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

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Motivation

Continuous Normalizing Flows (CNFs)

A normalizing flow [1] is an invertible mapping $f\colon \mathbb{R}^d \to \mathbb{R}^d$ between an arbitrary probability distribution and a standard normal distribution whose densities we denote by ρ_0 and ρ_1, respectively.

By change of variables,

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

In CNFs, f solves the neural ordinary differential equation (ODE) [2, 3]

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

where, for artificial time $t \in [0,T]$,

- $\boldsymbol{x}$ maps to $f(\boldsymbol{x}) = \boldsymbol{z}(\boldsymbol{x},T)$ following trajectory $\boldsymbol{z}\colon \mathbb{R}^d \times [0,T] \to \mathbb{R}^d$
- $\mathbf{v}\colon \mathbb{R}^d \times [0,T] \to \mathbb{R}^d$ is a neural network layer parameterized by $\boldsymbol{\theta}$
- $\ell(\boldsymbol{x},T) = \log\det \nabla f(\boldsymbol{x})$, derived from Jacobi's Formula [2]

Microscale: an arbitrary sample $\boldsymbol{x}$ maps to a normally distributed $f(\boldsymbol{x})$
Macroscale: ρ_0 maps to ρ_1

CNFs are trained by solving the optimization problem [1, 3]

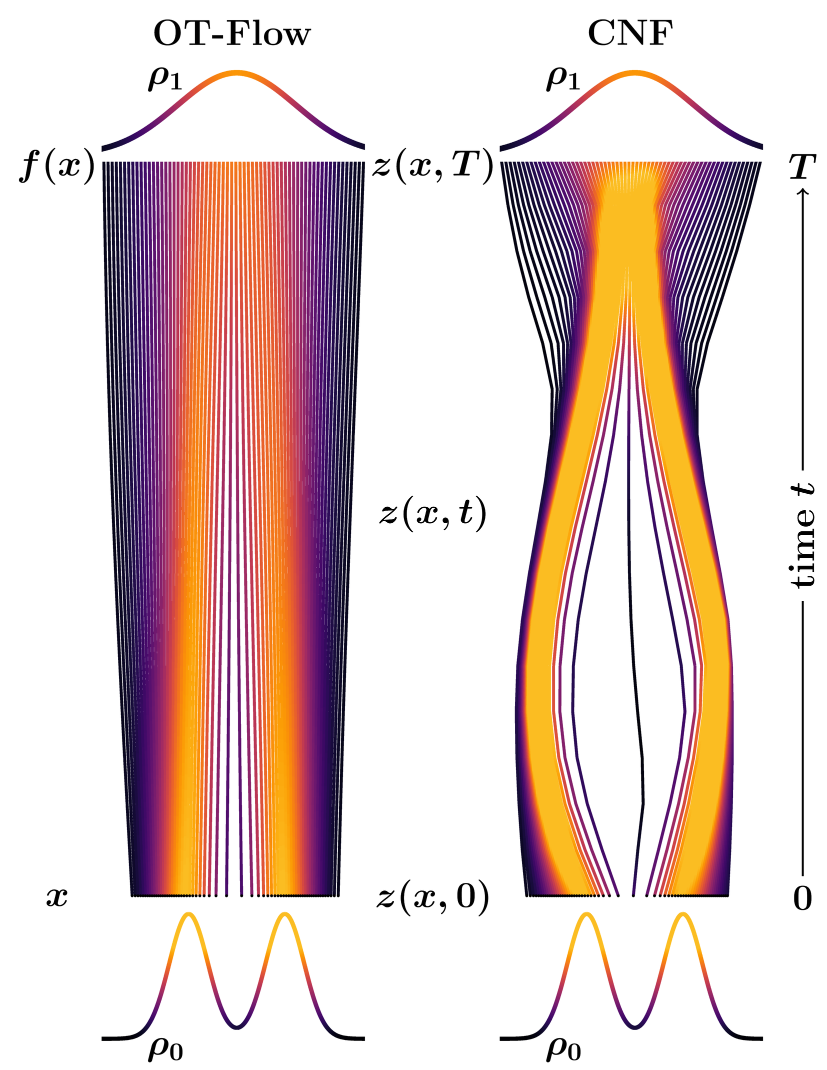


Figure 1: While a CNF can have curved trajectories, OT-Flow's are straight (modification of Fig. 1 in [3, 4]).

$$\min_{\boldsymbol{\theta}} \; \mathbb{E}_{\rho_0(\boldsymbol{x})} \left\{ C(\boldsymbol{x},T) := \frac{1}{2}\|\boldsymbol{z}(\boldsymbol{x},T)\|^2 - \ell(\boldsymbol{x},T) + \frac{d}{2}\log(2\pi) \right\} \quad \text{s.t.} \quad (2). \qquad (3)$$

High Training Costs

- Many functions evaluations are needed to solve (2)
- Computing the trace with automatic differentiation (AD) requires vector-Jacobian products with all d standard basis vectors, costing $\mathcal{O}(d^2)$ FLOPs total

Our Contributions

Optimal Transport (OT) Incorporating OT, we regularize the CNF so it has a unique solution (Figure 1).

Analytic Exact Trace We derive formulae for an exact trace computation with complexity $\mathcal{O}(d)$ FLOPs.

Optimal Transport

L_2 Transport Costs Add transport costs

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

to (3) to penalize the arc-length of the trajectories.

Potential Function By the Pontryagin maximum principle [5], there exists a scalar potential function $\Phi\colon \mathbb{R}^d \times [0,T] \to \mathbb{R}$ such that

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

Idea: Analogous to classical physics, samples move to minimize their potential
$\Rightarrow$ We parameterize potential Φ instead of $\mathbf{v}$.

HJB Regularizer At optimality, Φ satisfies the Hamilton-Jacobi-Bellman (HJB) equation [6]

$$-\partial_t\Phi(\boldsymbol{x},t) = -\frac{1}{2}\|\nabla\Phi(\boldsymbol{z}(\boldsymbol{x},t),t)\|^2,$$

$$\Phi(\boldsymbol{x},T) = 1 + \log\left(\rho_0(\boldsymbol{x})\right) - \log\left(\rho_1(\boldsymbol{z}(\boldsymbol{x},T))\right) - \ell(\boldsymbol{x},T)$$

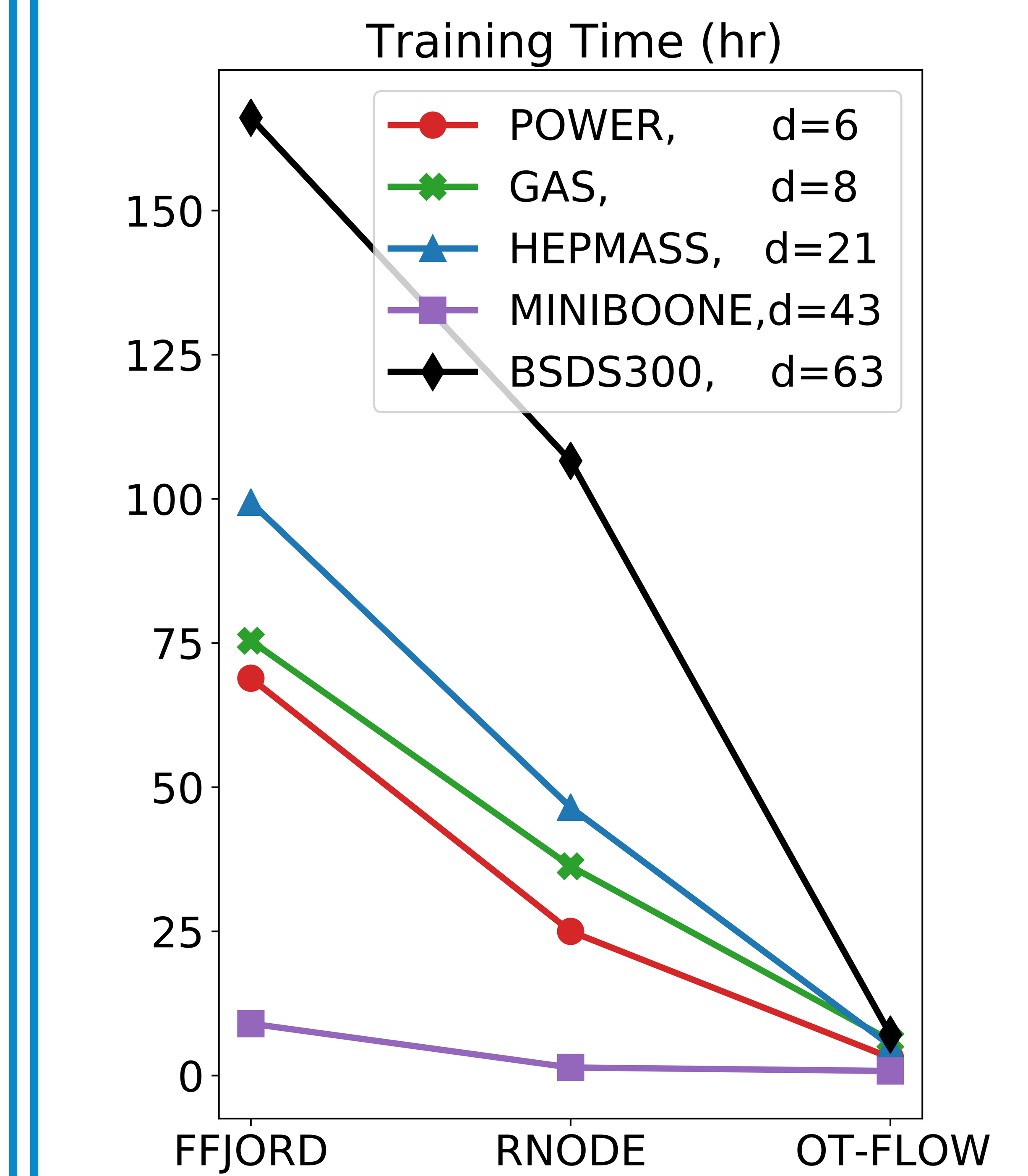
To penalize sub-optimality, use HJB regularizer

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

OT-Flow Optimization Problem

$$\min_{\boldsymbol{\theta}} \; \mathbb{E}_{\rho_0(\boldsymbol{x})} \left\{ C(\boldsymbol{x},T) + L(\boldsymbol{x},T) + R(\boldsymbol{x},T) \right\} \text{ s.t. } (2)$$

Results



8x speedup in training and 24x speedup in inference relative to the state-of-the-art RNODE [4] on five real datasets of dimensionality $d = 6, 8, 21, 43, 63$

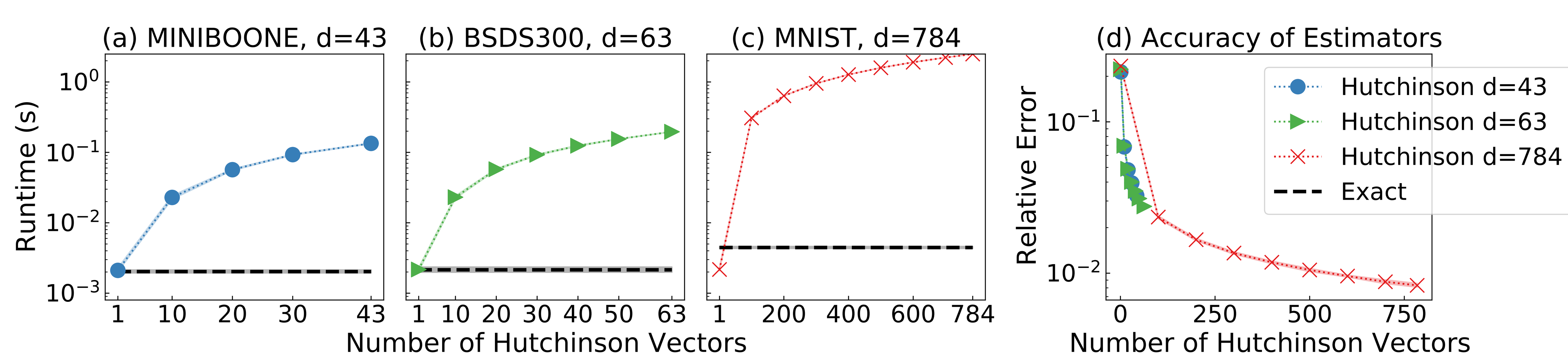
Exact Trace

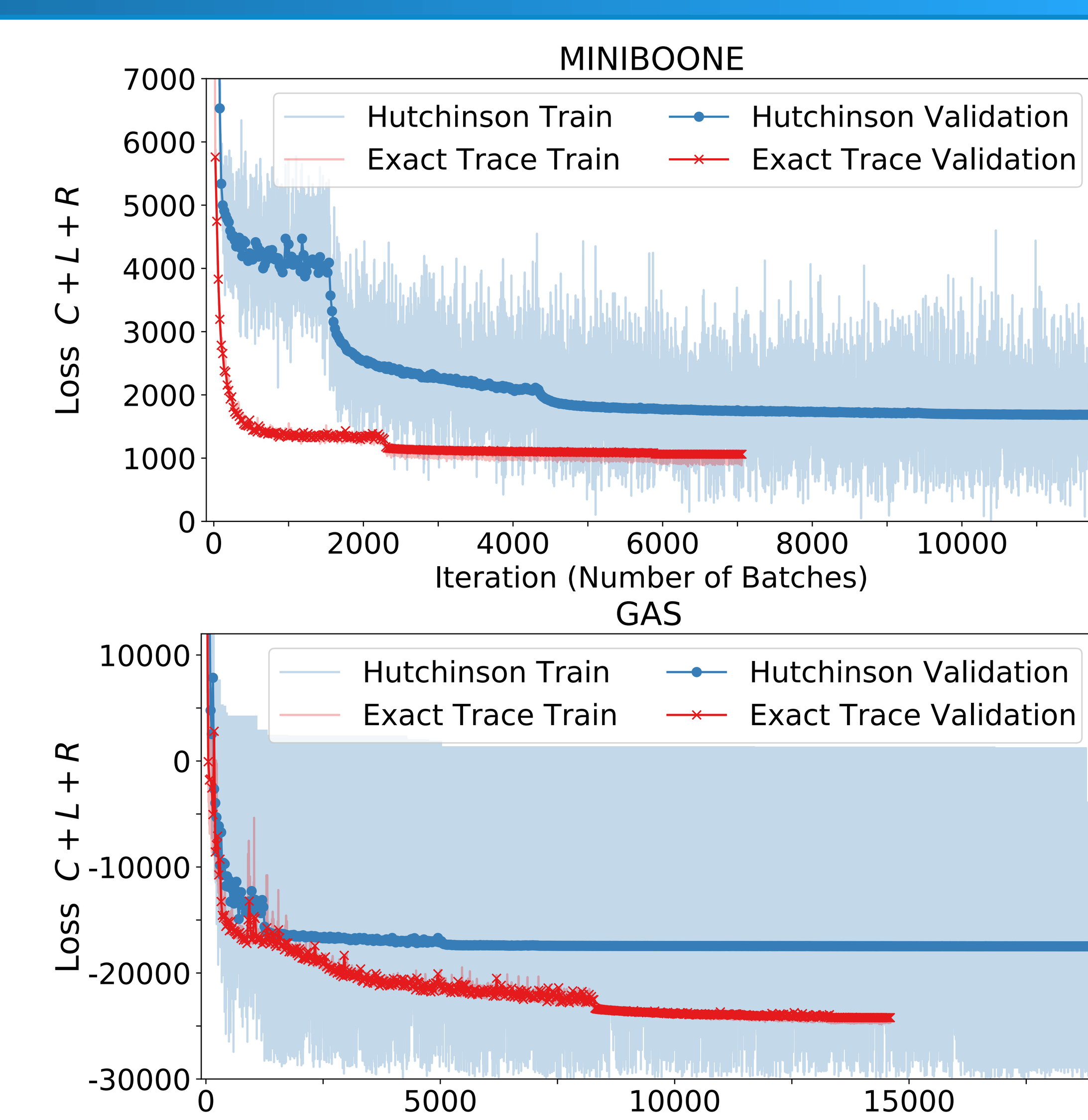
We devise an efficient analytic method for computing the trace by exploiting

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

In runtime, the exact trace is competitive with estimators used in other CNFs.

In convergence, the exact trace during training achieves 1) quicker validation convergence than using an estimator and 2) less variance in training loss than using an estimator





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Code

github.com/EmoryMLIP/OT-Flow