A dynamical systems view of learners, samplers and forecasters

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December 15, 2023
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- Potential consequences:
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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?

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

Non-converging optimization

(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:

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

where

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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 $\mu$ on $M$ is ergodic for the training dynamics if for all continuous functions $f : M \rightarrow \mathbb{R}$, and $\mu$-a.e. $w_0$,

$$\frac{1}{T} \sum_{t=0}^{T-1} f(w_t) \rightarrow \mathbb{E}_{w \sim \mu}[f(w)].$$
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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 $w_0$.

Orbits of four different initializations of a VGG16 training with SGD.
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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 $\beta$ 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 $\beta$ with error bars computed as sample mean. Test loss vs. time (epoch).
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Lower bound on $\beta$

Generalization error
Generalization of a non-converging algorithm

- Training error, $\hat{R}_S := (1/n) \sum_{z \in S} \langle \ell_z \rangle_S$

Theorem 1 (SAS implies generalization)
For an algorithm with SAS coefficient $\beta$ and large number of samples $n$, the generalization gap $R_S - \hat{R}_S = O(\beta \sqrt{n})$ with high probability.

Smaller $\beta \equiv$ more SAS $\Rightarrow$ better generalization.
Training error, $\hat{R}_S := (1/n) \sum_{z \in S} \langle \ell_z \rangle_S$

Test/generalization error, $R_S := \mathbb{E}_{z \sim \mathcal{D}} \langle \ell_z \rangle_S$.
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What makes an algorithm statistically stable?

Pointwise approach [Hardt et al 2016] toward algorithmic stability

\[ w_{t+1}^S - w_{t+1}^{S'} = w_t^S - w_t^{S'} - \eta(\hat{\nabla} L_S(w_t^S) - \hat{\nabla} L_{S'}(w_t^{S'})) \]

- Uninformative for SAS, which is a time-independent notion
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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
Theorem 2 (**Slower convergence of loss statistics implies larger $\beta$**) Let $\lambda$ be the slowest mixing rate of the transition operators on loss space. Then, the corresponding training algorithm with $n$ samples has SAS coefficient

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

where $L_D = \sup_w \text{Lip}(\nabla \ell(\cdot, w))$.
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- exploit perturbation theory of uniformly ergodic Markov chains (see e.g. [Mitraphanov 2005])
Predicting generalization gap from timeseries data

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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

Learning algorithms in which loss time-averages converge slower, e.g., correlations in the loss persist, are less SAS.
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SGD with constant step size of 0.01 on ResNet18 model trained on corrupted CIFAR10 dataset.

![Graph showing test loss autocorrelation and generalization gap over time for different noise levels.](image)
More long-term stability in the training algorithm leads to better generalization
Goal: Transport-based Bayesian Inference and Sampling
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Today: New transport construction.
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\textbf{score} of a probability distribution with density \( \rho := \nabla \log \rho \)
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Introduce a new transport map construction.
Sampling via measure transport

- Target measure: $\nu$ with density $\rho^\nu$.
- Tractable source measure $\mu$ with density $\rho^\mu$.
- $\text{supp}(\mu) = X$ and $\text{supp}(\nu) = Y$. 

A transport map $T: X \rightarrow Y$ is an invertible transformation such that $T^\# \mu = \nu$. 

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The score operator

Goal: new transport map that exploits availability of **scores**.
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Idea: Define an infinite-dimensional score matching problem

\[ \rho_{\nu} = \rho_{\mu} \circ T - 1 |\det \nabla T| \circ T - 1 \]

Pushforward operation on scores:

\[ G(s, U) = s(\nabla U) - 1 - \nabla \log |\det \nabla U| (\nabla U) - 1 \circ U - 1 = s(\nabla U) - 1 - \text{tr} \nabla^2 U (\nabla U) - 1 \circ U - 1, \]
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Change of variables/pushforward operation:

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Pushforward operation on scores:

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Some properties of $\mathcal{G}$

- $\mathcal{G}(s, \text{Id}) = s$
- $\mathcal{G}(s, U_2 \circ U_1) = \mathcal{G}(\mathcal{G}(s, U_1), U_2)$
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Infinite-dimensional score matching problem: Find $T$ such that

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

where,

- $p$: Source score $= \nabla \log \rho^\mu$
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- $q$: Target score = $\nabla \log \rho^\gamma$.

- Want to avoid parameterization
- Use Newton-type method
A zero of the score residual

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

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$$\mathcal{G}(p, T) = \mathcal{G}(q, \text{Id}) + D_1 \mathcal{G}(q, \text{Id})(p - q) + D_2 \mathcal{G}(q, \text{Id})(T - \text{Id}) + \Delta(p, T)$$
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$$\mathcal{L}(q) \nu := -D_2 \mathcal{G}(q, \text{Id}) \nu = \nabla q \nu + q \nabla \nu + \text{tr}(\nabla^2 \nu).$$
The zero of the score residual operator

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

\[(p - q) = \mathcal{L} \, v \] (1)

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**Newton**-type update:

\[T_{n+1} \leftarrow (\text{Id} + \nu_n) \circ T_n\]
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Score Operator Newton (SCONE) iteration for transport maps

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- Conceptually different from empirical, parametric score-matching [Koehler et al 2022].
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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.
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- Transport map implicitly obtained via particle paths

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- Optimize distance functional on probability measure space
- Find an optimal map in an ansatz space
- Triangular transport [Moselhy and Marzouk 2012], normalizing flows [Papamakarios et al. 2021], neural ODEs [Grathwohl et al. 2018]
- Gradient flow of appropriate distance functional
- Transport map implicitly obtained via particle paths
- [Jordan et al. 1998], [Wibisono 2018]

SCONE gives an iterative construction as the limit of a sequence of compositions. Based on finding zero of a score-residual operator.
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Existence of a $C^r$ transport and convergence of SCONE iteration

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

$$\mathcal{J}(\nu) = \mathcal{L}^{-1}(g(q + \mathcal{L}\nu, \text{Id + } \nu) - q),$$

- 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 $\nu$ helps avoid mode collapse
- Tail behavior captured due to score matching
Score Operator Newton Transport

**Input:** $p_0$ (src score), $q$ (tar score)

**Output:** Target samples

$\nu = \mathcal{L}^{-1}(p_0 - q)$

Solve PDE

Maps

- $T_0$
- $T_1$

$\text{Id} + \nu$

Scores

- src score, $p_0$
- tar score, $q$
- $p_1$

$\mathcal{G}(p_0, \text{Id} + \nu)$

Densities

- source, $\rho_0$
- target

$\left(\text{Id} + \nu\right)_\#$

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

▶ A deterministic nonparametric transport method derived with an operator root-finding principle.
Score Operator Newton construction: can be used for sampling, generative modeling, Bayesian inference and filtering in chaotic systems

- A deterministic nonparametric transport method derived with an operator root-finding principle.
- Convergence in Hölder norms using elliptic regularity

Next steps: nonparametric PDE solves e.g. particle vortex methods, smooth particle hydrodynamics, PINNs etc.

Low-rank approximations of elliptic PDE solution?

C, Schäfer, Marzouk 2023

https://arxiv.org/abs/2305.09792
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Learning chaotic dynamics from data

▶ Neural ODE [Chen et al 2018]:

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

▶ ERM problem to minimize loss of the form

$$\ell(x_0, h) = \| \varphi^{\delta t}_h(x_0) - x_\delta t \|^2_2$$

▶ Training and test errors (for one-step predictions) small, but does not generalize
Learning chaotic dynamics from data

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Learning the Lorenz ’63 system

Loss Behavior of MSE Loss

Train Loss
Test Loss

Good “generalization” performance. Three layer feed forward network trained with AdamW
Generalization => learning dynamics?

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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

▶ Can Neural ODEs learn statistics from timeseries data alone?
Learning ergodic dynamics from data using Neural ODEs

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Learning: Statistical stability implies generalization

C, Loukas, Gutmiry 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