Perspectives on Contraction Theory and Neural Networks



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- S. Jafarpour, A. Davydov, A. V. Proskurnikov, and F. Bullo. Robust implicit networks via non-Euclidean contractions. In *Advances in Neural Information Processing Systems*, Dec. 2021. URL http://arxiv.org/abs/2106.03194
- A. Davydov, S. Jafarpour, and F. Bullo. Non-Euclidean contraction theory for robust nonlinear stability. *IEEE Transactions on Automatic Control*, July 2021. URL https://arxiv.org/abs/2103.12263. Conditionally accepted
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Artificial and Biological Neural Networks





artificial neural network AlexNet '12

C. elegans connectome '17

Aim: understand the dynamics of neural networks, so that

- reproducible behavior, i.e., equilibrium response as function of stimula
- robust behavior in face of uncertain stimuli and dynamics
- learning models, efficient computational tools, periodic behaviors ...

A. Krizhevsky, I. Sutskever, and G. E. Hinton. Imagenet classification with deep convolutional neural networks. Advances in Neural Information Processing Systems, 25, 2012 G. Yan, P. E. Vértes, E. K. Towlson, Y. L. Chew, D. S. Walker, W. R. Schafer, and A.-L. Barabási. Network control principles predict neuron function in the Caenorhabditis elegans connectome. Nature, 550(7677):519–523, 2017.

Fixed point computation



Fixed point strategies in data science = simplifying and unifying framework to model, analyze, and solve advanced convex optimization methods, Nash equilibria, monotone inclusions, etc. P. L. Combettes and J.-C. Pesquet. Fixed point strategies in data science. *IEEE Transactions on Signal Processing*, 2021. Scientific and engineering problems from neural networks

2 Contraction theory

• Banach contractions and infinitesimal counterparts

Application to recurrent neural networks and implicit ML models
 Implicit neural networks in machine learning

④ Conclusions and future research

Contraction theory: historical notes

Origins

S. Banach. Sur les opérations dans les ensembles abstraits et leur application aux équations intégrales. *Fundamenta Mathematicae*, 3(1):133–181, 1922.

S. M. Lozinskii. Error estimate for numerical integration of ordinary differential equations. I. *Izvestiya Vysshikh Uchebnykh Zavedenii. Matematika*, 5:52–90, 1958. URL http://mi.mathnet.ru/eng/ivm2980. (in Russian)

C. A. Desoer and H. Haneda. The measure of a matrix as a tool to analyze computer algorithms for circuit analysis. *IEEE Transactions on Circuit Theory*, 19(5):480–486, 1972.

 Application in dynamics and control: W. Lohmiller and J.-J. E. Slotine. On contraction analysis for non-linear systems. *Automatica*, 34(6):683–696, 1998.

Reviews:

Z. Aminzare and E. D. Sontag. Contraction methods for nonlinear systems: A brief introduction and some open problems. In *IEEE Conf. on Decision and Control*, pages 3835–3847, Dec. 2014.

M. Di Bernardo, D. Fiore, G. Russo, and F. Scafuti. Convergence, consensus and synchronization of complex networks via contraction theory. In J. Lü, X. Yu, G. Chen, and W. Yu, editors, *Complex Systems and Networks*, pages 313–339. Springer, 2016. ISBN 978-3-662-47824-0.

H. Tsukamoto, S.-J. Chung, and J.-J. E. Slotine. Contraction theory for nonlinear stability analysis and learning-based control: A tutorial overview. *Annual Reviews in Control*, 52:135–169, 2021.





Given $\dot{x} = F(t, x)$, F is *infinitesimally strongly contractive* if its flow is a Banach contraction

On fixed point algorithms and Banach contractions

$$x = \mathsf{G}(x)$$

Banach Contraction Theorem If Lip(G) < 1 that is $\|G(u) - G(v)\| \le \text{Lip}(G)\|u - v\|$, then *Picard iteration* $x_{k+1} = G(x_k)$ is a Banach contraction



For $Lip(G) \ge 1$, define the *average iteration*

$$x_{k+1} = (1 - \alpha)x_k + \alpha \mathsf{G}(x_k)$$

Infinitesimal Contraction Theorem

Q there exists $0 < \alpha < 1$ such that the average iteration is a Banach contraction

- the map G satisfies osLip(G) < 1</p>
- **3** the dynamics $\dot{x} = -x + G(x)$ is infinitesimally strongly contracting

Robustness of fixed point algorithms

Robustness based upon Contraction x_u^* is a fixed point of x = G(x, u) and $Lip_x G < 1$, then

$$\|x_u^* - x_v^*\| \leq \frac{\operatorname{Lip}_u \mathsf{G}}{1 - \operatorname{Lip}_x \mathsf{G}} \|u - v\|$$



Robustness based upon Infinitesimal Contraction x_u^* is a fixed point of x = G(x, u) x_v^* is a fixed point of x = G(x, v) + D(x, v), and $osLip_x(G + D) < 1$, then

$$\|x_{u}^{*} - x_{v}^{*}\| \leq \frac{1}{1 - \mathsf{osLip}_{x}(\mathsf{G} + \mathsf{D})} \Big(\mathsf{Lip}_{u}(\mathsf{G} + \mathsf{D}) \|u - v\| + \|\mathsf{D}(x_{u}^{*}, u)\| \Big)$$

Properties of contracting dynamical systems

Highly ordered transient and asymptotic behavior:



- time-invariant F: unique globally exponential stable equilibrium two natural Lyapunov functions
- eriodic F: contracting system entrain to periodic inputs
- Ontractivity rate is natural measure/indicator of robust stability
- In modularity and interconnection properties,
- accurate numerical integration, and

there exist efficient methods for their equilibrium computation

The log norm of $A \in \mathbb{R}^{n \times n}$ wrt to $\| \cdot \|$:

$$\mu(A) := \lim_{h \to 0^+} \frac{\|I_n + hA\| - 1}{h}$$

Basic properties:

subadditivity:	$\mu(A+B) \le \mu(A) + \mu(B)$	
scaling:	$\mu(bA) = b\mu(A),$	$\forall b \geq 0$
norm/spectrum:	$\operatorname{Re}(\lambda) \le \mu(A) \le \ A\ ,$	$\forall \lambda \in \operatorname{spec}(A)$

Convexity and quasi-convexity:

$$\begin{split} \mu_{2,P^{1/2}(A)} &\leq -c & \iff & PA + A^{\top}P \preceq -2cP \\ \mu_{\infty,\eta}(A) &\leq -c & \iff & a_{ii}\eta_i + \sum_{j \neq i} |a_{ij}|\eta_j \leq -c\eta_i \text{ for all } i \end{split}$$

Contraction equivalences on normed vector spaces

For $x \in \mathbb{R}^n$ and continuously differentiable

 $\dot{x} = \mathsf{F}(x)$

For norm $\|\cdot\|$ with log norm $\mu(\cdot)$

$$\mathsf{osLip}(\mathsf{F}) := \sup_{x \in \mathbb{R}^n} \mu(D\mathsf{F}(x))$$

Main equivalences: for c > 0

d-osL : $osLip(F) \leq -c$

2 d-IS :
$$D^+ ||x(t) - y(t)|| \le -c ||x(t) - y(t)||$$
 for solthing $x(\cdot), y(\cdot)$

3 IS : $||x(t) - y(t)|| \le e^{-c(t-t_0)} ||x(t_0) - y(t_0)||$, for all soltns $x(\cdot), y(\cdot)$

Equilibria of contracting vector fields:

For a time-invariant F, c-strongly contracting with respect to $\|\cdot\|$

I flow of F is a contraction,

i.e., distance between solutions exponentially decreases with rate \boldsymbol{c}

2 there exists an equilibrium x^* , that is unique, globally exponentially stable with global Lyapunov functions

 $x \mapsto \|x - x^*\|$ and $x \mapsto \|\mathsf{F}(x)\|$



Computing equilibria

Given $\mathsf{F}:\mathbb{R}^n\to\mathbb{R}^n$

$$x^* \in \operatorname{zero}(\mathsf{F}) \qquad \iff x^* \in \operatorname{fixed}(G), \text{ where } \mathsf{G} = \mathsf{Id} + \mathsf{F}$$

consider forward step = Euler integration for F = averaged iteration for G:

$$x_{k+1} = (\mathsf{Id} + \alpha \mathsf{F})x_k = x_k + \alpha \mathsf{F}(x_k) \qquad = (1 - \alpha) \, \mathsf{Id} + \alpha \mathsf{G}$$

Given contraction rate c and Lipschitz constant ℓ , define condition number $\kappa = \ell/c \ge 1$ • the map Id $+\alpha F$ is a contraction map with respect to $\|\cdot\|$ for

$$0 < \alpha < \frac{1}{c\kappa(1+\kappa)}$$

2 the optimal step size minimizing and minimum contraction factor:

$$\alpha^* \approx \frac{1}{2c\kappa^2}, \qquad \ell^* \approx 1 - \frac{1}{4\kappa^2}$$

Application: ℓ_{∞} -contracting neural networks



lf

$$\mu_{\infty}(A) < 1$$
 (i.e., $a_{ii} + \sum_{j} |a_{ij}| < 1$ for all i)

- dynamics is contracting with rate $1 \mu_{\infty}(A)_+$
- average iteration is Banach with factor $1 \frac{1 \mu_{\infty}(A)_{+}}{1 \min_{i}(a_{ii})_{-}}$ at $\alpha = \frac{1}{1 \min_{i}(a_{ii})_{-}}$ • input-output Lipschitz constant $\operatorname{Lip}_{u \to y} = \frac{\|B\|_{\infty} \|C\|_{\infty}}{1 - \mu_{\infty}(A)_{+}}$

Scientific and engineering problems from neural networks

2 Contraction theory

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Application to recurrent neural networks and implicit ML models
 Implicit neural networks in machine learning

4 Conclusions and future research

Detour: a bit more detail

Continuous-time recurrent neural networks:

$$\begin{split} \dot{x} &= -x + A\Phi(x) + u \\ \dot{x} &= -x + \Phi(Ax + u) =: f_{\mathsf{FR}}(x) \\ \dot{x} &= A\Phi(x) \\ \dot{x} &= Ax - \Phi(x) \end{split}$$



activation functions are locally-Lip and slope-restricted: for all i $d_{\min} := \operatorname{ess\,inf}_{y \in \mathbb{R}} \frac{\partial \Phi_i(y)}{\partial y} \geq 0$ and $d_{\max} := \operatorname{ess\,sup}_{y \in \mathbb{R}} \frac{\partial \Phi_i(y)}{\partial y} < \infty$

$$f_{\mathsf{FR}}(x) = -x + \Phi(Ax + u)$$

Tight transcription.

$$\mathsf{osLip}_{\infty}(f_{\mathsf{FR}}) = \underset{x \in \mathbb{R}^n}{\operatorname{ess \, sup}} \, \mu_{\infty} \big(-I_n + (D\Phi(x))A \big) = -1 + \underset{d \in [d_{\min}, d_{\max}]^n}{\operatorname{max}} \, \mu_{\infty}(\operatorname{diag}(d)A)$$

Max log norms over hypercubes. For $A \in \mathbb{R}^{n \times n}$ and $0 \le d_{\min} \le d_{\max}$

$$\max_{\substack{d \in [d_{\min}, d_{\max}]^n}} \mu_{\infty}(\operatorname{diag}(d)A) = \max\left\{\mu_{\infty}(d_{\min}A), \mu_{\infty}(d_{\max}A)\right\}$$
$$\max_{\substack{d \in [d_{\min}, d_{\max}]^n}} \mu_1(\operatorname{diag}(d)A) = \max\{\mu_1(d_{\max}A), \mu_1(d_{\max}A - (d_{\max} - d_{\min})(I_n \circ A))\}$$
$$\max_{\substack{d \in [d_{\min}, d_{\max}]^n}} \mu_{\infty}(A\operatorname{diag}(d)) = \dots$$
$$\max_{\substack{d \in [d_{\min}, d_{\max}]^n}} \mu_1(A\operatorname{diag}(d)) = \dots$$

NonEuclidean contractivity of firing rate model

$$\dot{x} = -Cx + \Phi(Ax + u) =: f_{\mathsf{FR}}(x)$$

• for arbitrary $\eta \in \mathbb{R}^n_{>0}$

$$\mathsf{osLip}_{\infty,[\eta]^{-1}}(f_{\mathsf{FR}}) = \max\{\mu_{\infty,[\eta]^{-1}}(-C + d_{\mathsf{min}}A), \mu_{\infty,[\eta]^{-1}}(-C + d_{\mathsf{max}}A)\}$$

2 optimal weight η and minimim value of $\operatorname{osLip}_{\infty,[\eta]^{-1}}(f_{\mathsf{FR}})$ from quasiconvex opt:

$$\begin{split} & \inf_{b \in \mathbb{R}, \eta \in \mathbb{R}^n_{>0}} b \\ & \text{s.t.} \quad (-C + d_{\min} |A|_{\mathsf{M}}) \eta \leq b \eta \\ & (-C + d_{\max} |A|_{\mathsf{M}}) \eta \leq b \eta \end{split}$$

Explicit solution (from PF theory) when $d_{\min} = 0$

$$\inf_{\eta \in \mathbb{R}^n_{>0}} \mathrm{osLip}_{\infty,[\eta]}(f_{\mathsf{FR}}) = \max\left\{\alpha(-C), \alpha(-C + d_{\max}|A|_{\mathsf{M}})\right\}$$

Example: ℓ_{∞} -contracting neural networks



$$\mu_{\infty}(A) < 1$$
 (i.e., $a_{ii} + \sum_{j} |a_{ij}| < 1$ for all i)

• dynamics is contracting with rate $1 - \mu_{\infty}(A)_+$

lf

• average iteration is Banach with factor $1 - \frac{1 - \mu_{\infty}(A)_{+}}{1 - \min_{i}(a_{ii})_{-}}$ at $\alpha = \frac{1}{1 - \min_{i}(a_{ii})_{-}}$

• input-output Lipschitz constant $\operatorname{Lip}_{u \to y} = \frac{\|B\|_{\infty} \|C\|_{\infty}}{1 - \mu_{\infty}(A)_{+}}$

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Implicit neural networks in machine learning



ML advantages of implicit/equilibrium/fixed point formulation:

- bio-inspired
- 2 expressivity and ability to model I/O behavior, instead of modalities
- simplicity and memory efficiency
- accuracy
- input-output robustness

Motivation #1: Generalizing FF to fully-connected synaptic matrices $x^{i+1} = \Phi(A_ix^i + B_iu + b_i) \iff x = \Phi(Ax + Bu + b)$, where A has upper diagonal structure.



Motivation #2: Weight-tied infinite-depth NN \rightarrow fixed-point of INN

$$u \longrightarrow x_1 \xrightarrow{A} x_2 \xrightarrow{A} x_3 \xrightarrow{A} x_k \xrightarrow{} y$$

 $x^{i+1} = \Phi(Ax^i + Bu + b) \implies \lim_{i \to \infty} x^i = x^*$ solution to the INN

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- 2 L. El Ghaoui, F. Gu, B. Travacca, A. Askari, and A. Tsai. Implicit deep learning. SIAM Journal on Mathematics of Data Science, 3(3):930–958, 2021.
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Implicit Neural Networks (INNs)

- Training INNs:
 - $\textcircled{0} \text{ loss function } \mathcal{L}$
 - 2 training data $(\widehat{u}_i, \widehat{y}_i)_{i=1}^N$
 - **③** training optimization problem

$$\min_{A,B,C,b,x} \sum_{i=1}^{N} \mathcal{L}(\widehat{y}_i, Cx_i + c)$$
$$x_i = \Phi(Ax_i + B\widehat{u}_i + b)$$

- Efficient back-propagation through implicit differentiation
- Stochastic gradient descent: at each step solve $x = \Phi(Ax + Bu + b)$.

Robustness of INNs

Adversarial examples: small input change can cause large output change!



Robustness measures: input-output Lipschitz constant

- **1** ℓ_2 -norm Lipschitz constant: not informative in many scenarios
- **2** ℓ_{∞} -norm Lipschitz constant: large-scale input wrt wide-spread perturbations

Robustness of INNs

Adversarial examples: small input change can cause large output change!



Robustness measures: input-output Lipschitz constants

- NP-hard to compute exactly
- Q Approximations provide only coarse certified robustness guarantees

Training optimization problem:

$$\min_{A,B,C,b} \sum_{i=1}^{N} \mathcal{L}(\hat{y}_i, Cx_i + c) + \lambda \quad \mathsf{Lip}_{u \to y}$$
$$x_i = \Phi(Ax_i + B\hat{u}_i + b)$$
$$\mu_{\infty}(A) \le \gamma$$

- $\lambda \ge 0$ is a regularization parameter
- $\gamma < 1$ is a hyperparameter

Parametrization of μ_{∞} constraint:

$$\mu_{\infty}(A) \leq \gamma \quad \iff \quad \exists T \text{ s.t. } A = T - \operatorname{diag}(|T|\mathbb{1}_n) + \gamma I_n.$$

Graph-Theoretic Regularization

Synaptic matrix A encodes interactions between neurons



• A_{dropout} is a principal submatrix of A_{complete}

- $\mu_{\infty}(A_{\text{dropout}}) \leq \mu_{\infty}(A_{\text{complete}})$
 - Well-posedness of original INN implies well-posedness of INN with subset of neurons
 - Promotes compression and sparsity of overparametrized models

Numerical Experiments

- MNIST handwritten digit dataset (60K+10K, 28x28, grayscale)
- implicit neural network order: n = 100



Numerical Experiments

Robustness of INNs

Tradeoff between accuracy and robustness



Pareto-optimal curve

• Clean performance vs. robustness

Mixed monotonicity for INN reachability

Idea: mixed monotone systems theory for reachability analysis of RNN dynamics



 $\begin{array}{c} \text{Embedded INN} \\ \text{INN with } u \in [\underline{u}, \overline{u}] \\ x = \phi(Ax + Bu + b), \\ y = Cx + d, \end{array} \qquad \qquad \left[\begin{matrix} \underline{x} \\ \overline{x} \end{matrix} \right] = \phi \left(\begin{bmatrix} [A]^{\text{Mzr}} & [A]^{\text{Mzr}} \\ [A]^{\text{Mzr}} & [A]^{\text{Mzr}} \end{bmatrix} \begin{bmatrix} \underline{x} \\ \overline{x} \end{bmatrix} + \begin{bmatrix} [B]^+ & [B]^- \\ [B]^- & [B]^+ \end{bmatrix} \begin{bmatrix} \underline{u} \\ \overline{u} \end{bmatrix} + \begin{bmatrix} b \\ b \end{bmatrix} \right), \\ \begin{bmatrix} \underline{y} \\ \overline{y} \end{bmatrix} = \begin{bmatrix} [C]^+ & [C]^- \\ [C]^- & [C]^+ \end{bmatrix} \begin{bmatrix} \underline{x} \\ \overline{x} \end{bmatrix} + \begin{bmatrix} d \\ d \end{bmatrix}.$

Training provably robust INNs

Training INNs

- ${\rm 1}{\rm 1}$ training data $(\widehat{u}^i,\widehat{y}^i)_{i=1}^N,$
- **2** loss function \mathcal{L}
- optimization problem

$$\begin{split} \min_{\Theta} & \sum_{i=1}^{N} (1-\kappa) \mathcal{L}(y^{i}, \widehat{y}^{i}) + \kappa \mathcal{L}(\underline{y}^{i}, \widehat{y}^{i}), \\ & x^{i} = \phi(Ax^{i} + Bu^{i} + b), \quad y^{i} = Cx^{i} + d, \\ & \underline{y}^{i} = [T^{i}C]^{+} \underline{x}^{i} + [T^{i}C]^{-} \overline{x}^{i} + T^{i}c, \quad \mu_{\infty, [\eta]^{-1}}(A) \leq \gamma \end{split}$$

where $\kappa \in [0,1]$ and $\gamma < 1$ are hyperparameters.

- Stochastic gradient descent: at each step solve $2 \mbox{ fixed-point problems}$
- Backpropagation through fixed-point equations

Numerical Experiments

Robustness of INNs

- Tradeoff between accuracy and robustness
- implicit neural network order: n = 100 vs 5-layer feedforward network



Scientific and engineering problems from neural networks

2 Contraction theory

• Banach contractions and infinitesimal counterparts

3 Application to recurrent neural networks and implicit ML models

- Implicit neural networks in machine learning
- 4 Conclusions and future research

Conclusions

From Contracting Dynamics to Contracting Algorithms:

- O contraction theory, monotone operator theory, convex optimization
 - effective methodologies to tackle control, optimization and learning problems
 - extensions to network dynamics
- Irom Euclidean to non-Euclidean norms
- application to recurrent and implicit neural networks
 - existence, uniqueness, and computation of fixed-points
 - robustness analysis and robust training via Lipschitz bounds
 - https://github.com/davydovalexander/Non-Euclidean_Mon_Op_Net

From Contracting Dynamics to Contracting Algorithms:

- implicit graph neural architectures
- Ø bio-inspired Hebbian learning
- opustness of implicit models

Supplementary slides

Background on Infinitesimal Contraction Theorem

- () there exists $0 < \alpha < 1$ such that the average iteration is a Banach contraction
- **2** the map G satisfies osLip(G) < 1
- **3** the dynamics $\dot{x} = F(x) := -x + G(x)$ is infinitesimally contracting
- the equivalence (2) \iff (3) is just a transcription:
 - F = Id +G contracting with rate $c \iff {\rm osLip}({\rm F}) < -c \iff {\rm osLip}({\rm G}) < 1-c$, for c>0
 - in (ℓ_2, P) , osLip(F) < -c is usual Krasovskii: $PJ(x) + J(x)^\top P \preceq -2cP$ for all x and J = DF
- (2) ⇒ (1): known in monotone operator theory (page 15 "forward step method" in¹)
 vector field F is contracting with rate c ⇔ -F is strongly monotone with parameter c
- Theorem 1 in² proves the equivalence (1) ⇐⇒ (2) for any norm, i.e., the implication (2) ⇒ (1) for any norm (with proper osLip definitions) and the converse direction (1) ⇒ (2) for l₂, P. Theorem 3 in² proves the one-sided Lim Lemma (see next slide).

¹E. K. Ryu and S. Boyd. Primer on monotone operator methods. *Applied Computational Mathematics*, 15(1):3–43, 2016

²S. Jafarpour, A. Davydov, A. V. Proskurnikov, and F. Bullo. Robust implicit networks via non-Euclidean contractions. In Advances in Neural Information Processing Systems, Dec. 2021. URL http://arxiv.org/abs/2106.03194

Most foundational results in systems theory are based on ℓ_2 linear-quadratic theory;

their ℓ_1/ℓ_∞ analogs are yet to be worked out.

Advantages of non-Euclidean approach

- computational advantages: non-Euclidean log-norm constraints lead to LPs, whereas l₂ constraints leads to LMIs. Parametrization of log-norm constrained matrices is polytopic.
 A. Rantzer. Scalable control of positive systems. European Journal of Control, 24:72–80, 2015. ^C
- **2** guaranteed robustness to structural perturbations: ℓ_{∞} contractivity ensures:
 - 0 absolute contractivity = with respect to a class of activation functions
 - **2** total contractivity = remove any node and all its incident connections
 - connective contractivity = remove any set of edges

adversarial input-output analysis

 ℓ_∞ better suited for the analysis of adversarial examples than ℓ_2 : in high dimensions, large inner product between two vectors is possible even when one vector has small ℓ_∞ norm

I. J. Goodfellow, J. Shlens, and C. Szegedy. Explaining and harnessing adversarial examples. In International Conference on Learn Representations (ICLR), 2015. URL https://arxiv.org/abs/1412.6572

Literature on recurrent NN ODEs

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