
“Hey, that’s not an ODE”: Faster ODE Adjoint via Seminorms

Patrick Kidger^{1,2} Ricky T. Q. Chen^{3,4} Terry Lyons^{1,2}

Abstract

Neural differential equations may be trained by backpropagating gradients via the adjoint method, which is another differential equation typically solved using an adaptive-step-size numerical differential equation solver. A proposed step is accepted if its error, *relative to some norm*, is sufficiently small; else it is rejected, the step is shrunk, and the process is repeated. Here, we demonstrate that the particular structure of the adjoint equations makes the usual choices of norm (such as L^2) unnecessarily stringent. By replacing it with a more appropriate (semi)norm, fewer steps are unnecessarily rejected and the backpropagation is made faster. This requires only minor code modifications. Experiments on a wide range of tasks—including time series, generative modeling, and physical control—demonstrate a median improvement of 40% fewer function evaluations. On some problems we see as much as 62% fewer function evaluations, so that the overall training time is roughly halved.

1. Introduction

We begin by recalling the usual set-up for neural differential equations.

1.1. Neural ordinary differential equations

The general approach of neural ordinary differential equations (E, 2017; Chen et al., 2018) is to use ODEs as a learnable component of a differentiable framework. Typically the goal is to approximate a map $x \mapsto y$ by learning functions $\ell_1(\cdot, \phi)$, $\ell_2(\cdot, \psi)$ and $f(\cdot, \cdot, \theta)$, which

are composed such that

$$\begin{aligned} z(\tau) &= \ell_1(x, \phi), \\ z(t) &= z(\tau) + \int_{\tau}^t f(s, z(s), \theta) \, ds \\ y &\approx \ell_2(z(T), \psi). \end{aligned} \tag{1}$$

The variables ϕ , θ , ψ denote learnable parameters and the ODE is solved over the interval $[\tau, T]$. We include the (often linear) maps $\ell_1(\cdot, \phi)$, $\ell_2(\cdot, \psi)$ for generality, as in many contexts they are important for the expressiveness of the model (Dupont et al., 2019; Zhang et al., 2020), though our contributions will be focused around the ODE component and will not depend on these maps.

Here we will consider neural differential equations that may be interpreted as a neural ODE.

1.2. Applications

Neural differential equations have, to the best of our knowledge, three main applications:

1. Time series modeling. Rubanova et al. (2019) interleave Neural ODEs with RNNs to produce ODEs with jumps. Kidger et al. (2020) take $f(t, z, \theta) = g(z, \theta) \frac{dX}{dt}(t)$, dependent on some time-varying input X , to produce a neural *controlled* differential equation.
2. Continuous Normalising Flows as in Chen et al. (2018); Grathwohl et al. (2019), in which the overall model acts as coupling or transformation between probability distributions,
3. Modeling or controlling physical environments, for which a differential equation based model may be explicitly desired, see for example Zhong et al. (2020).

1.3. Adjoint equations

The integral in equation (1) may be backpropagated through either by backpropagating through the internal operations of a numerical solver, or by solving the backwards-in-time *adjoint equations* with respect to some

¹Mathematical Institute, University of Oxford, Oxford, United Kingdom ²The Alan Turing Institute, The British Library, London, United Kingdom ³University of Toronto ⁴The Vector Institute. Correspondence to: Patrick Kidger <kidger@maths.ox.ac.uk>.

(scalar) loss L :

$$\begin{aligned}
 a_z(T) &= \frac{dL}{dz(T)}, \\
 a_\theta(T) &= 0, \\
 a_t(T) &= \frac{dL}{dT}, \\
 a_z(t) &= a_z(T) - \int_T^t a_z(s) \cdot \frac{\partial f}{\partial z}(s, z(s), \theta) ds, \\
 a_\theta(t) &= a_\theta(T) - \int_T^t a_z(s) \cdot \frac{\partial f}{\partial \theta}(s, z(s), \theta) ds, \\
 a_t(t) &= a_t(T) - \int_T^t a_z(s) \cdot \frac{\partial f}{\partial s}(s, z(s), \theta) ds, \\
 \frac{dL}{dz(\tau)} &= a_z(\tau), \\
 \frac{dL}{d\theta} &= a_\theta(\tau), \\
 \frac{dL}{d\tau} &= a_t(\tau).
 \end{aligned} \tag{2}$$

These equations are typically solved together as a joint system $a(t) = [a_z(t), a_\theta(t), a_t(t)]$. (They are already coupled; the equations for a_θ and a_t depend on a_z .) As additionally their integrands require $z(s)$, and as the results of the forward computation of equation (1) are usually not stored, then the adjoint equations are typically additionally augmented by recovering z by solving backwards-in-time

$$z(t) = z(T) + \int_T^t f(s, z(s), \theta) ds. \tag{3}$$

1.4. Contributions

We demonstrate that the particular structure of the adjoint equations implies that numerical equation solvers will typically take too many steps, that are too small, wasting time during backpropagation. Specifically, the accept/reject step of adaptive-step-size solvers is too stringent.

By applying a correction to account for this, our method reduces the number of steps needed to solve the adjoint equations a median of 40%. On some problems we observe a reduction in function evaluations by as much as 62%.

Factoring in the forward pass (which is unchanged), the overall training procedure is roughly twice as fast.

The procedure we describe is simple to implement, does not affect model performance, and is hyperparameter-free and requires no tuning.

2. Method

2.1. Numerical solvers

Both the forward pass given by equation (1), and the backward pass given by equations (2) and (3), are solved by invoking a numerical differential equation solver. Our interest here is in adaptive-step-size solvers. Indeed the default choice for solving many equations is the adaptive-step-size Runge–Kutta 5(4) scheme of Dormand–Prince (Dormand & Prince, 1980), for example as implemented by `dopri5` in the `torchdiffeq` package or `ode45` in `MATLAB`.

A full discussion of the internal operations of these solvers is beyond our scope here; the part of interest to us is the accept/reject scheme. Consider the case of solving the general ODE

$$y(t) = y(\tau) + \int_\tau^t f(s, y(s)) ds,$$

with $y(t) \in \mathbb{R}^d$.

Suppose for some fixed t the solver has computed some estimate $\hat{y}(t) \approx y(t)$, and it now seeks to take a step $\Delta > 0$ to compute $\hat{y}(t + \Delta) \approx y(t + \Delta)$. A step is made, and some candidate $\hat{y}_{\text{candidate}}(t + \Delta)$ is generated. The solver additionally produces $y_{\text{err}} \in \mathbb{R}^d$ representing an estimate of the numerical error made in each channel during that step.

Given some prespecified absolute tolerance $ATOL$ (for example 10^{-9}), relative tolerance $RTOL$ (for example 10^{-6}), and (semi)norm $\|\cdot\| : \mathbb{R}^d \rightarrow [0, \infty)$ (for example $\|y\| = \sqrt{\frac{1}{d} \sum_{i=1}^d y_i^2}$ the RMS norm), then an estimate of the size of the solution to the equation is given by

$$\begin{aligned}
 SCALE &= \\
 &ATOL + RTOL \cdot \max(\hat{y}(t), \hat{y}_{\text{candidate}}(t + \Delta)) \in \mathbb{R}^d,
 \end{aligned} \tag{4}$$

where the maximum is taken channel-wise, and the error ratio r is computed (with an element-wise division):

$$r = \left\| \frac{y_{\text{err}}}{SCALE} \right\| \in \mathbb{R}. \tag{5}$$

If $r \leq 1$ then the error is deemed acceptable, the step is accepted and we take $\hat{y}(t + \Delta) = \hat{y}_{\text{candidate}}(t + \Delta)$. If $r > 1$ then the error is deemed too large, the candidate $\hat{y}_{\text{candidate}}(t + \Delta)$ is rejected, and the procedure is repeated with a smaller Δ .

Note the dependence on the choice of norm $\|\cdot\|$: in particular this determines the relative importance of each channel towards the accept/reject criterion.

2.2. Adjoint seminorms

Not an ODE The key observation is that a_θ (and in fact also a_t) does not appear anywhere in the vector fields of equation (2).

This means that (conditioned on knowing z and a_z), the integral corresponding to a_θ is just an integral—not an ODE. As such, it is arguably inappropriate to solve it with an ODE solver, which makes the implicit assumption that small errors now may propagate to create large errors later.

Accept/reject This is made manifest in the accept/reject step of equation (5). Typical choices of norm $\|\cdot\|$, such as L^2 , will usually weight each channel equally. But we have just established that to solve the adjoint equations accurately, it is far more important that z and a_z be accurate than it is that a_θ be accurate.

Seminorms Thus, when solving the adjoint equations equation (2), we propose to use a $\|\cdot\|$ that scales down the effect in those channels corresponding to a_θ .

In practice, in our experiments, we scale $\|\cdot\|$ all the way down by applying zero weight to the offending channels, so that $\|\cdot\|$ is in fact a seminorm. This means that the integration steps are chosen solely for the computation of a_z and z , and the values of a_θ are computed just by integrating with respect to those steps.

Example As an explicit example, note that $a_\theta(T) = 0$. When solving the adjoint equation numerically, this means for t close to T that the second term in equation (4) is small. As $ATOL$ is typically also small, then $SCALE$ is additionally small, and the error ratio r in equation (5) is large.

This implies that it becomes easy for the error ratio r to violate $r \leq 1$, and it is easy for the step to be rejected. Now there is nothing intrinsically bad about a step being rejected—we would like to solve the ODE accurately, after all—the problem is that this is a *spurious rejection*, as the rejection occurred to ensure the accuracy of a_θ , which is as already established unnecessary.

In practice, we observe that spurious rejections may occur for any t , not just those near T .

Other channels In fact, essentially the same argument applies to a_t as well: this does not affect the value of the vector field either. In a continuous normalising flow, the log-probability channel is also only an integral, rather than an ODE, and again the same argument may be applied.

Does this reduce the accuracy of parameter gradients?

One obvious concern is that we are typically ultimately

interested in the parameter gradients a_θ , in order to train a model; with respect to this our approach seems counter-intuitive.

However, we verify empirically that models still train without a reduction in performance. We explain this by noting that the z , a_z channels truly are ODEs, so that small errors now do propagate to create larger errors later. Thus these are likely the dominant source of error overall.

Code `torchdiffeq` (Chen et al., 2018) now supports adjoint seminorms as a built-in option. This may be used by passing `odeint_adjoint(..., adjoint_options=dict(norm="seminorm"))`.

The code for all our experiments can be found at <https://github.com/patrick-kidger/FasterNeuralDiffEq/>.

3. Experiments

We compare our proposed technique against conventionally-trained neural differential equations, across multiple tasks—time series, generative, and physics-informed. These are each drawn from the main applications of neural differential equations, discussed in Section 1.2. In every case, the differential equation solver used is the Dormand–Prince 5(4) solver “`dopri5`”. The default norm is a mixed L^∞/L^2 norm used in `torchdiffeq`; see Appendix A. For the sake of an interesting presentation, we investigate different aspects of each problem.

In each case see Appendix B for details on hyperparameters, optimisers and so on.

3.1. Neural Controlled Differential Equations

Consider the Neural Controlled Differential Equation (Neural CDE) model of Kidger et al. (2020).

To recap, given some (potentially irregularly sampled) time series $\mathbf{x} = ((t_0, x_0), \dots, (t_n, x_n))$, with each $t_i \in \mathbb{R}$ the timestamp of the observation $x_i \in \mathbb{R}^v$, let $X: [t_0, t_n] \rightarrow \mathbb{R}^{1+v}$ be an interpolation such that $X(t_i) = (t_i, x_i)$. For example X could be a natural cubic spline.

Then take $f(t, z, \theta) = g(z, \theta) \frac{dX}{dt}(t)$ in a Neural ODE model, so that changes in \mathbf{x} provoke changes in the vector field, and the model incorporates the incoming information \mathbf{x} . This may be thought of as a continuous-time RNN; indeed Kidger et al. (2020) use this to learn functions of (irregular) time series.

We apply a Neural CDE to the Speech Commands dataset (Warden, 2020). This is a dataset of one-second audio recordings of spoken words such as ‘left’, ‘right’ and

Table 1: Results for Neural CDEs. The number of function evaluations (NFE) used in the adjoint equations—accumulated throughout training—are reported. Test set accuracy is additionally reported. Mean \pm standard deviation over five repeats. Every model has 88,940 parameters.

RTOL, ATOL	Default norm		Seminorm	
	Accuracy (%)	Bwd. NFE (10^6)	Accuracy (%)	Bwd. NFE (10^6)
$10^{-3}, 10^{-6}$	92.6 ± 0.4	14.36 ± 1.09	92.5 ± 0.5	8.67 ± 1.60
$10^{-4}, 10^{-7}$	92.8 ± 0.4	30.67 ± 2.48	92.5 ± 0.5	12.75 ± 2.00
$10^{-5}, 10^{-8}$	92.4 ± 0.7	77.95 ± 4.47	92.9 ± 0.4	29.39 ± 0.80

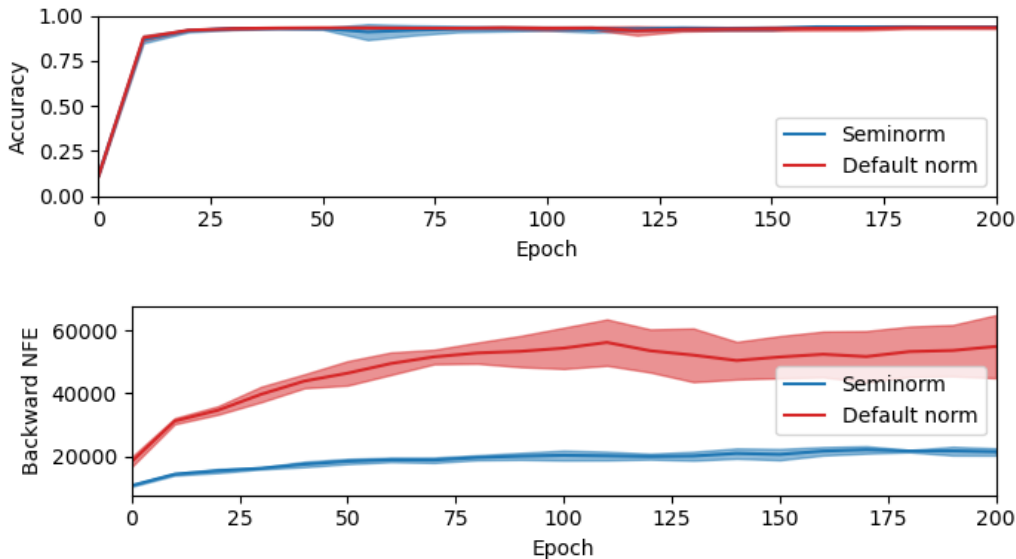


Figure 1: Mean \pm standard deviation, for accuracy and the number of function evaluations (NFE) for the backward pass, during training, for Neural CDEs.

so on. We take 34975 time series corresponding to 10 words, to produce a balanced classification problem. We preprocess the dataset by computing mel-frequency cepstrum coefficients so that each time series is then regularly spaced with length 161 and 20 channels. The data was then normalised to have zero mean and unit variance. We used the `torchcde` package (Kidger, 2020), which wraps `torchdiffeq`.

The initial map ℓ_1 (of equation (1)) is taken to be linear on (t_0, x_0) . The terminal map ℓ_2 is taken to be linear on $z(t_n)$.

We investigate how the effect changes for varying tolerances by varying the pair $(RTOL, ATOL)$ over $(10^{-3}, 10^{-6})$, $(10^{-4}, 10^{-7})$, and $(10^{-5}, 10^{-8})$. For each such pair we run five repeated experiments.

See Table 1 for results on accuracy and number of function evaluations. We see that the accuracy of the model is unaffected by our proposed change, whilst the backward

pass uses 40%–62% fewer steps, depending on tolerance.

Next, we investigate how accuracy and function evaluations change during training. See Figure 1. We see that accuracy quickly gets close to its maximum value during training, with only incremental improvements for most of the training procedure. In particular, this statement is true of both approaches, and we do not see any discrepancy between them. Additionally, we see that the number of function evaluations is much lower for the seminorm throughout training.

3.2. Continuous Normalising Flows

Continuous Normalising Flows (CNF) (Chen et al., 2018) are a class of generative models that define a probability distribution as the transformation of a simpler distribution by following the vector field parameterised by a Neural ODE. Let $p(z_0)$ be an arbitrary base distribution that we can efficiently sample from, and compute its density. Then

Table 2: Results for Continuous Normalising Flows. The number of function evaluations (NFE) used in the adjoint equations—accumulated throughout training—are reported. Test set bits/dim and number of parameters are additionally reported. Mean \pm standard deviation over three repeats.

Model	Parameters	Default norm		Seminorm	
		Test bits/dim	Bwd. NFE (10^6)	Test bits/dim	Bwd. NFE (10^6)
CIFAR-10 ($d_h = 64$)	1,200,600	3.3492 \pm 0.0059	41.65 \pm 1.97	3.3428 \pm 0.0121	38.93\pm1.32
MNIST ($d_h = 32$)	281,928	0.9968 \pm 0.0020	41.50 \pm 2.35	0.9942 \pm 0.0013	37.03\pm0.96
MNIST ($d_h = 64$)	1,005,384	0.9623 \pm 0.0020	44.24 \pm 1.78	0.9603 \pm 0.0021	37.85\pm0.94
MNIST ($d_h = 128$)	3,779,400	0.9439 \pm 0.0030	48.60 \pm 2.30	0.9466 \pm 0.0048	41.84\pm1.92

let $z(t)$ be the solution of the initial value problem

$$\begin{aligned} z(0) &\sim p(z_0), \\ \frac{dz(t)}{dt} &= f(t, z(t), \theta), \\ \frac{d \log p(z(t))}{dt} &= -\text{tr} \left(\frac{\partial f}{\partial z}(t, z(t), \theta) \right), \end{aligned}$$

for which the initial point is randomly sampled from $p(z_0)$, and for which the change in log probability density is also tracked as the sample is transformed through the vector field.

The distribution at an arbitrary time value T can be trained with maximum likelihood to match data samples, resulting in a generative model of data with the distribution $p(z(T))$. Furthermore, Grathwohl et al. (2019) combines this with a stochastic trace estimator (Hutchinson, 1989) to create an efficient and unbiased estimator of the log probability for data samples x :

$$\begin{aligned} \log p(z(T) = x) &= \log p(z(0)) + \\ \mathbb{E}_{v \sim \mathcal{N}(0,1)} &\left[\int_T^0 v^T \left(\frac{\partial f}{\partial z}(t, z(t), \theta) \right) v dt \right]. \end{aligned} \tag{6}$$

In Table 2 we show the final test performance and the total number of function evaluations (NFEs) used in the adjoint method over 100 epochs. We see substantially fewer NFEs in experiments on both MNIST and CIFAR-10. Next, we investigate changing model size, by varying the complexity of the vector field f , which is a CNN with d_h hidden channels. We find that using the seminorm, the backward NFE does not increase as much as when using the default norm. In particular, we can use roughly same NFEs as the smaller ($d_h = 32$) model to train a larger ($d_h = 128$) model and in doing so achieve a substantial gain in performance (1.00 \rightarrow 0.95).

3.3. Hamiltonian dynamics

We consider the problem of learning Hamiltonian dynamics, using the Symplectic ODE-Net model of Zhong et al. (2020). Under Hamiltonian mechanics, the vector field is parameterised as

$$f(t, z, \theta) = \begin{bmatrix} \frac{dH}{dp}(q, p, \theta) \\ g(q, \theta)u - \frac{dH}{dq}(q, p, \theta) \\ 0 \end{bmatrix},$$

where $z = (q, p, u)$ is the state decomposed into (generalised) positions q , momenta p , and control u . H is a Hamiltonian and g is an input term, both parameterised as neural networks. The input g offers a way to control the system, which can be understood via energy shaping.

This parameterisation lends itself to being interpretable. H learns to encode the physics of the system in the form of Hamiltonian mechanics, whilst g learns to encode the way in which inputs affect the system. This can then be used to construct controls u driving the system to a desired state. In this context (unlike the other problems we consider here), z is not a hidden state but instead the output of the model. The evolution of z is matched against the observed state at multiple times $z(t_1), z(t_2), \dots$, and trained with L^2 loss.

We consider the fully-actuated double pendulum (“acrobot”) problem. Training data involves small oscillations under constant forcing.

We investigate several quantities of interest.

First we investigate the number of function evaluations. See Table 3. We see that the model successfully learns the dynamics, with very small loss (order $\mathcal{O}(10^{-4})$) in both cases. However, under our proposed change the model is trained using 43% fewer function evaluations on the backward pass.

Next, we verify that the end goal of controlling the system is still achievable, using a seminorm-trained model. See Figures 2 and 3, in which the double pendulum is

Table 3: Results for Symplectic ODE-Net on a fully-actuated double pendulum. The number of function evaluations (NFE) used in the adjoint equations—accumulated throughout training—are reported. Test set loss is additionally reported. Mean \pm standard deviation over five repeats. The model has 509,108 parameters.

Default norm		Seminorm	
Test L^2 loss (10^{-4})	Bwd. NFE (10^4)	Test L^2 loss (10^{-4})	Bwd. NFE (10^4)
1.247 \pm 0.520	46.45 \pm 0.01	2.995 \pm 2.190	26.55\pm0.01

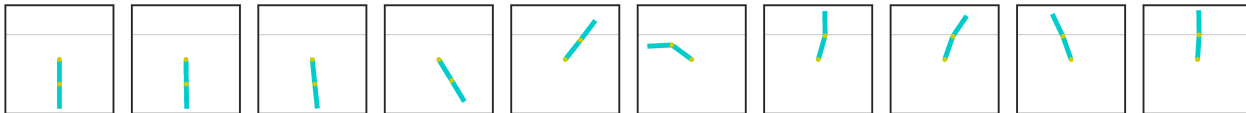


Figure 2: Frames from controlling the fully-actuated double pendulum to the full-upright position.

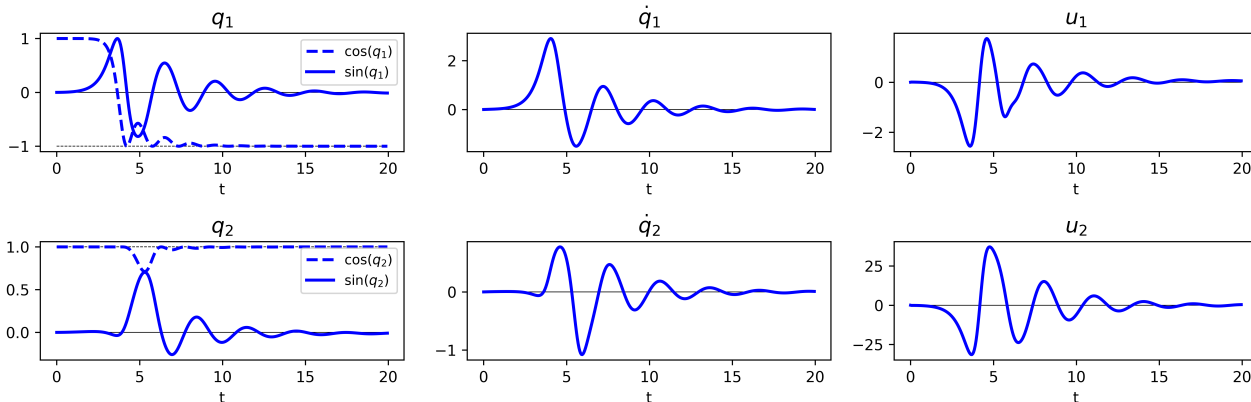


Figure 3: Evolution of the state $z = (q, \dot{q}, u)$ whilst controlling the fully-actuated double pendulum from the full-down to the full-upright position. q_1 denotes the angle of the first joint, and q_2 denotes the angle of the second joint.

successfully controlled from the full-down to the full-upright position, using the seminorm-trained model.

Third, we investigate the locations of the function evaluations. See Figure 4. We see that the default norm makes consistently more evaluations for every time t . This is interesting as our initial hypothesis was that there would be more spurious rejections for t near the terminal time T , where $a_\theta(t)$ is small, as $a_\theta(T) = 0$. In fact we observe consistent improvements for all t .

Fourth and finally, we investigate the locations of the rejected steps. See Figure 5. We see that the seminorm produces almost no rejected steps. This accounts for the tight grouping seen in Figure 4, as for each batch the evaluations times are typically at the same locations. Moreover, we observe an interesting structure to the the location of the rejected steps with the default norm. We suspect this is due to the time-varying physics of the problem. Note that the Dormand–Prince solver makes 6 function evaluations per step, which is the reason for the

difference in scale between Figures 4 and 5.

3.4. Where do improvements come from?

Parameter-state ratio We hypothesised that the ratio between size of state and number of parameters may explain the differences between the smaller improvements for continuous normalising flows against the substantial improvements for Hamiltonian neural networks and neural CDEs (corresponding to the proportion of channels that can no longer cause rejections). Given a model with p parameters and state $z(t) \in \mathbb{R}^d$, then seminorms reduce the number of rejection-causing channels from $1 + 2d + p$ to just $1 + 2d$.

We plot the (log) ratio $1+2d+p/1+2d$ against the percentage improvement in backward steps. See Figure 6. We see that this hypothesis partly explains things: broadly speaking continuous normalising flows (which have $\mathcal{O}(10^3)$ state variables) see small improvements, whilst the neural CDEs

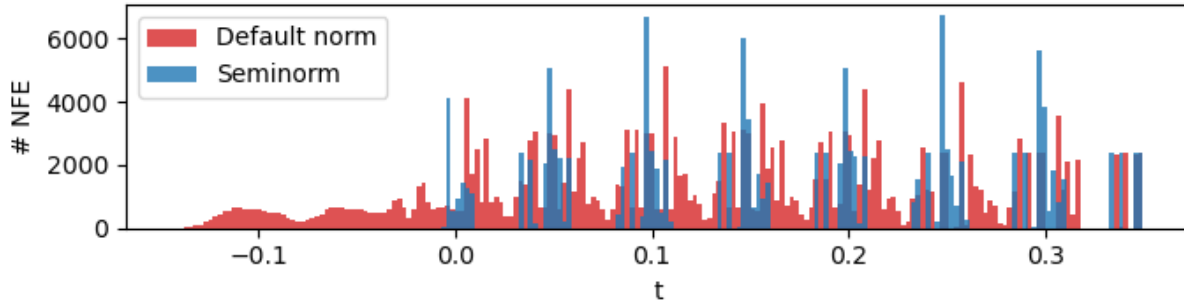


Figure 4: Location of function evaluations for the adjoint equations, during training for the fully-actuated double pendulum problem. All evaluations over five runs are shown.

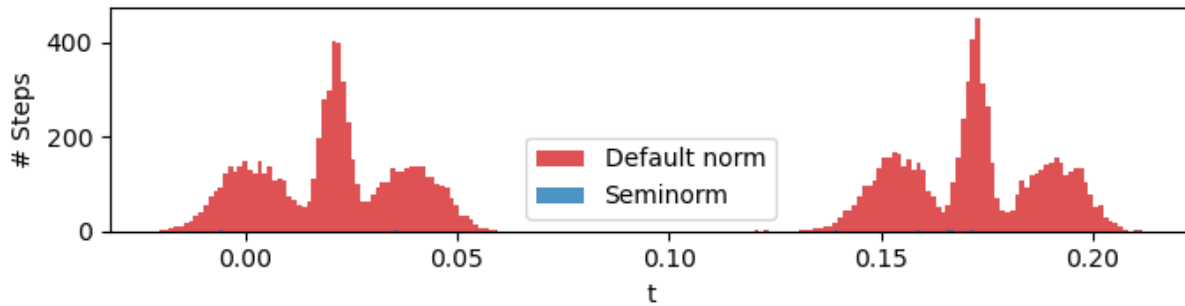


Figure 5: Location of rejected steps during training for the fully-actuated double pendulum problem. All steps over five runs are shown. There were no rejected steps for the seminorm.

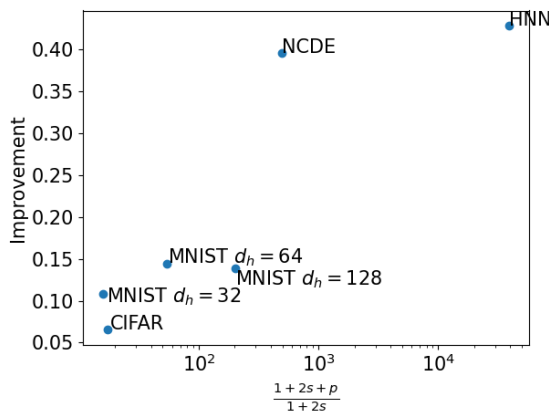


Figure 6: Parameter-state ratio against improvement, as given by the relative decrease in backward NFE. Only one neural CDE experiment (RTOL=10⁻³, ATOL=10⁻⁶) is shown as the others use different tolerances. CNFs are averaged over their different blocks.

and Hamiltonian neural networks (with $\mathcal{O}(10^1)$ state variables) see larger improvements.

There are still many differences between problems (tolerances, complexity of vector field, and so on); see for example the variation amongst the continuous normalising flows. Thus for any given problem this serves more as a rule-of-thumb.

Number of accepted/rejected steps Next we investigate the improvements for each problem, broken down by accepted and rejected steps (over a single backward pass). See Table 4. We begin by noting that the absolute number of accepted and rejected steps nearly always decreased. (In the case of modelling Hamiltonian dynamics, the seminorm actually produced *zero* rejected steps.) However beyond this, the *proportion* of rejected steps nearly always decreased.

This highlights that the benefit of seminorms is two-fold. First, that the number of accepted steps is reduced indicates that use of seminorms means systems are treated as smaller and so easier-to-solve, allowing larger step sizes. Second, the reduced proportion of rejected steps means that the differential equation solve is more efficient, with fewer wasted steps.

Table 4: Number of rejected and accepted backward steps on one pass over the test set.

Experiment	Rejected steps (10^3)		Accepted steps (10^3)		Proportion rejected	
	Default	Seminorm	Default	Seminorm	Default	Seminorm
NCDE (small)	0.13 \pm 0.02	0.15 \pm 0.02	3.45 \pm 0.26	1.92 \pm 0.18	3.63%	7.25%
NCDE (medium)	1.01 \pm 0.18	0.17 \pm 0.05	8.38 \pm 0.86	3.25 \pm 0.43	10.76%	4.97%
NCDE (large)	10.91 \pm 1.03	1.16 \pm 0.13	28.86 \pm 2.15	8.61 \pm 0.45	27.43%	11.87%
CIFAR-10	11.04 \pm 0.29	9.30 \pm 1.92	23.50 \pm 1.19	22.82 \pm 1.34	31.96%	28.95%
MNIST ($d_h = 32$)	5.54 \pm 0.99	4.51 \pm 1.01	20.91 \pm 0.90	19.93 \pm 0.42	20.95%	18.45%
MNIST ($d_h = 64$)	7.79 \pm 0.81	4.29 \pm 0.69	22.95 \pm 1.02	19.73 \pm 0.99	38.53%	17.86%
MNIST ($d_h = 128$)	8.88 \pm 0.21	7.40 \pm 1.17	26.54 \pm 0.91	25.01 \pm 1.17	25.07%	22.83%
HNN	0.11 \pm 0.00	0.00 \pm 0.00	0.18 \pm 0.00	0.16 \pm 0.00	37.93%	0.00%

4. Related work

Several works have sought techniques for speeding up training of neural differential equations.

4.1. Techniques included here

Dupont et al. (2019) and Massaroli et al. (2020a) note that adding extra dimensions to the Neural ODE improve expressivity and training. Indeed this has arguably now become a standard part of the model; we include this via the linear ℓ_1 in equation (1).

Chen et al. (2018) mention regularizing the differential equation using weight decay; we include this throughout our experiments.

When backpropagating through the internal operations of the solver (so not the adjoint method used here), Zhuang et al. (2020) note that backpropagating through rejected steps is unnecessary. This is implicitly used here as this is now the default behaviour in `torchdiffeq`.

4.2. Model-specific techniques

For Neural ODEs only, Ghosh et al. (2020) regularise the neural ODE by randomly selecting the terminal integration time. Much like this work, this is a simple change with immediate benefit.

Specialised for Continuous Normalising Flows, Finlay et al. (2020) and Kelly et al. (2020) investigate regularising the higher-order derivatives of the model. The idea is that this encourages simpler trajectories that are easier to integrate. However, this improvement must be weighed against the extra cost of computing the regularisation term. Thus whilst Finlay et al. (2020) describe speed improvements for CNFs, Kelly et al. (2020) describe slower training as a result of this extra cost.

For Continuous Normalizing Flows, Grathwohl et al. (2019), Chen & Duvenaud (2019), and Onken et al. (2020)

have proposed specific architectural choices to reduce training cost.

4.3. Other techniques

Quaglino et al. (2020) describe speeding up training via spectral approximation. Unfortunately, this method is rather involved, and to our knowledge does not have a reference implementation.

Massaroli et al. (2020b) discuss hypersolvers, which are hybrids of neural networks and numerical differential equation solvers, trained to efficiently solve a desired Neural ODE. However the Neural ODE changes during training, making these most useful after training, to speed up inference.

Independent of modifications to the model or training procedure, Rackauckas & Nie (2017) and Rackauckas et al. (2019) claim speed-ups simply through an improved implementation.

5. Further work

Our seminorm-based approach means that the integrals for a_θ, a_t in equation (2) are estimated based on the points selected to solve the equation for a_z . One can sensibly imagine refinements of the technique described here, by combining ODE solvers for z and a_z with quadrature rules for a_θ and a_t .

6. Conclusion

We have introduced a method for reducing the number of function evaluations required to train a neural differential equation, by reducing the number of rejected steps during the adjoint (backward) pass. Doing so offers substantial speed-ups across a variety of applications with no observed downsides.

ACKNOWLEDGMENTS

PK was supported by the EPSRC grant EP/L015811/1. PK and TL were supported by the Alan Turing Institute under the EPSRC grant EP/N510129/1.

References

- Chen, R. T. and Duvenaud, D. K. Neural networks with cheap differential operators. In *Advances in Neural Information Processing Systems*, pp. 9961–9971, 2019.
- Chen, R. T. Q., Rubanova, Y., Bettencourt, J., and Duvenaud, D. K. Neural Ordinary Differential Equations. In *Advances in Neural Information Processing Systems 31*, pp. 6571–6583. Curran Associates, Inc., 2018.
- Dormand, J. R. and Prince, P. J. A family of embedded Runge–Kutta formulae. *J. Comp. Appl. Math*, 6:19–26, 1980.
- Dupont, E., Doucet, A., and Teh, Y. W. Augmented neural odes. In *Advances in Neural Information Processing Systems 32*, pp. 3140–3150. Curran Associates, Inc., 2019.
- E, W. A Proposal on Machine Learning via Dynamical Systems. *Commun. Math. Stat.*, 5(1):1–11, 2017.
- Finlay, C., Jacobsen, J.-H., Nurbekyan, L., and Oberman, A. M. How to train your neural ODE: the world of Jacobian and kinetic regularization. *ICML 2020*, 2020.
- Ghosh, A., Behl, H. S., Dupont, E., Torr, P. H. S., and Nambodiri, V. STEER: Simple Temporal Regularization For Neural ODEs. *Neural Information Processing Systems*, to appear, 2020.
- Grathwohl, W., Chen, R. T. Q., Bettencourt, J., Sutskever, I., and Duvenaud, D. Ffjord: Free-form continuous dynamics for scalable reversible generative models. *International Conference on Learning Representations*, 2019.
- Hutchinson, M. F. A stochastic estimator of the trace of the influence matrix for laplacian smoothing splines. *Communications in Statistics-Simulation and Computation*, 18(3):1059–1076, 1989.
- Kelly, J., Bettencourt, J., Johnson, M. J., and Duvenaud, D. Learning Differential Equations that are Easy to Solve. *arXiv:2007.04504*, 2020.
- Kidger, P. torchcde, 2020. <https://github.com/patrick-kidger/torchcde>.
- Kidger, P., Morrill, J., Foster, J., and Lyons, T. Neural Controlled Differential Equations for Irregular Time Series. *arXiv:2005.08926*, 2020.
- Kingma, D. and Ba, J. Adam: A method for stochastic optimization. *ICLR*, 2015.
- Massaroli, S., Poli, M., Park, J., Yamashita, A., and Asama, H. Dissecting Neural ODEs. *arXiv:2002.08071*, 2020a.
- Massaroli, S., Poli, M., Yamashita, A., Asama, H., and Park, J. Hypersolvers: Toward Fast Continuous-Depth Models. *arXiv:2007.09601*, 2020b.
- Onken, D., Fung, S. W., Li, X., and Ruthotto, L. Ot-flow: Fast and accurate continuous normalizing flows via optimal transport. *arXiv preprint arXiv:2006.00104*, 2020.
- Paszke, A., Gross, S., Massa, F., Lerer, A., Bradbury, J., Chanan, G., Killeen, T., Lin, Z., Gimelshein, N., Antiga, L., Desmaison, A., Kopf, A., Yang, E., DeVito, Z., Raison, M., Tejani, A., Chilamkurthy, S., Steiner, B., Fang, L., Bai, J., and Chintala, S. PyTorch: An Imperative Style, High-Performance Deep Learning Library. In *Advances in Neural Information Processing Systems 32*, pp. 8024–8035. Curran Associates, Inc., 2019.
- Quaglino, A., Gallieri, M., Masci, J., and Koutník, J. Snode: Spectral discretization of neural odes for system identification. In *International Conference on Learning Representations*, 2020.
- Rackauckas, C. and Nie, Q. Differentialequations.jl—a performant and feature-rich ecosystem for solving differential equations in julia. *Journal of Open Research Software*, 5(1), 2017.
- Rackauckas, C., Innes, M., Ma, Y., Bettencourt, J., White, L., and Dixit, V. Diffeqflux.jl—a julia library for neural differential equations. *arXiv preprint arXiv:1902.02376*, 2019.
- Rubanova, Y., Chen, T. Q., and Duvenaud, D. K. Latent Ordinary Differential Equations for Irregularly-Sampled Time Series. In *Advances in Neural Information Processing Systems 32*, pp. 5320–5330. Curran Associates, Inc., 2019.
- Warden, P. Speech commands: A dataset for limited-vocabulary speech recognition. *arXiv:1804.03209*, 2020.
- Zhang, H., Gao, X., Unterman, J., and Arodz, T. Approximation capabilities of neural odes and invertible residual networks. *International Conference on Machine Learning*, 2020.

Zhong, Y. D., Dey, B., and Chakraborty, A. Symplectic ode-net: Learning hamiltonian dynamics with control. In *International Conference on Learning Representations*, 2020.

Zhuang, J., Dvornik, N., Li, X., Tatikonda, S., Papademetris, X., and Duncan, J. Adaptive checkpoint adjoint method for gradient estimation in neural ode. *International Conference on Machine Learning*, 2020.

A. Code

Built-in to torchdiffeq `torchdiffeq` (Chen et al., 2018) has chosen to support adjoint seminorms as a built-in option. This may be used by passing `odeint_adjoint(..., adjoint_options=dict(norm='seminorm'))`.

PyTorch reference implementation A reference implementation, using PyTorch (Paszke et al., 2019) and `torchdiffeq` (Chen et al., 2018), is shown in Figure 7.

By default, `torchdiffeq` uses a (somewhat unusual) mixed L^∞ -RMS norm. Given the adjoint state $[a_t, z, a_z, a_\theta]$, then the norm used is

$$\| [a_t, z, a_z, a_\theta] \| = \max \{ \|a_t\|_{\text{RMS}}, \|z\|_{\text{RMS}}, \|a_z\|_{\text{RMS}}, \|a_\theta\|_{\text{RMS}} \},$$

where for $x = (x_1, \dots, x_n)$,

$$\|x\|_{\text{RMS}} = \sqrt{\frac{1}{n} \sum_{i=1}^n x_i^2}.$$

Respecting this convention, the code provided reduces this to the seminorm

$$\| [a_t, z, a_z, a_\theta] \| = \max \{ \|z\|_{\text{RMS}}, \|a_z\|_{\text{RMS}} \}.$$

Other similar approaches such as pure-RMS over $[z, a_z]$ should be admissible as well.

Julia The `DifferentialEquation.jl` library (Rackauckas & Nie, 2017) library offers an argument `internalsnorm` which may be used to implement seminorms in a manner analogous to the reference implementation provided here.

B. Experimental details

B.1. Neural Controlled Differential Equations

We use the same setup and hyperparameters as in Kidger et al. (2020). The loss function is cross entropy. The optimiser used was Adam (Kingma & Ba, 2015), with learning rate 1.6×10^{-3} , batch size of 1024, and 0.01-weighted L^2 weight regularisation, trained for 200 epochs. The number of hidden channels (the size of z) is 90, and f is parameterised as a feedforward network, of width 40 with 4 hidden layers, ReLU activation, and tanh final activation.

```

1 import torchdiffeq
2
3 def rms_norm(tensor):
4     return tensor.pow(2).mean().sqrt()
5
6 def make_norm(state):
7     state_size = state.numel()
8
9     def norm(aug_state):
10        y = aug_state[1:1 + state_size]
11        adj_y = aug_state[1 + state_size:1 + 2 * state_size]
12        return max(rms_norm(y), rms_norm(adj_y))
13    return norm
14
15 torchdiffeq.odeint_adjoint(func=..., y0=..., t=...,
16                            adjoint_options=dict(norm=make_norm(y0)))

```

Figure 7: Reference PyTorch implementation for adjoint seminorms.

B.2. Continuous Normalising Flows

We follow Grathwohl et al. (2019) and Finlay et al. (2020). The loss function is the negative log likelihood $-\log(p(z(T) = x))$ of equation (6). The optimiser used was Adam, with learning rate 10^{-3} and batch size 256, trained for 100 epochs. Relative and absolute tolerance of the solver are both taken to be 10^{-5} . We used a multi-scale architecture as in Grathwohl et al. (2019) and Finlay et al. (2020), with 4 blocks of CNFs at 3 different scales.

B.3. Symplectic ODE-Net

The optimiser used was Adam, with learning rate 10^{-3} , batch size of 256, and 0.01-weighted L^2 weight regularisation. Relative and absolute tolerance of the solver are both taken to be 10^{-4} . We use the same architecture as in Zhong et al. (2020): this involves parameterising H as a sum of kinetic and potential energy terms. These details of Symplectic ODE-Net are a little involved, and we refer the reader to Zhong et al. (2020) for full details.