OT-Flow: Fast and Accurate Continuous Normalizing Flows via Optimal Transport

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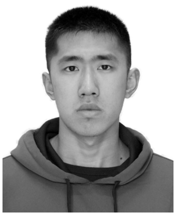

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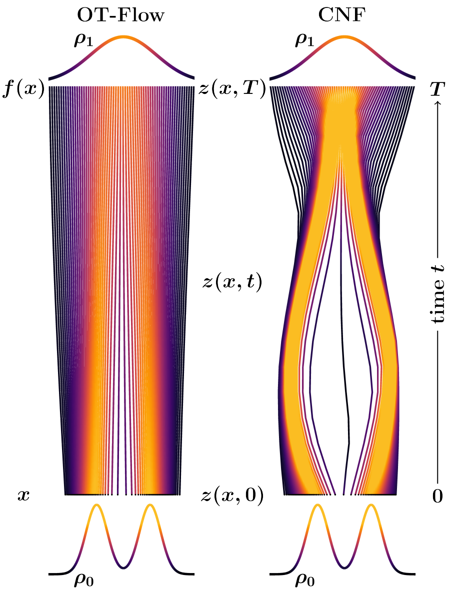
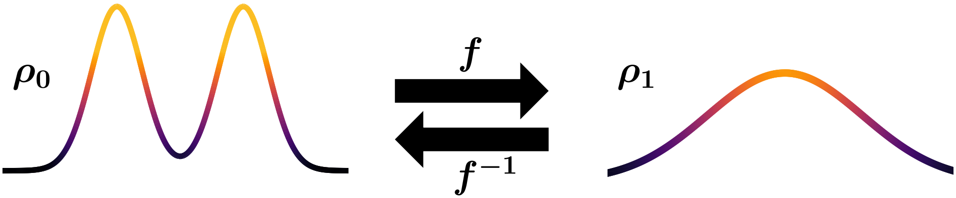
Overview

- **Background**
  - Normalizing Flows
  - Continuous Normalizing Flows
- **Mathematical Formulation**
  - Optimal Transport
  - Potential Function
  - Hamilton-Jacobi-Bellman (HJB) Regularizers
- **Numerical Implementation**
  - Efficient Exact Trace Computation
  - Discretize-then-Optimize
- **Results**
  - 8x training speed-up
  - 24x testing speed-up
- **Conclusion**



Normalizing Flows for Density Estimation

A normalizing flow[1,2] is an invertible mapping $f\colon \mathbb{R}^d \to \mathbb{R}^d$ between an arbitrary probability distribution and a standard normal distribution with respective densities ρ_0 and ρ_1



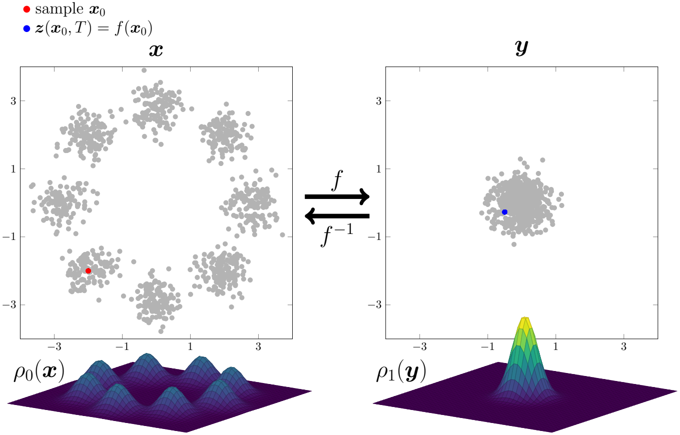
By the change of variables formula, the flow satisfies

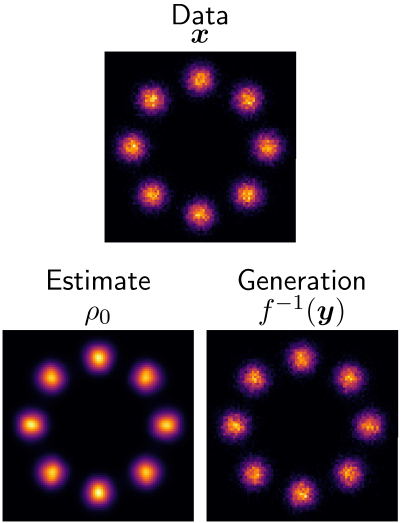
$$\log \rho_0(\boldsymbol{x}) = \log \rho_1(f(\boldsymbol{x})) + \log |\det \nabla f(\boldsymbol{x})| \quad \text{for all} \quad \boldsymbol{x} \in \mathbb{R}^d. \tag{1}$$

[1]Rezende and Mohamed. "Variational Inference with Normalizing Flows". 2015.
[2]Papamakarios et al. "Normalizing Flows for Probabilistic Modeling and Inference". 2019.

Two-Dimensional Example

Gaussian Mixture Problem





Continuous Normalizing Flows (CNFs)

Issue: log-determinants cost $\mathcal{O}(d^3)$ FLOPS in general
One Solution: replace the log-det with a trace computation for $\mathcal{O}(d^2)$ FLOPS in general

Using a neural ordinary differential equation (ODE)[3] leads to the CNF[4]

$$\partial_t \begin{bmatrix} \boldsymbol{z}(\boldsymbol{x},t) \\ \ell(\boldsymbol{x},t) \end{bmatrix} = \begin{bmatrix} \mathbf{v}\big(\boldsymbol{z}(\boldsymbol{x},t),t;\boldsymbol{\theta}\big) \\ \mathrm{tr}\left(\nabla \mathbf{v}(\boldsymbol{z}(\boldsymbol{x},t),t;\boldsymbol{\theta})\right) \end{bmatrix}, \quad \begin{bmatrix} \boldsymbol{z}(\boldsymbol{x},0) \\ \ell(\boldsymbol{x},0) \end{bmatrix} = \begin{bmatrix} \boldsymbol{x} \\ 0 \end{bmatrix}. \tag{2}$$

where

- $\boldsymbol{z}(\boldsymbol{x},t)$ are the features for initial state $\boldsymbol{x}$ at time $t \in [0,T]$
- $\mathbf{v}\colon \mathbb{R}^d \times [0,T] \to \mathbb{R}^d$ is a neural network layer with parameters $\boldsymbol{\theta}$
- $f(\boldsymbol{x}) = \boldsymbol{z}(\boldsymbol{x},T)$
- $\ell(\boldsymbol{x},T) \coloneqq \log \rho_0(\boldsymbol{x}) - \log \rho_1(f(\boldsymbol{x}))$

[3] Chen et al. "Neural Ordinary Differential Equations". 2018.
[4] Grathwohl et al. "FFJORD: Free-form Continuous Dynamics for Scalable Reversible . . . ". 2019.

CNF Optimization Problem

For expected negative log-likelihood[5,6]

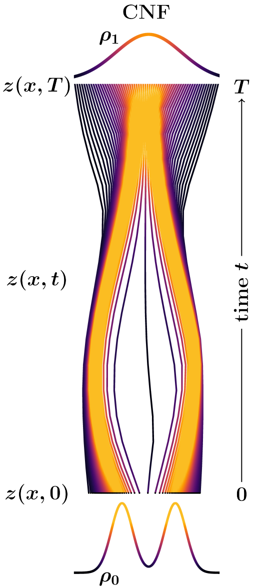
$$C(\boldsymbol{x},T) := \frac{1}{2}\|\boldsymbol{z}(\boldsymbol{x},T)\|^2 - \ell(\boldsymbol{x},T) + \frac{d}{2}\log(2\pi),$$

we optimize

$$\min_{\boldsymbol{\theta}} \quad \mathbb{E}_{\rho_0(\boldsymbol{x})} \{C(\boldsymbol{x},T)\}$$

subject to

$$\partial_t \begin{bmatrix} \boldsymbol{z}(\boldsymbol{x},t) \\ \ell(\boldsymbol{x},t) \end{bmatrix} = \begin{bmatrix} \mathbf{v}\big(\boldsymbol{z}(\boldsymbol{x},t),t;\boldsymbol{\theta}\big) \\ \operatorname{tr}\big(\nabla \mathbf{v}(\boldsymbol{z}(\boldsymbol{x},t),t;\boldsymbol{\theta})\big) \end{bmatrix}, \quad \begin{bmatrix} \boldsymbol{z}(\boldsymbol{x},0) \\ \ell(\boldsymbol{x},0) \end{bmatrix} = \begin{bmatrix} \boldsymbol{x} \\ 0 \end{bmatrix}.$$



[5] Rezende and Mohamed. "Variational Inference with Normalizing Flows". 2015.
[6] Papamakarios et al. "Normalizing Flows for Probabilistic Modeling and Inference". 2019.

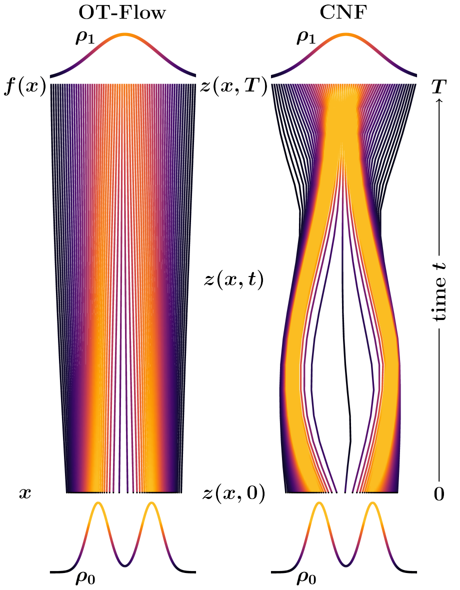
High Costs of CNFs

CNFs have high computation cost because

- Trajectories can be complicated leading to high number of function evaluations
- Expensive trace computation
  - State-of-the-art train with $\mathcal{O}(d)$ trace cost by using Hutchinson's trace estimator[7]

$$\mathrm{tr}(\nabla \mathbf{v}) = \mathop{\mathbb{E}}_{\phi(\epsilon)} \left\{ \epsilon^\top \, \nabla \mathbf{v} \, \epsilon \right\}$$

for noise vector ϵ w/ density $\phi(\epsilon)$, $\mathbb{E}\{\epsilon\} = 0$, $\mathrm{Cov}(\epsilon) = I$



[7] Hutchinson. "A Stochastic Estimator of the Trace of the Influence Matrix for . . . ". 1990.

Straight Trajectories

Include some optimal transport (OT)
$\Rightarrow$ model named OT-Flow

Arclength of the trajectories

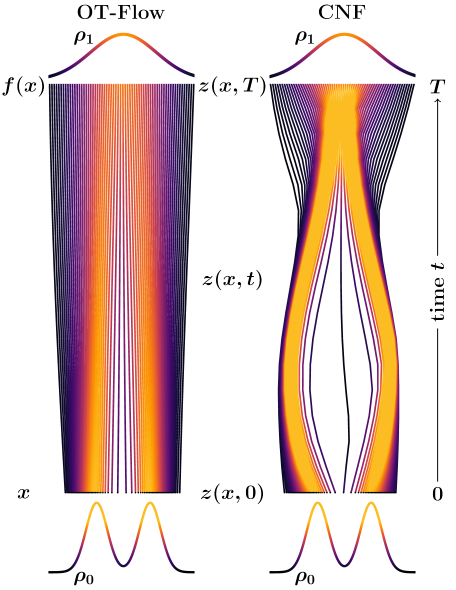
$$L(\boldsymbol{x},T) = \int_0^T \frac{1}{2} \|\mathbf{v}(\boldsymbol{z}(\boldsymbol{x},t),t;\boldsymbol{\theta})\|^2 \,\mathrm{d}t$$

We regularize the optimization problem

$$\min_{\boldsymbol{\theta}} \quad \mathop{\mathbb{E}}_{\rho_0(\boldsymbol{x})} \left\{ C(\boldsymbol{x},T) + L(\boldsymbol{x},T) \right\} \tag{3}$$

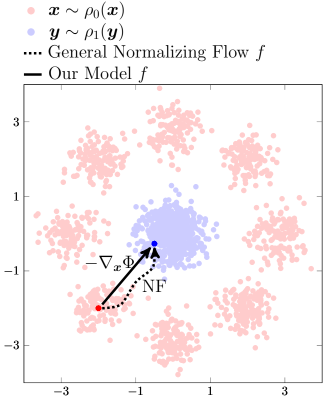
subject to (2).

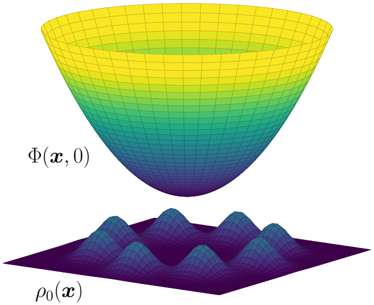
Now, a unique mapping exists.



Potential Function Φ

Apply the Pontryagin maximum principle[8] to (3)





There exists a scalar potential function $\Phi \colon \mathbb{R}^d \times [0, T] \to \mathbb{R}$ such that

$$\mathbf{v}(\boldsymbol{x}, t; \boldsymbol{\theta}) = -\nabla\Phi(\boldsymbol{x}, t; \boldsymbol{\theta}).$$

Analogous to classical physics, samples move in a manner to minimize their potential.

We parametrize potential Φ instead of $\mathbf{v}$.

[8]Pontryagin et al. *The Mathematical Theory of Optimal Processes*. 1962.

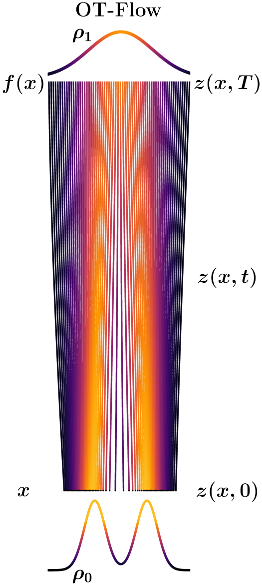
HJB Equations

The optimality conditions of (3) lead to another regularizer.

Potential Φ satisfies the Hamilton-Jacobi-Bellman (HJB) equations[9]

$$
\begin{aligned}
-\partial_t \Phi(\boldsymbol{z}(\boldsymbol{x},t),t) &= -\frac{1}{2}\|\nabla\Phi(\boldsymbol{z}(\boldsymbol{x},t),t)\|^2, \quad 0 < t < T \\
\Phi(\boldsymbol{z}(\boldsymbol{x},T),T) &= 1 + \log\left(\rho_0(\boldsymbol{x})\right) - \log\left(\rho_1(\boldsymbol{z}(\boldsymbol{x},T))\right) - \ell(\boldsymbol{x},T)
\end{aligned}
$$

Terminal condition $\Phi(\boldsymbol{z}(\boldsymbol{x},T),T)$ derives from the variational derivative of the Kullback-Leibler (KL) divergence



[9] Bellman. *Dynamic Programming*. 1957.

HJB Regularizer R

Penalize deviations from the HJB equation

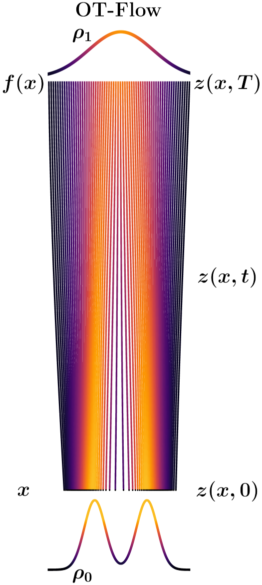
We add another regularizer, so the optimization problem is

$$\min_{\boldsymbol{\theta}} \mathop{\mathbb{E}}_{\rho_0(\boldsymbol{x})} \Big\{ C(\boldsymbol{x},T) + L(\boldsymbol{x},T) + R(\boldsymbol{x},T) \Big\}$$

subject to (2).

The HJB regularizer[10] is computed as

$$R(\boldsymbol{x},T) = \int_0^T \left| \partial_t \Phi(\boldsymbol{z}(\boldsymbol{x},t),t) - \frac{1}{2} \| \nabla \Phi(\boldsymbol{z}(\boldsymbol{x},t),t) \|^2 \right| \mathrm{d}t.$$



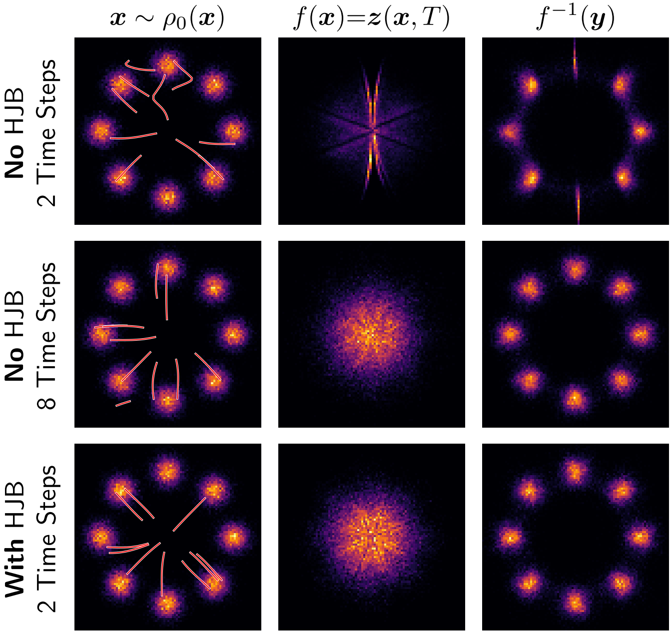
[10] Yang and Karniadakis. "Potential Flow Generator With L_2 Optimal Transport Regularity . . . ". 2020.

HJB Regularizer Effectiveness

Compare three models:

- No HJB regularizer with only 2 time steps
- No HJB regularizer with only 8 time steps
- Using HJB regularizer with only 2 time steps

HJB regularizer gives similar results to using many time steps



OT-Flow Formulation

We incorporate the time integration in the ODE solver.

$$\min_{\boldsymbol{\theta}} \quad \mathop{\mathbb{E}}_{\rho_0(\boldsymbol{x})} \left\{ C(\boldsymbol{x},T) + L(\boldsymbol{x},T) + R(\boldsymbol{x},T) \right\}$$

subject to

$$\partial_t \begin{pmatrix} \boldsymbol{z}(\boldsymbol{x},t) \\ \ell(\boldsymbol{x},t) \\ L(\boldsymbol{x},t) \\ R(\boldsymbol{x},t) \end{pmatrix} = \begin{pmatrix} -\nabla\Phi(\boldsymbol{z}(\boldsymbol{x},t),t;\boldsymbol{\theta}) \\ -\operatorname{tr}\left(\nabla^2\Phi(\boldsymbol{z}(\boldsymbol{x},t),t;\boldsymbol{\theta})\right) \\ \frac{1}{2}\|\nabla\Phi(\boldsymbol{z}(\boldsymbol{x},t),t;\boldsymbol{\theta})\|^2 \\ \left|\,\partial_t\Phi(\boldsymbol{z}(\boldsymbol{x},t),t;\boldsymbol{\theta}) - \frac{1}{2}\|\nabla\Phi(\boldsymbol{z}(\boldsymbol{x},t),t;\boldsymbol{\theta})\|^2\,\right| \end{pmatrix}$$

with initial conditions

$$\boldsymbol{z}(\boldsymbol{x},0) = \boldsymbol{x} \quad \text{and} \quad \ell(\boldsymbol{x},0) = L(\boldsymbol{x},0) = R(\boldsymbol{x},0) = 0$$

Trace Integration

Uniqueness of OT-Flow:

How we calculate $\ell(\boldsymbol{x}, T) = \int_0^T -\operatorname{tr}\left(\nabla^2 \Phi(\boldsymbol{z}(\boldsymbol{x}, t), t; \boldsymbol{\theta})\right) \mathrm{d}t$

OT-Flow:

- Trace
  - Exact Trace Computation
- Time Integration
  - Discretize-then-optimize (DTO)[11,12]

Comparatively, state-of-the-art:

- Trace (during training)
  - Hutchinson's Estimator
- Time Integration
  - Optimize-then-discretize (OTD)[11,12]

[11] Gholami, Keutzer, and Biros. "ANODE: Unconditionally Accurate Memory-Efficient Gradients for . . .". 2019.
[12] Onken and Ruthotto. "Discretize-Optimize vs. Optimize-Discretize for Time-Series . . .". 2020.

Improving the Trace Computation

Competitive in Time Complexity

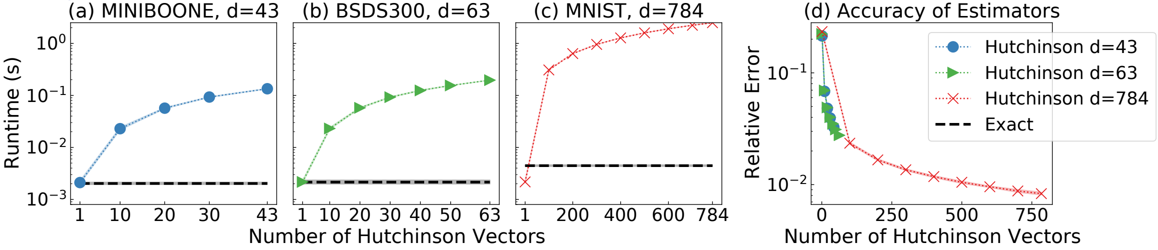
General Trace Computation: $\mathcal{O}(d^2)$ FLOPS

Trace Estimators: $\mathcal{O}(d)$ FLOPS

Our Exact Trace in OT-Flow $\mathcal{O}(d)$ FLOPS

$\Big\}$ assumes model's hidden dimension is fixed

Competitive in Runtime



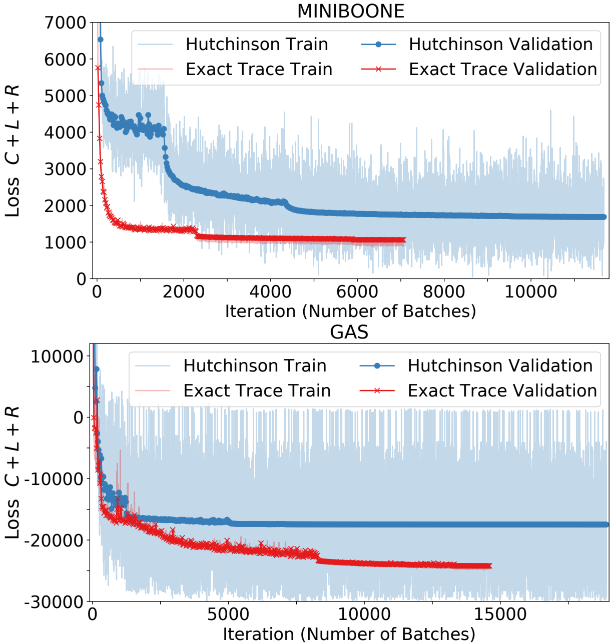
Improving the Trace Computation

Improved Convergence

Exact Trace ⇒ Improved Convergence

Compare OT-Flow (using exact trace) against a replicate model using Hutchinson's trace estimator

OT-Flow converges
1) in fewer iterations
2) with less training variance



Exact Trace Computation

Our model

Neural Network

$$\Phi(\boldsymbol{s};\boldsymbol{\theta}) = \boldsymbol{w}^\top N(\boldsymbol{s};\boldsymbol{\theta}_N) + \frac{1}{2}\boldsymbol{s}^\top(\boldsymbol{A}^\top\boldsymbol{A})\boldsymbol{s} + \boldsymbol{b}^\top\boldsymbol{s} + c,$$

$$\text{where} \quad \boldsymbol{\theta} = (\boldsymbol{w}, \boldsymbol{\theta}_N, \boldsymbol{A}, \boldsymbol{b}, c)$$

Gradient

$$\nabla_{\boldsymbol{s}}\Phi(\boldsymbol{s};\boldsymbol{\theta}) = \nabla_{\boldsymbol{s}}N(\boldsymbol{s};\boldsymbol{\theta}_N)\boldsymbol{w} + (\boldsymbol{A}^\top\boldsymbol{A})\boldsymbol{s} + \boldsymbol{b}$$

where

- space-time inputs $\boldsymbol{s} = (\boldsymbol{x}, t) \in \mathbb{R}^{d+1}$
- neural network $N(\boldsymbol{s};\boldsymbol{\theta}_N)\colon \mathbb{R}^{d+1} \to \mathbb{R}^m$ (we choose ResNet)
- $\boldsymbol{\theta}$ consists of all the trainable weights:
  $\boldsymbol{w} \in \mathbb{R}^m$, $\boldsymbol{\theta}_N \in \mathbb{R}^p$, $\boldsymbol{A} \in \mathbb{R}^{r\times(d+1)}$, $\boldsymbol{b} \in \mathbb{R}^{d+1}$, $c \in \mathbb{R}$ where $r = \min(10, d)$

Exact Trace Computation

Analytic Gradient and Trace Computation

N is an $(M+1)$-layer ResNet

Forward propagation

Compute $N(\boldsymbol{s};\boldsymbol{\theta}_N) = \boldsymbol{u}_M$.

$$\begin{aligned}
\boldsymbol{u}_0 &= \sigma(\boldsymbol{K}_0\boldsymbol{s} + \boldsymbol{b}_0) \\
\boldsymbol{u}_1 &= \boldsymbol{u}_0 + h\sigma(\boldsymbol{K}_1\boldsymbol{u}_0 + \boldsymbol{b}_1) \\
&\vdots \qquad\qquad \vdots \\
\boldsymbol{u}_M &= \boldsymbol{u}_{M-1} + h\sigma(\boldsymbol{K}_M\boldsymbol{u}_{M-1} + \boldsymbol{b}_M)
\end{aligned}$$

where

- fixed step size $h > 0$
- ResNet weights $\boldsymbol{\theta}_N$ are
  - $\boldsymbol{K}_0 \in \mathbb{R}^{m\times(d+1)}$
  - $\boldsymbol{K}_1, \ldots, \boldsymbol{K}_M \in \mathbb{R}^{m\times m}$
  - $\boldsymbol{b}_0, \ldots, \boldsymbol{b}_M \in \mathbb{R}^m$
- $\sigma(\boldsymbol{x}) = \log(\exp(\boldsymbol{x}) + \exp(-\boldsymbol{x}))$
  - the antiderivative of hyperbolic tangent
  - so, $\sigma'(\boldsymbol{x}) = \tanh(\boldsymbol{x})$

Exact Trace Computation

Analytic Gradient Computation

N is an $(M+1)$-layer ResNet

Forward propagation

Compute $N(\boldsymbol{s};\boldsymbol{\theta}_N) = \boldsymbol{u}_M$.

$$\begin{aligned} \boldsymbol{u}_0 &= \sigma(\boldsymbol{K}_0 \boldsymbol{s} + \boldsymbol{b}_0) \\ \boldsymbol{u}_1 &= \boldsymbol{u}_0 + h\sigma(\boldsymbol{K}_1 \boldsymbol{u}_0 + \boldsymbol{b}_1) \\ \vdots \quad & \quad \quad \vdots \\ \boldsymbol{u}_M &= \boldsymbol{u}_{M-1} + h\sigma(\boldsymbol{K}_M \boldsymbol{u}_{M-1} + \boldsymbol{b}_M) \end{aligned}$$

Backpropagation (chain rule)

Compute $\nabla_{\boldsymbol{s}} N(\boldsymbol{s};\boldsymbol{\theta}_N)\boldsymbol{w} = \boldsymbol{z}_0$ analytically

Laplacian

Compute

$$\operatorname{tr}\left(\nabla^2 \Phi(\boldsymbol{s};\boldsymbol{\theta})\right) = \operatorname{tr}\left(\boldsymbol{E}^\top \left(\nabla_{\boldsymbol{s}}^2 (N(\boldsymbol{s};\boldsymbol{\theta}_N)\boldsymbol{w}) + \boldsymbol{A}^\top \boldsymbol{A}\right) \boldsymbol{E}\right)$$
$$\text{for} \quad \boldsymbol{E} = \texttt{eye(d+1,d)}$$

with cost $\mathcal{O}(m^2 \cdot d)$ **FLOPS**.

(details in paper)

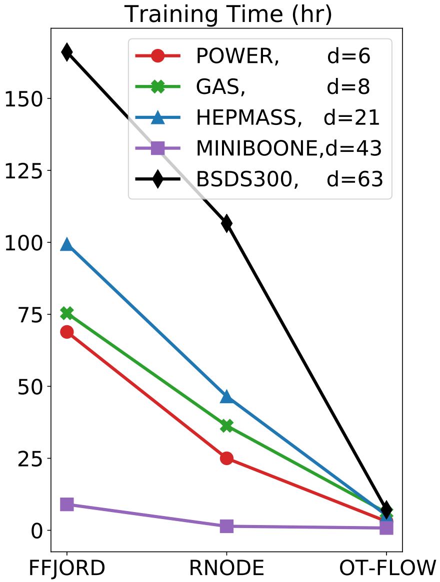
Other OT approaches in CNFs

Model	Formulation					Training Implementation			Inference
	ODEs (2)	Φ	L	R	$\|\nabla \mathbf{v}\|_F^2$	Solver	DTO/OTD	Trace	Trace
FFJORD[13]	✓	✗	✗	✗	✗	RK(4)5	OTD	Hutch w/ Rad	AD exact
RNODE[14]	✓	✗	✓	✗	✓	RK 4	OTD	Hutch w/ Rad	AD exact
M-A Flows[15]	✓	✓	✗	✗	✗	RK 4	DTO	Hutch w/ Gauss	
PFGs[16]	✓	✓	✗	✓	✗	RK 1	DTO	AD exact	
OT-Flow	✓	✓	✓	✓	✗	RK 4	DTO	efficient exact	

RK: Runge-Kutta, OTD: optimize-then-discretize, DTO: discretize-then-optimize, AD: automatic differentiation, Hutch: Hutchinson's trace estimator where ϵ from Rademacher or Gaussian distribution

[13] Grathwohl et al. "FFJORD: Free-form Continuous Dynamics for Scalable Reversible . . . ". 2019.
[14] Finlay et al. "How to Train your Neural ODE: the World of Jacobian and Kinetic Regularization". 2020.
[15] Zhang and Wang. "Monge-Ampére Flow for Generative Modeling". 2018.
[16] Yang and Karniadakis. "Potential Flow Generator With L_2 Optimal Transport Regularity . . . ". 2020.

Fast Training

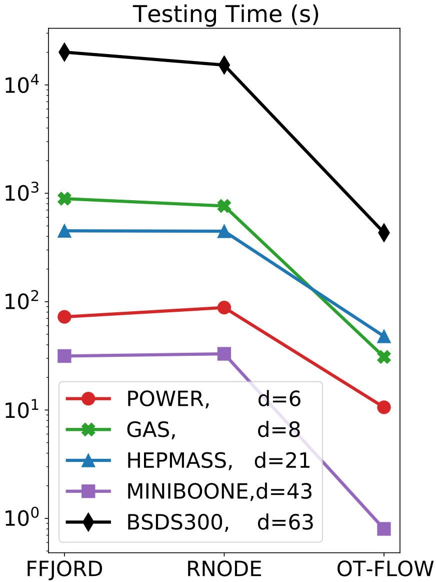


OT-Flow has 8x training speed-up on average

Reasons

- OT-inspired regularization leads to straight trajectories that are inexpensive to integrate.
- Exact trace computation
  - Competitive in time
  - Better in convergence
- The potential flows approach results in fewer weights and a smaller model.

Fast Inference

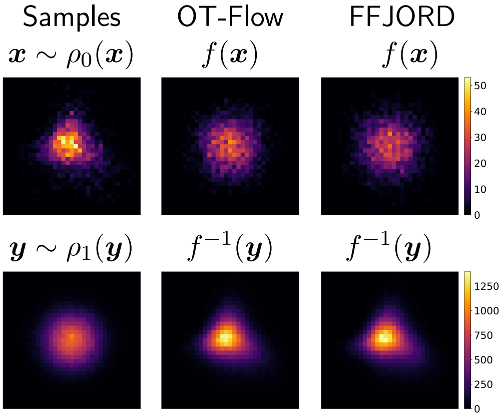


OT-Flow has 24x testing speed-up on average

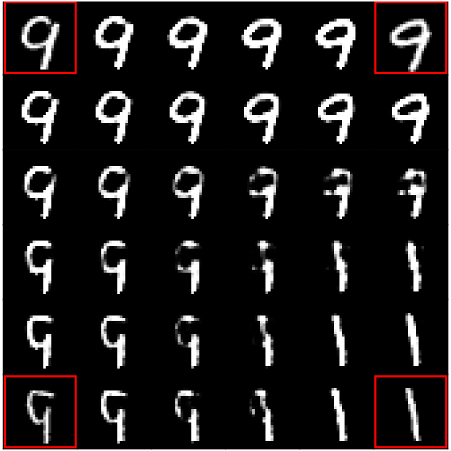
Reasons

- Inference uses exact trace (no estimates)
  - State-of-the-art approaches use AD to obtain exact trace with $\mathcal{O}(d^2)$
  - Meanwhile, our exact trace is $\mathcal{O}(d)$

More Results



Two of the 43 dimensions in the MINIBOONE CNF



MNIST synthetic generation. Original images boxed in red.

Conclusions

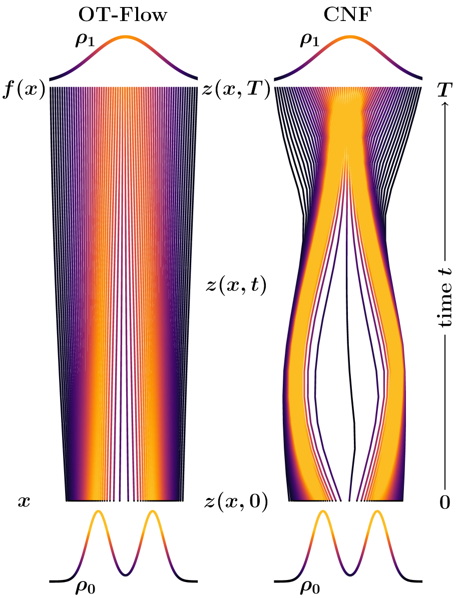
Formulation

- CNF + OT $\Rightarrow$ well-posed
- HJB regularizer reduces training costs

Implementation

- Discretize-then-optimize + Runge-Kutta 4
  $\Rightarrow$ efficient ODE solve
- Efficient exact trace improves CNF training

Public Code
github.com/EmoryMLIP/OT-Flow



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