A dynamical systems view of learners, samplers and forecasters

Nisha Chandramoorthy

Collaborators: **Andreas Loukas** (Genentech), **Khashayar Gatmiry** (MIT), **Stefanie Jegelka** (MIT), **Youssef Marzouk** (MIT), **Jeongjin Park** (Georgia Tech), **Thien Le** (MIT), **Evan Montoya** (Georgia Tech)

December 15, 2023

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  - dynamics-aware generalization

Intersections with areas of statistics

Generalization: The performance of a learning algorithm on unseen data (typically from the same distribution)

C, Loukas, Gatmiry and Jegelka, NeurIPS 2022

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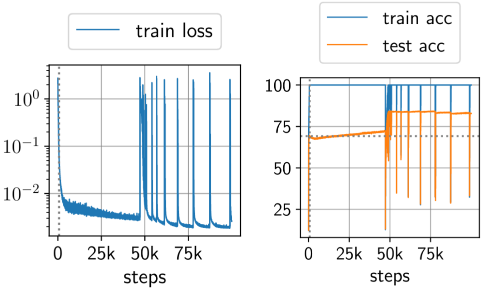
Forecasting: predicting chaotic timeseries from data

Park and C, 2023

More **long-term** stability in the training algorithm leads to better generalization

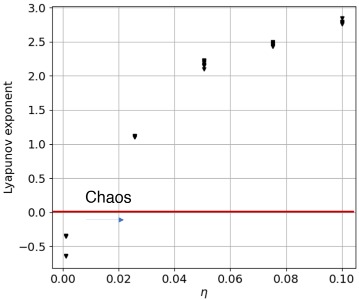
Non-converging optimization

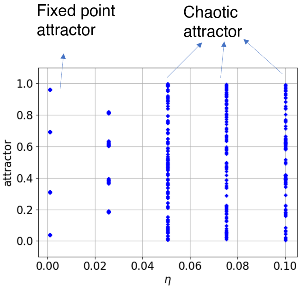
What happens in training beyond the stopping point?



Courtesy: [Lyu Li Arora 2022]. Recent interest [Kong and Tao 2021, Cohen et al 2021, Lobacheva et al 2021, Zhang Li Sra Jadbabaie 2022] in non-converging training algorithms

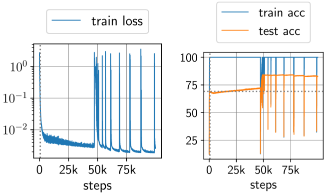
Training algorithms as nonlinear dynamical systems





- heavy-tailed fluctuations in SGD leads to better generalization [**Martin and Mahoney 2017, 2019, 2020**]
- generalization linked to fractal dimension of SGD attractor [**Şimşekli et al 2020**], data-dependent generalization [**Xu and Raginsky 2017**] based on Fernique-Talagrand functional [**Hodgkinson et al 2022**]

Non-converging optimization



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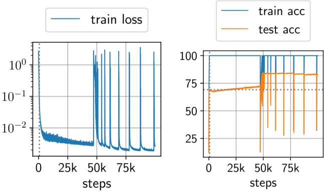

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(Q1) How can we *define* and *study* the generalization properties of a non-converging learning algorithm?

(Q2) Can the statistical/ergodic properties of the algorithm *predict* its generalization performance?

SGD/GD dynamics on weight space:

$$w_{t+1} = w_t - \eta \hat{\nabla} L_S(w_t),$$

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In general, deterministic/stochastic nonlinear dynamics on compact set. No guarantee of convergence to fixed points. There exist multiple invariant, ergodic distributions on weight space, M.

Ergodic properties of training

A probability measure μ on M is ergodic for the training dynamics if for all continuous functions $f : M \to \mathbb{R}$, and μ-a.e. w_0,

$$(1/T) \sum_{t=0}^{T-1} f(w_t) \to \mathbb{E}_{w\sim\mu}[f(w)].$$

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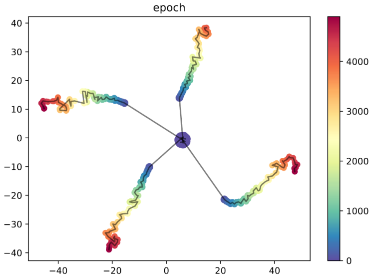
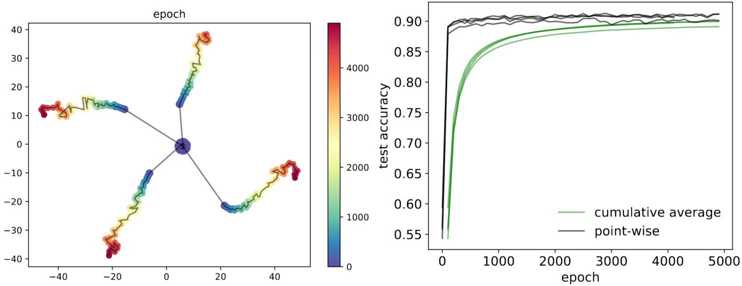


Convergence of loss time-averages

Assumption 1: For almost every w_0 and every z, time-average of $\ell(z, \cdot)$ converges to a constant $\langle \ell_z \rangle_S$, independent of w_0.



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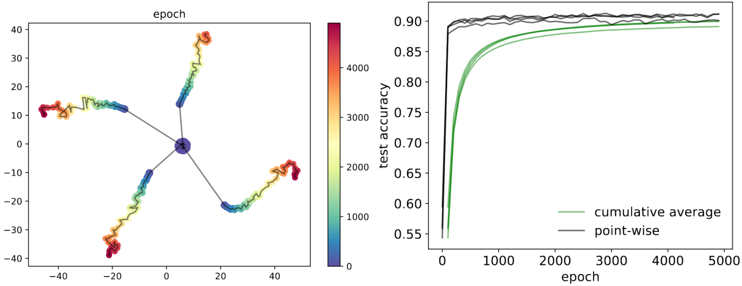

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Assumption allows us to extend algorithmic stability to *statistical algorithmic stability* (SAS).

Statistical Algorithmic Stability

Classical algorithmic stability [Bousquet and Elisseeff 2002]:

$$\beta := \sup_{z} \sup_{S,S'} |\ell(z, w_S^*) - \ell(z, w_{S'}^*)|.$$

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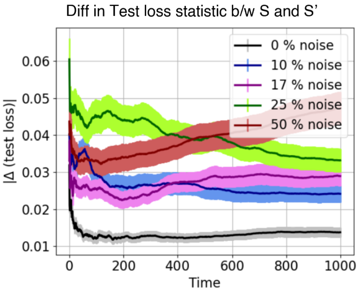
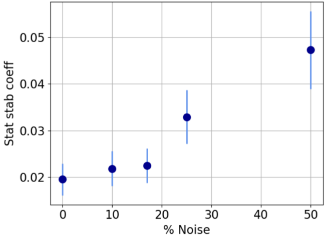
- applies to non-converging learning algorithms
- is constant on network function/parameter space

Numerical approximation of β for SGD on VGG16 model trained on CIFAR10





Noisy CIFAR10 labels.
Anticlockwise: Sample mean over 45 (S, S') pairs, with error bars, of time-averaged test loss difference. Lower bound on β with error bars computed as sample mean. Test loss vs. time (epoch).

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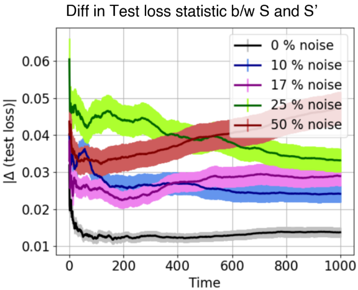

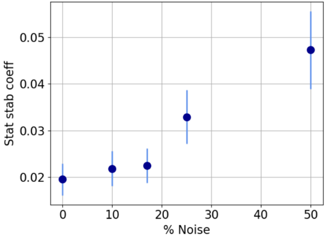

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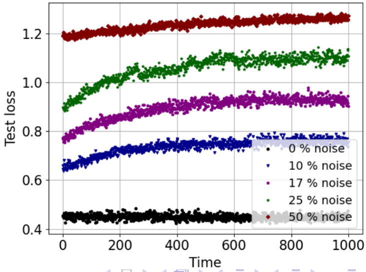

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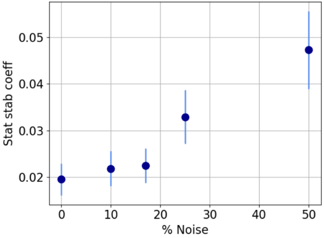

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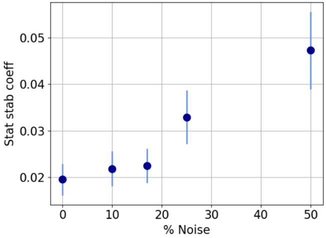
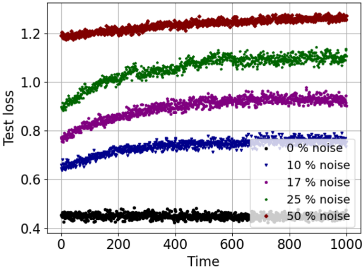


Generalization error



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Pointwise approach [**Hardt et al 2016**] toward algorithmic stability

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- Uninformative for SAS, which is a time-independent notion
- Early stopping based on the upper bound does not apply to non-converging algorithms
- Must take global **(operator-theoretic)** approach to SAS-based generalization

Predicting generalization gap from timeseries data

Theorem 2 (**Slower convergence of loss statistics implies larger** β) Let λ be the slowest mixing rate of the transition operators on loss space. Then, the corresponding training algorithm with n samples has SAS coefficient

$$\beta = \mathcal{O}\left(\frac{1}{n}\frac{L_D}{1-\lambda}\right),$$

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- exploit perturbation theory of uniformly ergodic Markov chains (see e.g. [Mitraphanov 2005])
- Under conditions of the above result, $\beta \sim \mathcal{O}(1/n)$.

Numerical verification of the connection between speed of convergence of statistics and SAS, and hence generalization

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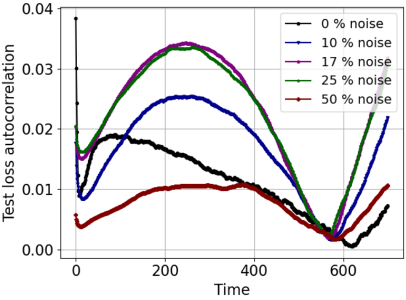
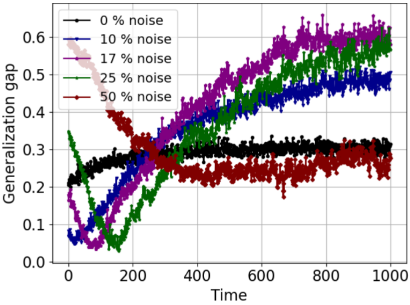
SGD with constant step size of 0.01 on ResNet18 model trained on corrupted CIFAR10 dataset.





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score of a probability distribution with density $\rho := \nabla \log \rho$

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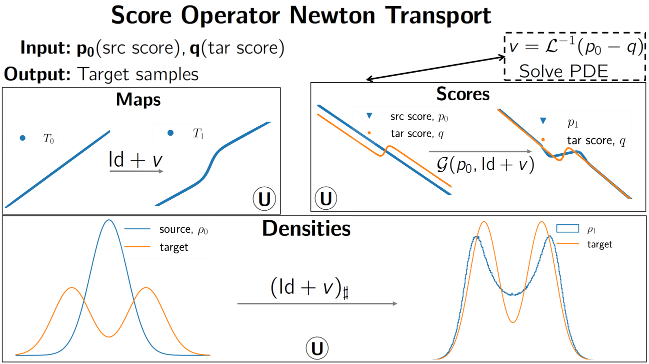

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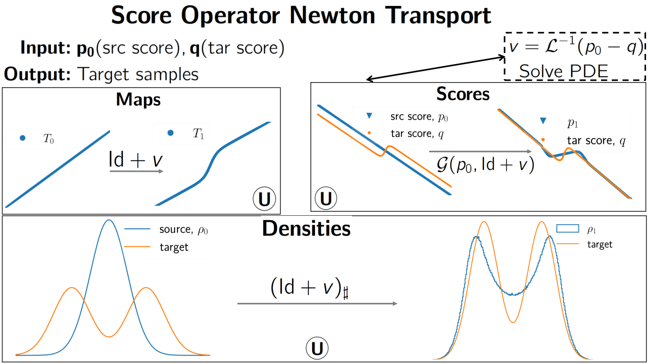

Introduce a new **transport map** construction

Sampling via measure transport

- Target measure: ν with density ρ^{ν}.
- Tractable source measure μ with density ρ^{μ}.
- $\mathrm{supp}(\mu) = \mathbb{X}$ and $\mathrm{supp}(\nu) = \mathbb{Y}$.

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A transport map $T : \mathbb{X} \to \mathbb{Y}$ is an invertible transformation such that $T_{\sharp}\mu = \nu$.

The score operator

Goal: new transport map that exploits availability of **scores**.

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Change of variables/pushforward operation:

$$\rho^{\nu} = \frac{\rho^{\mu} \circ T^{-1}}{|\det \nabla T| \circ T^{-1}}$$

Pushforward operation on **scores**:

$$\begin{aligned}\mathcal{G}(s, U) &= \left(s(\nabla U)^{-1} - \nabla \log |\det \nabla U| (\nabla U)^{-1}\right) \circ U^{-1} \\ &= \left(s\,(\nabla U)^{-1} - \mathrm{tr}\left((\nabla U)^{-1} \nabla^2 U\right)(\nabla U)^{-1}\right) \circ U^{-1},\end{aligned}$$

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Some properties of $\mathcal{G}$

- $\mathcal{G}(s, \mathrm{Id}) = s$
- $\mathcal{G}(s, U_2 \circ U_1) = \mathcal{G}(\mathcal{G}(s, U_1), U_2)$

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Infinite-dimensional score matching problem: Find **T** such that

$$\mathcal{G}(p, T) = q,$$

where,
p: Source score = $\nabla \log \rho^{\mu}$
q: Target score = $\nabla \log \rho^{\nu}$.

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Infinite-dimensional score matching problem: Find **T** such that

$$\mathcal{G}(p, T) = q,$$

where,
p: Source score = $\nabla \log \rho^{\mu}$
q: Target score = $\nabla \log \rho^{\nu}$.

- Want to avoid parameterization
- Use Newton-type method

A zero of the score residual

Infinite-dimensional score matching problem: Find a zero $\in \mathcal{C}^2(\mathbb{X}, \mathbb{Y})$ of the **score residual** operator

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$$\mathcal{L}(q)\, v := -D_2\mathcal{G}(q, \mathrm{Id})\, v = \nabla q\, v + q\, \nabla v + \mathrm{tr}(\nabla^2 v).$$

The zero of the score residual operator

The **linearized** score-matching problem: **Elliptic** PDE system

$$(p - q) = \mathcal{L}\, v \tag{1}$$

Newton-type step:

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SCONE gives an iterative construction as the limit of a sequence of compositions. Based on finding zero of a score-residual operator.

Existence of a $\mathcal{C}^r$ transport and convergence of SCONE iteration

Theorem [**SCONE**(informal)] For every $\epsilon > 0, s \in \mathbb{N}$, there exists a $\delta > 0$ such that $\|p - q\|_s \leqslant \epsilon$ implies $\exists\ T \in \mathcal{C}^{s+2,\cdot}(M)$ such that (i) $\mathcal{G}(p, T) = q$ and (ii) $\| T - \mathrm{Id}\|_{s+2} \leqslant \delta$. Moreover, $T = \lim_{n\to\infty} T_n$ and $q = \lim_{n\to\infty} p_n$ in $\mathcal{C}^{s+2,\cdot}(\bar{\Omega})$, where $(T_n)_{n\geqslant 0}$ and $(p_n)_{n\geqslant 0}$ are the sequences generated by the Score Operator Newton iteration.

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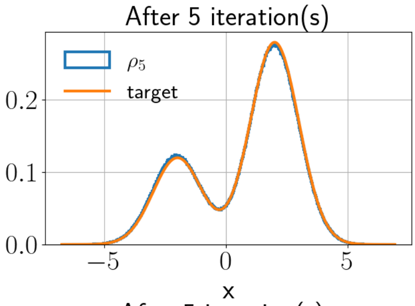
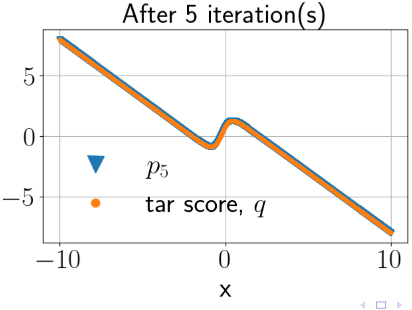
- Contraction mapping principle (Banach fixed point theorem) applied to

$$\mathcal{J}(v) = \mathcal{L}^{-1}(\mathcal{G}(q + \mathcal{L}v, \mathrm{Id} + v) - q),$$

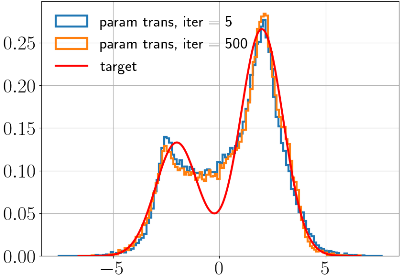
- Use elliptic regularity for proving continuity of derivative

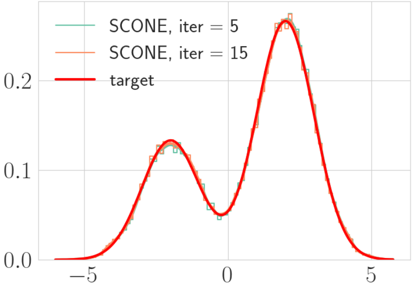
Numerical validation





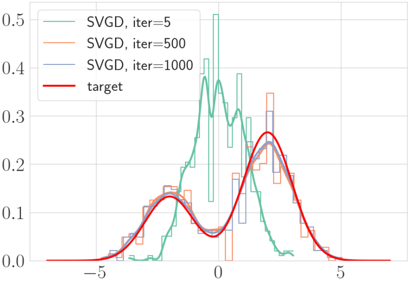
Comparison against parametric transport at the same computational cost

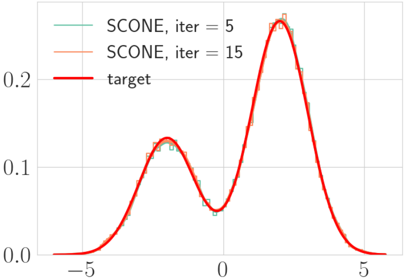




Left: Monotone transport [**Parno et al 2022**], up to 10th order Hermite polynomials, Number of parameters x Number of samples to approximate KL divergence = 11x(512*512/11). Right: SCONE with 512 grid points

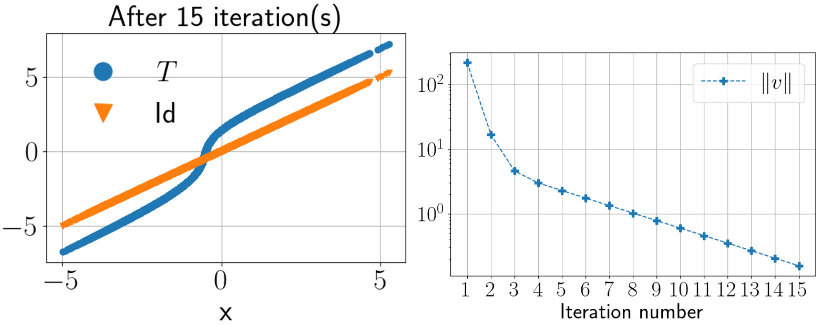
1D comparisons





Left: SVGD [**Liu and Wang 2016**] with 512 particles, RBF kernel, gradient descent with step size 0.01

Convergence of SCONE construction to the increasing rearrangement in 1D

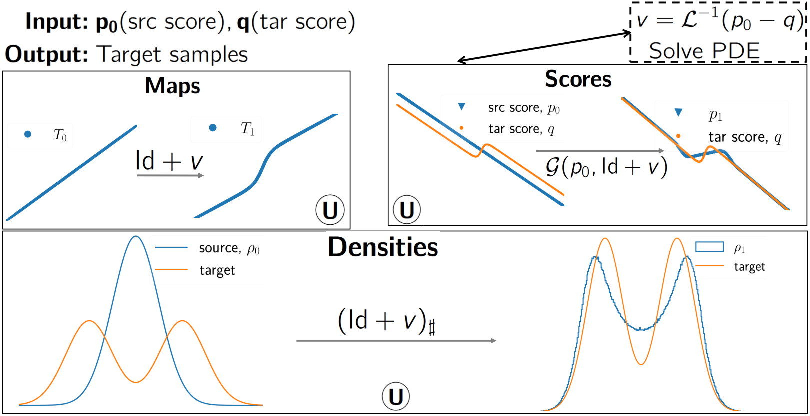


- Global dependence of v helps avoid mode collapse
- Tail behavior captured due to score matching

Score Operator Newton Transport

Input: $\mathbf{p_0}$(src score), $\mathbf{q}$(tar score)

Output: Target samples



Score Operator Newton construction: can be used for sampling, generative modeling, Bayesian inference and filtering in chaotic systems

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- Low-rank approximations of elliptic PDE solution?

C, Schäfer, Marzouk 2023 https://arxiv.org/abs/2305.09792

Learning chaotic dynamics from data

- Neural ODE [Chen et al 2018]:

$$\frac{d}{dt}\varphi_h^t(x) = h(\varphi_h^t(x)), \quad x \in \mathbb{R}^d. \tag{2}$$

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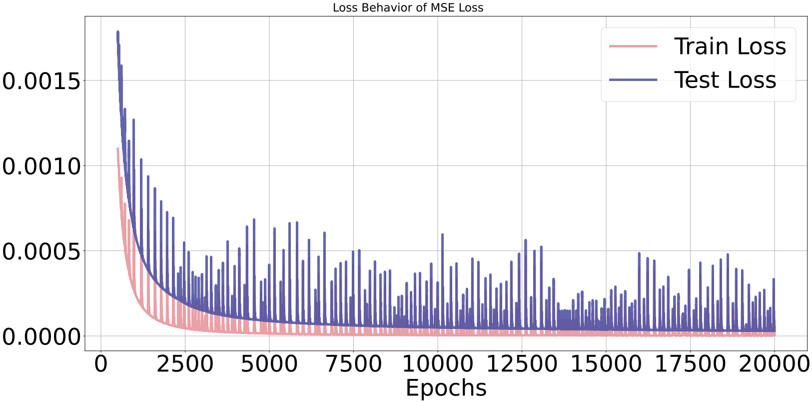
- Training and test errors (for one-step predictions) small, but does not generalize

Learning the Lorenz ’63 system



Good “generalization” performance. Three layer feed forward network trained with AdamW

Generalization => learning dynamics?

	Lyapunov Exponent
True LE	$\approx$ **[0.9, 0, -14.5]**
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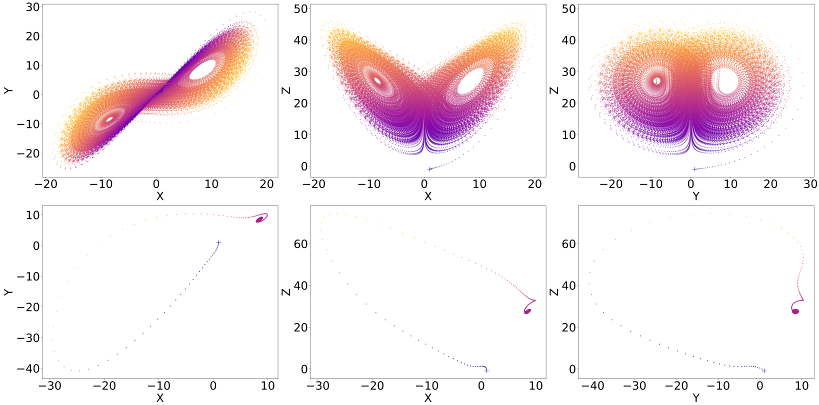

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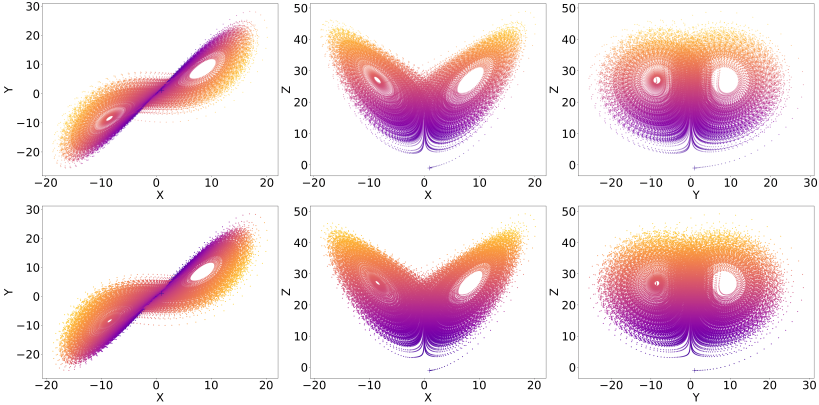
- With modified loss, statistical moments (correlations, LEs) are accurate

Learning out-of-attractor dynamics



Learning ergodic dynamics from data using Neural ODEs

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- How should generalization error be defined?
- Many more problems at the intersection of dynamics and learning theory!

Learning: Statistical stability implies generalization

C, Loukas, Gatmiry and Jegelka, NeurIPS 2022

Sampling: Score Operator Newton transport – root-finding principle for sampling

C, Schäfer and Marzouk, arxiv:2305.09792, 2023

Forecasting: context-dependent generalization analyses

Park and C, 2023