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Neural Controlled Differential Equations for Irregular Time Series

PATRICK KIDGER

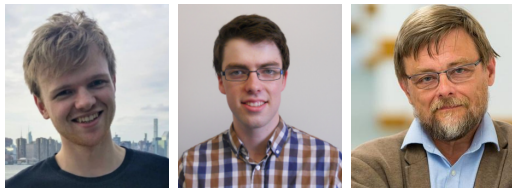
*Mathematical Institute
University of Oxford*

Market Generators 2020

Oxford
Mathematics



Joint work with...



James Morrill, James Foster, Terry Lyons

`https://github.com/patrick-kidger/NeuralCDE`
`https://arxiv.org/abs/2005.08926`

Summary

Neural Controlled Differential Equations



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- New tool for time series
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- Can be trained with memory-efficient adjoint backpropagation, even across observations
- Straightforward to implement with existing tools.
- Demonstrates state-of-the-art performance.

Recap

Controlled Differential Equations

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~~Controlled~~ ^{Ordinary} Differential Equations

(vector field) $f: \mathbb{R}^w \rightarrow \mathbb{R}^w$

Recap

~~Controlled~~ Ordinary Differential Equations

$$\begin{array}{ll} \text{(vector field)} & f: \mathbb{R}^w \rightarrow \mathbb{R}^w \\ \text{(solution)} & z: [0, T] \rightarrow \mathbb{R}^w \end{array}$$

(vector field)	$f: \mathbb{R}^w \rightarrow \mathbb{R}^w$
(solution)	$z: [0, T] \rightarrow \mathbb{R}^w$
(ODE)	$\frac{dz}{dt}(t) = f(z(t))$
	$z(0) = z_0$

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(control)	$X: [0, T] \rightarrow \mathbb{R}^v$
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(control)	$X: [0, T] \rightarrow \mathbb{R}^v$
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(response)	$z: [0, T] \rightarrow \mathbb{R}^w$
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Neural Ordinary Differential Equations



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Have an efficient training algorithm (adjoint backpropagation) that uses $\mathcal{O}(1)$ memory in the time horizon T .

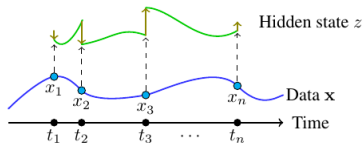
Recap

Neural Ordinary Differential Equations for time series



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Neural Controlled Differential Equations

Splines



Neural Controlled Differential Equations

Splines



Observe $\mathbf{x} = ((t_0, x_0), \dots, (t_n, x_n))$ with $t_i \in \mathbb{R}$ and $x_i \in \mathbb{R}^v$.

Neural Controlled Differential Equations

Splines

Observe $\mathbf{x} = ((t_0, x_0), \dots, (t_n, x_n))$ with $t_i \in \mathbb{R}$ and $x_i \in \mathbb{R}^v$.
(WLOG $t_0 = 0, t_n = T$)

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(WLOG $t_0 = 0, t_n = T$)

Let $X: [t_0, t_n] = [0, T] \rightarrow \mathbb{R}^v$ be the natural cubic spline interpolation of this data, so $X(t_i) = (x_i, t_i)$.

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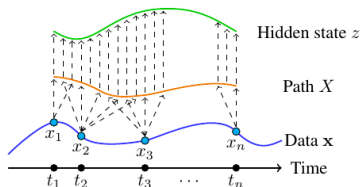
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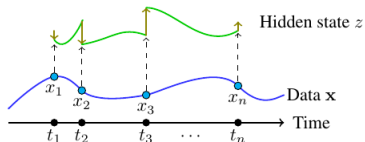
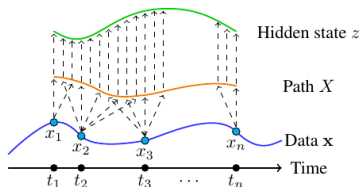
(once again z is “hidden state”)

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Neural Controlled Differential Equations

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- The equation $\frac{dz}{dt}(t) = f_{\theta}(z(t)) \frac{dX}{dt}(t)$ is still an ODE, so we can solve it with the same tools as for Neural ODEs.
 - In particular with the same software, hassle-free.

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- Neural CDEs demonstrate state-of-the-art performance.

Results!

CharacterTrajectories

Test accuracy (mean \pm std, computed across five runs) and memory usage on CharacterTrajectories. Memory usage is independent of repeats and of amount of data dropped.

Model	Test Accuracy			Memory usage (MB)
	30% dropped	50% dropped	70% dropped	
GRU-ODE	89.9% \pm 8.4%	89.6% \pm 5.6%	86.6% \pm 3.5%	1.5
GRU- Δt	94.4% \pm 1.7%	92.0% \pm 1.0%	91.1% \pm 1.1%	15.6
GRU-D	93.2% \pm 2.0%	92.7% \pm 2.8%	90.8% \pm 2.1%	16.9
ODE-RNN	97.9% \pm 0.4%	97.5% \pm 0.6%	96.7% \pm 0.9%	14.7
Neural CDE (ours)	99.2% \pm 0.3%	99.3% \pm 0.3%	99.4% \pm 0.4%	1.3

Results!

Speech Commands

Test Accuracy (mean \pm std, computed across five runs) and memory usage on Speech Commands. Memory usage is independent of repeats.

Model	Test Accuracy	Memory usage (GB)
GRU-ODE	47.9% \pm 2.9%	0.164
GRU- Δt	43.3% \pm 33.9%	1.54
GRU-D	32.4% \pm 34.8%	1.64
ODE-RNN	65.9% \pm 35.6%	1.40
Neural CDE (ours)	89.8% \pm 2.5%	0.167

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T. Lyons, M. Caruana, and T. Levy, *Differential equations driven by rough paths*. Springer, 2004. École d'Été de Probabilités de Saint-Flour XXXIV - 2004

R. T. Q. Chen, Y. Rubanova, J. Bettencourt, and D. K. Duvenaud, "Neural Ordinary Differential Equations," in *Advances in Neural Information Processing Systems 31*, pp. 6571–6583, Curran Associates, Inc., 2018.

Y. Rubanova, T. Q. Chen, and D. K. Duvenaud, "Latent Ordinary Differential Equations for Irregularly-Sampled Time Series," in *Advances in Neural Information Processing Systems 32*, pp. 5320–5330, Curran Associates, Inc., 2019