Abstract

Continuous–depth learning has recently emerged as a novel perspective on deep learning, improving performance in tasks related to dynamical systems and density estimation. Core to these approaches is the neural differential equation, whose forward passes are the solutions of an initial value problem parametrized by a neural network. Unlocking the full potential of continuous–depth models requires a different set of software tools, due to peculiar differences compared to standard discrete neural networks, e.g inference must be carried out via numerical solvers. We introduce TorchDyn, a PyTorch library dedicated to continuous–depth learning, designed to elevate neural differential equations to be as accessible as regular plug–and–play deep learning primitives. This objective is achieved by identifying and subdividing different variants into common essential components, which can be combined and freely repurposed to obtain complex compositional architectures. TorchDyn further offers step–by–step tutorials and benchmarks designed to guide researchers and contributors.

Keywords: continuous–depth learning, neural differential equations, dynamical systems.

1. Introduction

With foundational work now decades old (Cohen and Grossberg, 1983; Hopfield, 1984; Le-Cun et al., 1988; Zhang et al., 2014), the blend of differential equations, deep learning and dynamical systems has been rekindled by recent works on a novel computational primitive: neural differential equations (Chen et al., 2018). Often referred to as continuous–depth learning, this new paradigm has shown promise across a plethora of different machine learning tasks, such as density estimation (Chen et al., 2018; Grathwohl et al., 2018), forecasting (Rubanova et al., 2019; Poli et al., 2019; Portwood et al., 2019), time series classification (Kidger et al., 2020), image segmentation (Pinckaers and Litjens, 2019).

Continuous–depth models rely on additional machinery and supporting modules not present in standard deep learning libraries. Indeed, inspecting modern software implementations of state–of–the–art variants in the literature of neural differential equations reveals a pro-
hibitive amount of boilerplate code, with convoluted inheritance chains. As a result, advances in the field are hindered to be both slower and less reproducible, leading to longer onboarding times for researchers and practitioners interested in deploying neural differential equations in and outside academia. TorchDyn aims at filling these gaps, by providing a fully–featured library for continuous–depth models. Through TorchDyn neural differential equations and derivative models, e.g (Greydanus et al., 2019; Toth et al., 2019; Massaroli et al., 2020b; Lutter et al., 2019; Cranmer et al., 2020; Massaroli et al., 2020a; Li et al., 2020), including yet–to–be–published combinations, can effortlessly be obtained by ad hoc primitives in combination with the rich PyTorch (Paszke et al., 2019) ecosystem.

2. The TorchDyn Library

Design philosophy The main objective of TorchDyn is to offer a complete, intuitive access–point to the continuous–depth framework, which can be interfaced with PyTorch to obtain architectures going beyond modern literature on the topic. We follow core design ideals driving the success of modern deep learning frameworks such as PyTorch: namely, modular, object–oriented, and with a focus on GPUs and batched operations.

Software dependencies TorchDyn is embedded in Python and is built to be compatible with PyTorch, relying on a select number of supporting libraries. We utilize torchdiffeq (Chen et al., 2018) and torchsde (Li et al., 2020), along with recent learning–based approaches (Poli et al., 2020) as a source of numerical methods for differential equations, augmented by PyTorch–Lightning (Falcon et al., 2019) for logging and training loops. We note that TorchDyn is fully-functional without PyTorch–Lightning, included to improve quality of life and reduce boilerplate for practitioners who do not wish to work at a higher level of abstraction that native PyTorch.

3. The Elements of TorchDyn

We detail the core elements of the library highlighted in Figure 1 via specific examples.

NeuralDE and DEFunc At the core of TorchDyn lie the NeuralDE and DEFunc classes. NeuralDEs represent the primary model class which can interacted with in usual PyTorch fashion. Internally, DEFunc perform auxiliary operations required to preserve compatibility across NeuralDE variants, such as higher–order dynamics or handling additional dimensions for integral cost functions.

Utilities and depth–variance Neural differential equations can be defined to have parameters either fixed or varying in depth. This is achieved in a different way than regular

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1. An example is the original FFJORD (Grathwohl et al., 2018), where long inheritance chains are present due to intertwining of model details and boilerplate classes. TorchDyn preserves modularity by disentangling these factors, significantly simplifying extensions or modifications to the original model.
discrete neural networks, which store a separate parameter tensor for each layer and index them with the appropriate layer index. This methodology would be impossible for continuous models as the depth–variable indexing the parameters takes real values, and as such leads to an infinite number of layers and thus parameters. There exist several strategies to sidestep this issue; approximating depth–variance by concatenating to the state, usually achieved by defining modified torch.nn.Module, or utilizing spectral or depth discretizations (Massaroli et al., 2020b). TorchDyn includes dedicated layers for depth–variance: DepthCat and GalLinear, GalConv2d, which eliminate the need of defining additional modules to achieve the desired effect.

**Energy models** There exists a whole line of work of physics–inspired Neural ODE variants such as Hamiltonian Neural Networks (Greydanus et al., 2019), Lagrangian Neural Networks (Lutter et al., 2019; Cranmer et al., 2020) or general energy–based models (Massaroli et al., 2020a). TorchDyn fully supports these models by dedicated wrappers for any torch.nn.Modules parametrizing the Energy/Hamiltonian/Lagrangian function. These wrappers are further preserved to be compatible with other modules by DEFuncs, allowing several combinations as shown in Figure 4.

**Continuous normalizing flows** An additional fundamental member of the continuous–depth framework, continuous normalizing flows (CNFs) (Chen et al., 2018; Grathwohl et al., 2018) are treated as first–class primitives. Notably, this allows for an out–of–the–box definition of Hamiltonian CNFs (Toth et al., 2019) and other unpublished variants.

**Adjoint and integral losses** TorchDyn implements a complete sensitivity toolset for Neural ODEs. This includes standard back–propagation through the ODE solver (O(\(\tilde{S}\)) memory efficiency\(^2\)) and adjoint–based gradients (O(1) memory efficiency). Compared to torchdiffeq’s adjoint method, TorchDyn offers the capability to compute gradients of integral\(^3\) loss functions which are gaining increasing popularity in the Neural ODEs research community (Massaroli et al., 2020a; Finlay et al., 2020).

### 3.1 Tutorials and documentation

The continuous–depth framework requires a set of background theoretical developments less familiar to deep learning specialists. TorchDyn offers a series of step–by–step, tutorial notebooks guiding new users and contributors. Some examples include a complete cookbook for neural ordinary differential equation variants, and tutorials for Hamiltonian Neural Networks (Greydanus et al., 2019), FFJORD (Grathwohl et al., 2018), Neural Graph Ordinary Differential Equations (Poli et al., 2019) and more.

### 4. Related Software

To the best knowledge of the authors, TorchDyn represents the first Python–based library entirely dedicated to continuous–depth models and utilities. TorchDyn builds upon

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2. \(\tilde{S}\) represents the number of integration step of the numerical solver.

3. Integral loss functions are defined on the whole depth domain, e.g. \(\ell := \int_\mathbf{S} l(\theta, \mathbf{z}(\tau), \tau)d\tau\). See (Massaroli et al., 2020b) for further details on the derivation of the adjoint method for this type of losses.
```python
from torchdyn import *
import torch.nn as nn

# vector field parametrized by a NN
f = nn.Sequential(DepthCat(1),
nn.Linear(3, 64),
nn.Tanh(),
nn.Linear(64, 2))

model = NeuralODE(f,
sensitivity='adjoint',
solver='dopri5')

x = torch.rand(128, 2)
print(model(x).shape)
>> torch.Size([128, 2])

x = torch.rand(128, 2)
s_span = torch.linspace(0, 2, 50)
print(model.trajectory(x, s_span).shape)
>> torch.Size([50, 128, 2])

print(model)
```

**Figure 2:** Examples of the flexible NeuralDE API, compatible with PyTorch. The Neural ODE can instance can be passed tensor data directly, implicitly utilizing the .forward. Alternatively, the ODE can be evaluated at a predetermined set of depth points via a .trajectory method, resulting in an output of dimensions length, batch size, data dimension.

torchdiffeq (Chen et al., 2018) and torchsde (Li et al., 2020) as a source of numerical solvers for batched ODEs and SDEs on GPUs. Outside of Python, the SciML ecosystem provides a Julia-based alternative with a primary focus on scientific machine learning and smaller data regimes. DiffEqFlux (Rackauckas et al., 2019) provides some of the model classes present in TorchDyn, such as ANODEs (Dupont et al., 2019) and FFJORD (Grathwohl et al., 2018), though with less emphasis on modularity and composability. DiffEqFlux relies on Flux for its deep learning primitives, which is notably more limited and less established in its current form than Python-based frameworks such as PyTorch or TensorFlow. The advantage for DiffEqFlux in specialized scientific application is due to the extensive numerical method suite offered by SciML (Rackauckas and Nie, 2017).

![Support in torchdyn of different SOTA models.

- : fully supported as the original paper.
- : supported in torchdyn but not present in the original paper.
- : Hamiltonian-type energy functions.
- : Lagrangian-type energy functions.
- : autograd trace.
- : Hutchinson estimator.](image)
5. Conclusions

We introduce TorchDyn, the first fully–featured library for continuous–depth models compatible with PyTorch. TorchDyn is designed to provide an intuitive, modular and powerful interface for neural differential equations and derivative models. The library further provides a complete set of tutorials to guide new practitioners and researchers.

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