Variational Integrator Networks for Physically Structured Embeddings

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What is *Neural Differential Equation* anyway?

Neural Differential Equation

A *neural differential equation* is a differential equation using a neural network to parameterise the vector field. The canonical example is a *neural ordinary differential equation*.

$$y(0) = y_0 \tag{1}$$

$$\frac{\mathrm{d}y}{\mathrm{d}t}(t) = f_\theta(t, y(t)) \tag{2}$$

Where θ is some vector of learnt parameters. Usually, f_θ is a feedforward network.

[1] Chen et al. 2019.
[2] Kidger 2022.

Residual Network (ResNet)

$$y_{j+1} = y_j + f_\theta(j, y_j) \tag{3}$$

Where $f_\theta(j, \cdot)$ is j-th residual block. With θ as vector of parameters from all layers.

If we try the discretization of neural ODE, it might start looking familiar.

$$\frac{y(t_{j+1}) - y(t_j)}{\Delta t} \approx \frac{\mathrm{d}y}{\mathrm{d}t}(t) = f_\theta(t_j, y(t_j)) \tag{4}$$

If we absorb the discretization step into the f_θ, we can derive:

$$y(t_{j+1}) = y(t_j) + f_\theta(t, y_j) \tag{5}$$

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Neural Differential Equations

Comparison of RN[3] and NDE

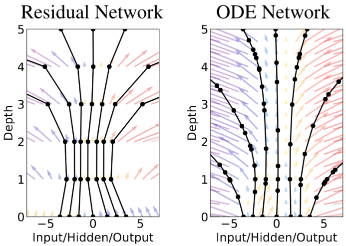

Figure 1: *Left:* A Residual network defines a discrete sequence of finite transformations. *Right:* A ODE network defines a vector field, which continuously transforms the state. *Both:* Circles represent evaluation locations.

Why to bother with constant discrete number of hidden layers?
Continuous-layer architecture allows:

1. Precision+Accuracy tuning
2. Constant memory
3. Fast backprop
4. Continuous evaluation

[3] Yin et al. 2019.

1. *Neural ODEs* are the continuous limit of residual networks.
2. **GRU** and **LSTM** updates rules suspiciously similar to discretised differential equations.
3. **StyleGAN2** is simply discretised *SDE*
4. Invertible NN coupling layers are reversible DE solvers

Many of the DL architectures resemble DEs.

Neural Network $\Leftrightarrow$ Differential Equation

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Variational Integrator Networks[4]

A Bridge

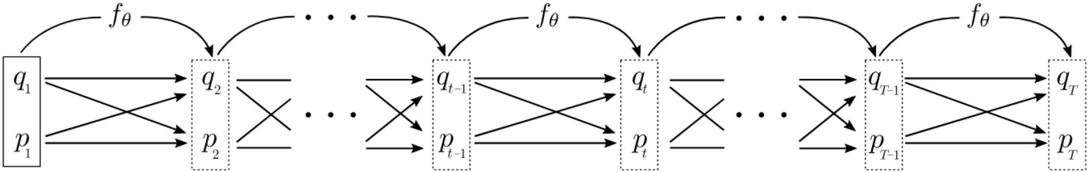
VIN is the bridge between the viewpoint of representing deep residual networks as discretisation of differential equations and the viewpoint of geometric embeddings.

Geometric Embeddings

Geometric Embeddings[a,b,c] is the way of embedding data into it's natural geometry, preserving relational information.

[a] Chamberlain, Clough, and Deisenroth 2017.
[b] Davidson et al. 2022.
[c] Xiong et al. 2023.

[4] Saemundsson et al. 2020.



Overall structure of the VIN resembles the residual network we seen before. We consider it to be a multilayered (discretised) dynamics of the system. $(\mathbf{q}, \mathbf{p})$ is the hidden space, which is 2-form of position-momentum phase-space and f_θ we have seen earlier.

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