Data Analytics and Machine Learning Group
Department of Informatics
Technical University of Munich

Neural Flows: Efficient Alternative to Neural ODEs

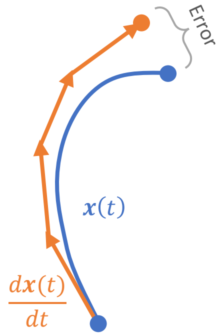
Marin Biloš[1], Johanna Sommer[1], Syama Sundar Rangapuram[2], Tim Januschowski[2] and Stephan Günnemann[1]
[1]Technical University of Munich, [2]AWS AI Labs, Germany

TL;DR

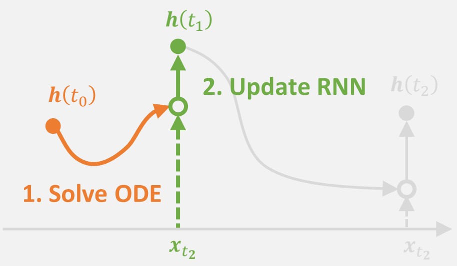
- We **directly model** the neural ODE **solutions** with neural flows
- This is **much faster**, since we avoid using expensive numerical solvers
- We achieve **better results** on time series and density estimation applications

Neural ordinary differential equations

- Describe the instantaneous change in the system $dx(t)/dt = f(t, x(t))$, f is a neural network
- Given initial condition $x(t_0)$, want to evaluate the solution curve $x(t)$ – usually solved numerically
- Trade-off between speed and precision

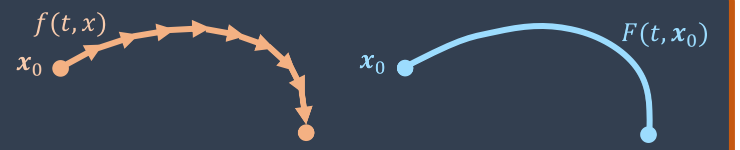


Example: Irregular time series



Neural flows

- Model the solution curve directly!
- Function $F(t, x_0)$ is the solution to some ODE with the initial condition x_0 iff:
  1. $F(0, x_0) = x_0$ (initial condition)
  2. $F(t, \cdot)$ is invertible, $\forall t$ (unique solution)




```
# ODE: multiple steps
f = NeuralNetwork()
y = SolveODE(f, t, x)
```

```
# Flow: single pass
F = NeuralNetwork()
y = F(t, x)
```

Implementation

- Neural networks need to satisfy conditions *1.* and *2.*
- Models: **ResNet flow, GRU flow, coupling flow**

```
# ResNet flow
F(t, x) = x + phi(t) * g(t, x)
spectral_norm(g) # Lip(g) < 1
```

```
# Coupling flow
F(t, xa) = xa * u(t, xb) + v(t, xb)
```

Irregularly-sampled time series

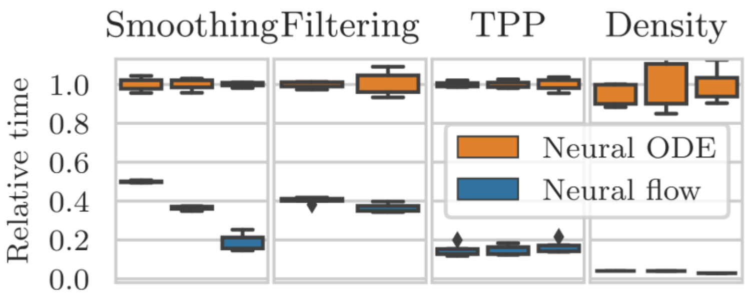
- Previous works: evolve the RNN state in between observations with neural ODE – we use neural flows
- Experiments: smoothing, filtering, temporal point process
- **Neural flows outperform neural ODEs** across different experimental setups at a fraction of the computation cost

Density estimation in continuous time

- Density changes with time, e.g. modeling spatial data
- Previous works: continuous normalizing flow (ODE-based)
- We use coupling flow that provides closed-form density
- **Coupling flow outperforms CNF** on spatio-temporal data

Speed comparison

- How much time it takes to run one training epoch?
- With similar number of parameters (same hyperparam)



Thirty-fifth Conference on Neural Information Processing Systems (2021)

www.daml.in.tum.de/neural-flows