D Murari, F Sherry, CB Schönlieb, *Contractive Systems Improve Graph Neural Networks Against Adversarial Attacks* arXiv preprint arXiv:2311.06942.
- Where you can find more experiments on adversarial robustness.

Applications in imaging

- **Variational regularization in image processing**
  clean images $\hat{u}$ are recovered from measurements y by minimising a trade-off between
  1. $E_y(u) := d(A(u), y)$ the **data fit** and
  2. $R(u)$ **penalty function** encoding prior knowledge

$$\hat{u} = \arg\min_u E_y(u) + R(u).$$

- **Splitting methods for optimisation**: split the objective function in two or more terms, each easier to optimise.
- **Proximal gradient** is a variant of gradient descent where the gradient flow is approximated by an implicit-explicit time-stepping. The implicit part corresponds to the **proximal operator**:

Proposition:

$$\mathrm{prox}_{hR}\, u = \arg\min_{u'} \|u - u'\|_2 + h\, R(u').$$

To solve the optimization problem

$$\hat{u} = \arg\min_u E_y(u) + R(u)$$

we use

Proximal gradient descent

Input: measurements y, initial estimate u_0

for $\ell = 1, \ldots, N$ **do**

$$u^{[\ell+1]} = \mathrm{prox}_{hR}(u^{[\ell]} - h\nabla E_y(u^{[\ell]}))$$

end for

Plug-and-Play: replace prox_{hR} with a (non-expansive) neural network $\widehat{\mathrm{prox}}_{h,\ell}$, learning the de-noiser form data.

Definition An operator $\mathcal{A} : \mathbb{R}^d \to \mathbb{R}^d$ is α-averaged if $\exists$ a non expansive operator $T : \mathbb{R}^d \to \mathbb{R}^d$ s.t.

$$\mathcal{A} = \alpha T + (1 - \alpha) I_d, \quad \alpha \in (0, 1).$$

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Theorem (Hertrich, Neumayer, Steidl)
Let $E:\mathbb{R}^m \to \mathbb{R}$ be convex and differentiable with L-Lipschitz continuous gradient and let $\widehat{\mathrm{prox}}_{h,\ell}:\mathbb{R}^m \to \mathbb{R}^m$ be averaged. Then, for any $0 < h < \frac{2}{L}$, the sequence $\{u^{[\ell]}\}_\ell$ generated by

Proximal gradient descent-PnP:

for $\ell = 1,\ldots,N$ **do**

$$u^{[\ell+1]} = \widehat{\mathrm{prox}}_{h,\ell}(u^{[\ell]} - h\nabla E_y(u^{[\ell]}))$$

end for

converges.

- J Hertrich, S Neumayer, G Steidl, *Convolutional Proximal Neural Networks and Plug-and-Play Algorithms* , Lin. Alg. and Appl.

PnP with ResNet and non-expansive networks

- Using $f(t, y) = -A^T \sigma(Ay + b)$ we can construct residual neural networks that are provably non-expansive (1-Lipschitz) and averaged.
- **J Hertrich, S Neumayer, G Steidl.** Averagedness together with $E_y(u)$ convex, differentiable and ∇E_y is L-Lipschitz, is sufficient to prove convergence of PnP algorithms.

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Theorem (Sherry)
Let σ non decreasing and L-Lipschitz, $A \in \mathbb{R}^{n\times k}$, $b \in \mathbb{R}^n$ and let $\alpha \in (0,1)$. A single layer mapping $\mathcal{A} : x \to \varphi(x)$,

$$\varphi(x) = x - hA^{\top}\sigma(Ax + b)$$

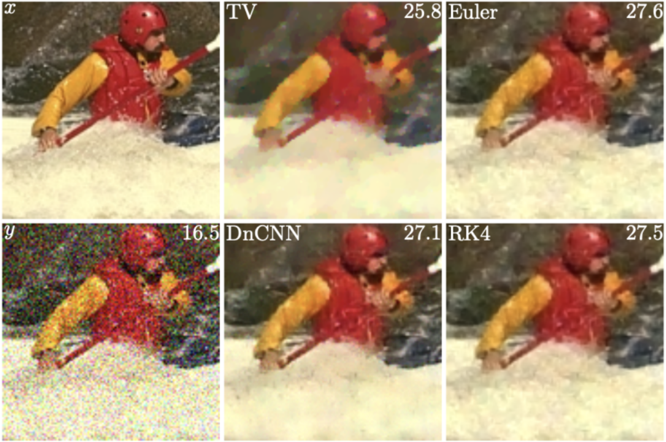
is α-averaged if

$$h \leq \frac{2\alpha}{L\|A\|^2}. \tag{1}$$

Remark Composition of m operators $\mathcal{A}_i$, $i = 1, \ldots, m$ which are α_i averaged is α averaged for a certain α.

- Sherry, EC, Ehrhardt, Murari, Owren and Schönlieb, *Designing Stable Neural Networks using Convex Analysis and ODEs*, 2024, Physica D

Denoising with PnP (Courtesy of F. Sherry)



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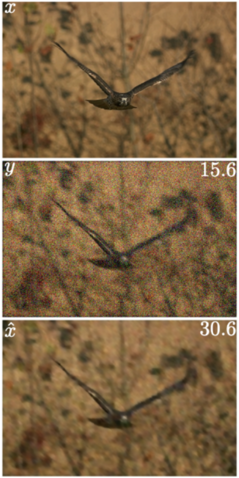
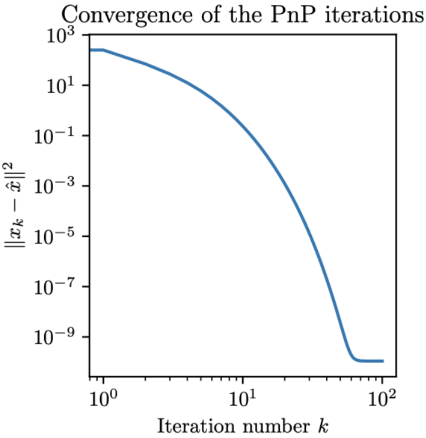
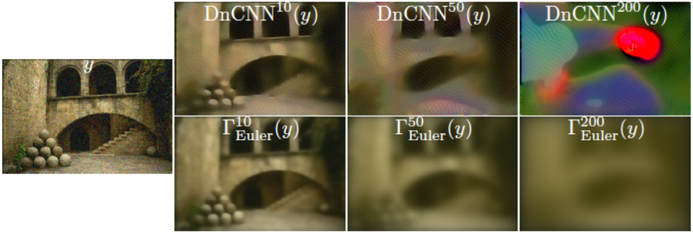
Convergence with PnP (Courtesy of F. Sherry)





- Sherry, EC, Ehrhardt, Murari, Owren and Schönlieb, *Designing Stable Neural Networks using Convex Analysis and ODEs*, 2023, arXiv:2306.17332

Convergence vs Divergence of Learned Denoisers



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Contractivity of numerical integrators on Riemannian manifolds

Diffusion tensor imaging

Manifold valued images: $s = (s_{1,1}, \ldots, s_{l,m}) \in \mathcal{M}$, $\mathcal{M} = (\mathrm{Sym}^+(3))^{m \times l}$.

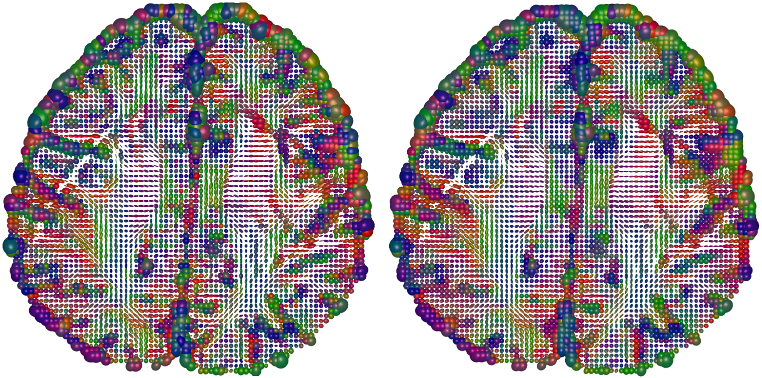
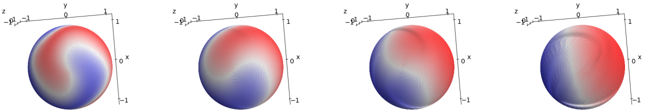


Figure: DTI scan, axial slice. Left: Noisy image. Right: Denoised with $\beta = 2$, $\lambda = 0.05$.

- E.C., S. Eidnes, B. Owren, **T. Ringholm**, *Dissipative numerical schemes on Riemannian manifolds with applications to gradient flows*, SISC 2019.

Neural Networks on Manifolds

- Model order reduction via Autoencoders implies the Latent space is a Manifold
- Covariance matrices are symmetric positive (semi) definite
- Diffusion Tensor Imaging, SPD voxels
- Robotics require rotations and roto-translations
- Message passing neural networks require hyperbolic geometry
- Graph data in biology, network science, computer graphycs/vision can be handled much more efficiently when embedded in hyperbolic space [Ganea et al 2018] e.g. for learning low-dimensional embeddings.



Layer 0 **Layer 3** **Layer 6** **Layer 10**

There are a number of open questions:

- How to construct neural networks on manifolds.
- How to obtain **stability and robustness**.

Recall the contractivity condition in flat spaces

Contractivity condition: a vector field $X(t, y)$ is contractive in ℓ^2-norm if there is $\nu > 0$ such that for all y_1, y_2 and $t \in [0, T]$:

$$\langle X(t, y_2) - X(t, y_1), y_2 - y_1 \rangle \leq -\nu \|y_2 - y_1\|^2.$$

This implies that for any two integral curves $y(t)$ and $z(t)$

$$\|y(t) - z(t)\| \leq e^{-t\nu} \|y(0) - z(0)\|.$$

Recall also

Cocoercivity condition:

$$\langle X(t, y_2) - X(t, y_1), y_2 - y_1 \rangle \leq -\bar{\nu} \|X(t, y_2) - X(t, y_1)\|^2, \quad \bar{\nu} > 0,$$

used to obtain contractivity of the forward Euler method for small enough step-sizes.

Contractivity of numerical integrators on Riemannian manifolds

- $(\mathcal{M}, g)$ a Riemannian manifold, $g_p(u,v) = \langle u, v\rangle_p$
- $\ell(\gamma) = \int_a^b \sqrt{\langle\dot\gamma(t), \dot\gamma(t)\rangle} dt, \quad d(p,q) = \inf_{\gamma_{p\to q}} \ell\left(\gamma_{p\to q}\right),$
- *geodesic*: $\gamma(t) = \exp_p(t\, v_p)$, $\exp_p : T_p\mathcal{M} \to \mathcal{M}$ Riemannian exponential
- ∇ is the Levi-Civita connection induced by g
- X and Y vector fields on $\mathcal{M}$: $\nabla_X Y$ denotes the covariant derivative on $\mathcal{M}$
- a curve $\gamma(t)$ on $\mathcal{M}$ is a geodesic if it satisfies the equation $\nabla_{\dot\gamma}\dot\gamma = 0$

Contractivity of numerical integrators on Riemannian manifolds

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- $\ell(\gamma) = \int_a^b \sqrt{\langle \dot\gamma(t), \dot\gamma(t)\rangle} dt, \quad d(p,q) = \inf_{\gamma_{p\to q}} \ell(\gamma_{p\to q})$,
- *geodesic*: $\gamma(t) = \exp_p(t\, v_p)$, $\exp_p : T_p\mathcal{M} \to \mathcal{M}$ Riemannian exponential
- ∇ is the Levi-Civita connection induced by g
- X and Y vector fields on $\mathcal{M}$: $\nabla_X Y$ denotes the covariant derivative on $\mathcal{M}$
- a curve $\gamma(t)$ on $\mathcal{M}$ is a geodesic if it satisfies the equation $\nabla_{\dot\gamma}\dot\gamma = 0$

Contractivity condition: for $\mathcal{U} \subset \mathcal{M}$ a vector field X satisfies the monotonicity condition on $\mathcal{U}$ if there is $\alpha_0 > 0$ st

$$\langle \nabla_{v_x} X, v_x\rangle \le -\alpha_0 \|v_x\|^2, \quad \forall x \in \mathcal{U}, \quad v_x \in T_x\mathcal{M}.$$

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Gronwall: Assume $\mathcal{U}$ geodesically convex, let $y(t)$ and $z(t)$ be two integral curves of the vector field X with $y(0) = y_0$ and $z(0) = z_0$ both contained in $\mathcal{U}$ $\forall t \in [0, T]$ then

$$d(y(t), z(t)) \le e^{-t\alpha_0} d(y_0, z_0), \quad \forall t \in [0, T].$$

Non-expansiveness when X is forward complete, $\mathcal{U}$ is forward X-invariant and $\nu \le 0$.

- M. Kunzinger et al., 2006, Revista Matemática Complutense.
- J. W. Simpson-Porco and F. Bullo, Contraction theory on Riemannian manifolds, Sys. Cont.Lett. 2014

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Cocoercivity condition: is satisfied by X on $\mathcal{U}$, if there is $\alpha > 0$ s.t.

$$\langle \nabla_{v_x} X, v_x\rangle \leq -\alpha \|\nabla_{v_x} X\|^2, \quad \forall x \in \mathcal{U} \quad v_x \in T_x\mathcal{M}.$$

Definition: Suppose

- X is contractive on $\mathcal{U} \subset \mathcal{M}$,
- $\phi_{h,X} : \mathcal{M} \to \mathcal{M}$ is a numerical method approximating the solution of $\dot{y} = X(y)$ and $y(0) = p$ and $\phi_{h,X}$ is well defined for all $h \geq 0$,
- $\mathcal{U}$ is forward $\phi_{h,X}$-invariant for all $h \geq 0$ and forward X-invariant

then the method is said to be **B-stable** iff

$$d(\phi_{h,X}(y_0), \phi_{h,X}(z_0)) \leq d(y_0, z_0), \quad \forall h \geq 0.$$

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B-stability of Geodesic Implicit Euler

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B-stability of Geodesic Implicit Euler

$$y_n = \exp_{y_{n+1}}(-hX(y_{n+1})).$$

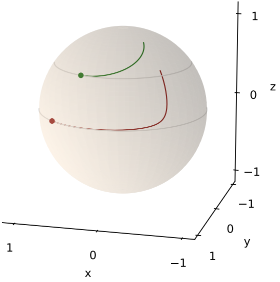
Theorem
If $\mathcal{M}$ is a Riemannian manifold with **non-positive sectional curvature** then the geodesic implicit Euler method is B-stable.

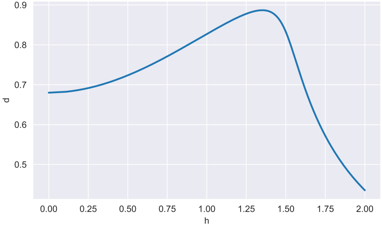
Example Space of $n \times n$ symmetric positive definite matrices.

- Arnold, EC, Cokaj, Owren, Tumiotto, *Contractivity of numerical integrators on Riemannian manifolds*, JCD, 2024.

Geodesic Implicit Euler is not B-stable on the sphere. Counterexample.

The sphere has positive sectional curvature equal to 1:





- Non-expansive vector field (on the northern hemisphere)

$$\dot{y} = X(y) = a \times y, \qquad a = [0, 0, 1].$$

- (Left) One step of Geodesic Implicit Euler applied with increasing step size h, starting from two different initial values.
- (Right) Geodesic distance: $d(y_1, z_1)$ plotted as a function of h, where $y_0 = \exp_{y_1}(-hX(y_1)), \quad z_0 = \exp_{z_1}(-hX(z_1))$.

We assume constant sectional curvature and we seek a bound of the step-size h that makes the geodesic explicit Euler non-expansive.

Projected cocoercivity conditions

- positive curvature $\rho > 0$: project tangent vectors onto the orthogonal complement of X_{y_n}:

$$\langle \nabla_v X, (I - P_X)v \rangle \geq -\mu^+ \|\nabla_v X\|^2 \tag{2}$$

- negative curvature $\rho < 0$: project tangent vectors on the span of X_{y_n}

$$\langle \nabla_v X, P_X v \rangle \geq -\mu_- \|\nabla_v X\|^2 \tag{3}$$

Theorem (manifolds of constant positive sectional curvature)

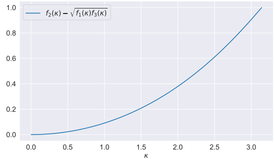
- Let $(\mathcal{M}, g)$ have positive sectional curvature.
- Let X be a vector field with ∇X invertible, and satisfying the contractivity condition with constant $\alpha > 0$
- Also let X satisfy the projected cocoercivity condition (2) with constant μ^+
- Let $\kappa = h\|X\|\sqrt{\rho}$, $\rho > 0$ being the curvature of $\mathcal{M}$.

Then the Geodesic Explicit Euler method applied to X with stepsize h is nonexpansive whenever

$$h \leq 2\alpha - 2\mu^+ f(\kappa)$$

where

$$f(\kappa) = 1 - \cos(\kappa)\mathrm{sinc}(\kappa) - \sin(\kappa)\sqrt{1 - \mathrm{sinc}(\kappa)^2}$$



Theorem (manifolds of constant negative sectional curvature)

- Let $(\mathcal{M}, g)$ have negative sectional curvature.
- Let X be a vector field with ∇X invertible, and satisfying the non-expansivity condition with constant $\alpha > 0$
- Also let X satisfy the projected cocoercivity condition (3) with constant μ_-
- Let $\kappa = h\|X\|\sqrt{-\rho}$, $\rho < 0$ being the curvature of $\mathcal{M}$.

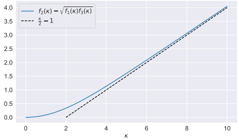
Then the Geodesic Explicit Euler method applied to X with stepsize h is nonexpansive whenever

$$0 < h \leq \frac{2}{1 + \sigma^2 C\rho}\left(\alpha\kappa \coth(\kappa) - \mu_- \frac{f(\kappa)}{\phi(\kappa)}\right)$$

where

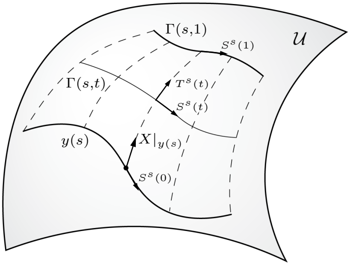
$$f(\kappa) = (\cosh(\kappa)\phi(\kappa) - 1) - \sinh(\kappa)\sqrt{\phi(\kappa)^2 - 1}$$

$$\phi(\kappa) = \frac{\sinh(\kappa)}{\kappa}$$



Conditional stability of the Geodesic Explicit Euler method

$$\Gamma(s,t) = \exp_{y(s)}(t\,h\,X(y(s))), \quad t \in [0,1]$$



- $y(s)$ curve of initial points.
- Dahsed lines: numerical flow.
- $\Gamma(s,1)$: $y(s)$ as transported by the numerical flow at time $t = 1$.
- $S(s,t)$ and $T(s,t)$ tangent vector fields along s and t.

Objective: to ensure that the length of $\Gamma(s,1)$ is not bigger than the length of $\Gamma(s,0) = y(s)$.

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Thank you for listening!