NEURAL NETWORKS AS ORDINARY DIFFERENTIAL EQUATIONS

Presenter: Jodie Zhu (Dessa)

Facilitator: Helen Ngo & Lindsay Brin

The Paper

Neural Ordinary Differential Equations

Ricky T. Q. Chen, Yulia Rubanova, Jesse Bettencourt, David Duvenaud

10/22/2018 (v1: 6/19/2018) cs.LG | cs.AI | stat.ML

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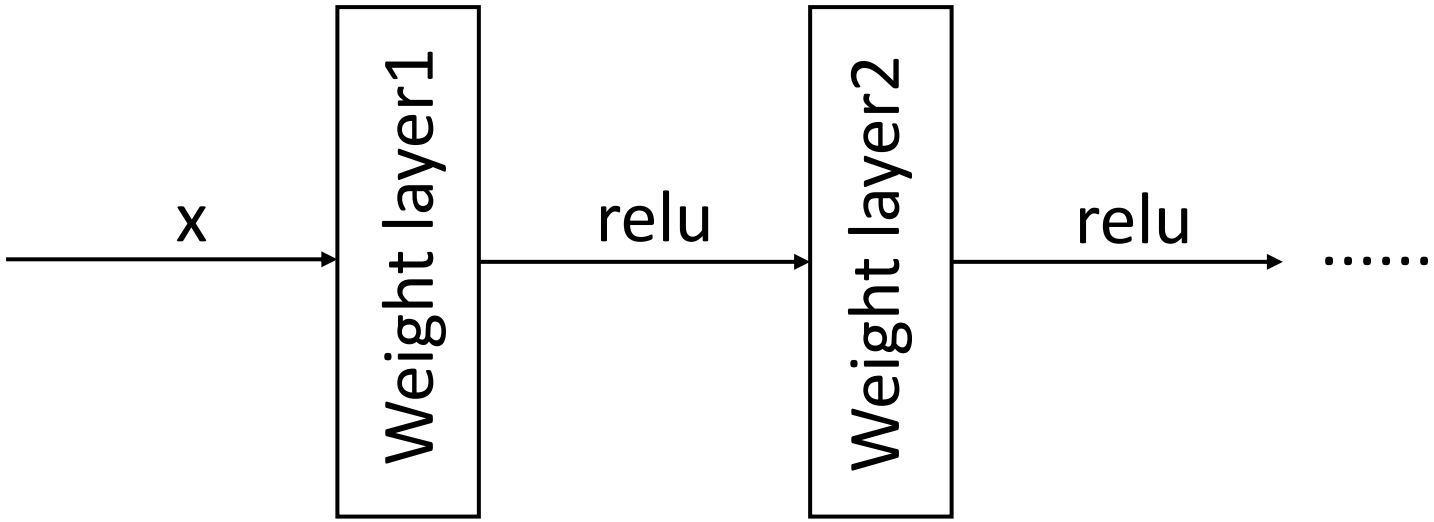
Neural nets as discrete layers

New state Old state

$$h_{t+1} = f(h_t)$$

State: $h_1 = f(x)$ $h_2 = f(h_1)$ ……



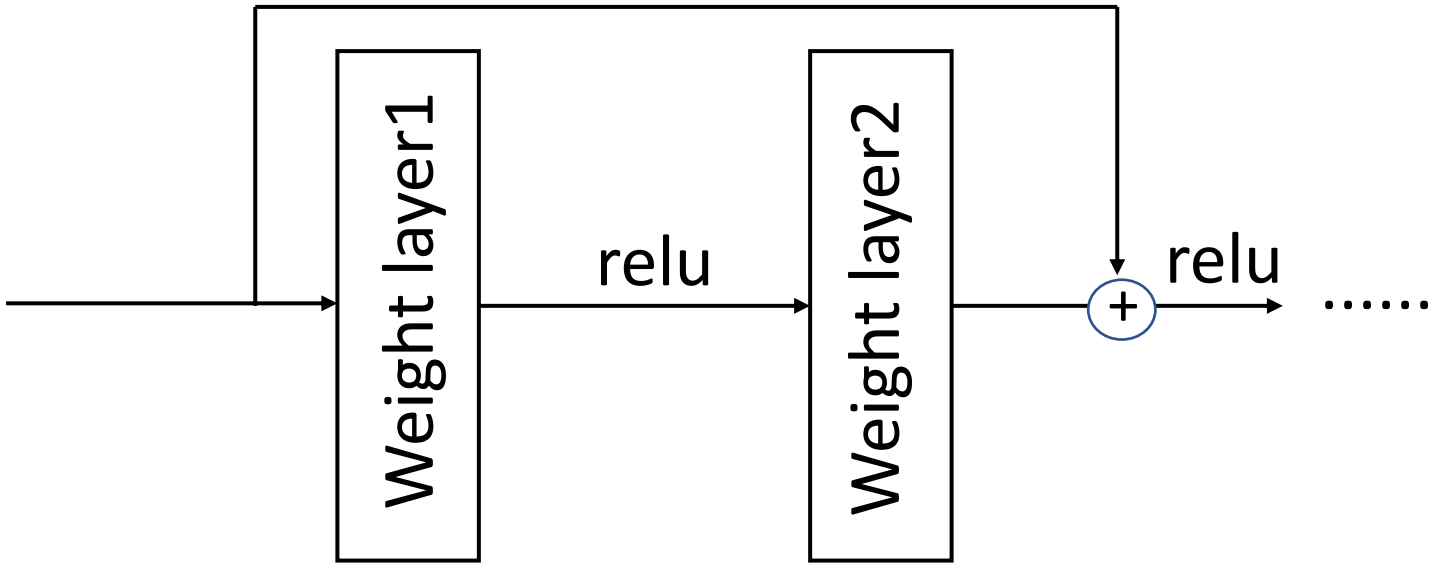
Residual neural networks

New state Old state

$$h_{t+1} = f(h_t)$$

Residuals

State: h_1 $h_2 = h_1 + f(h_1)$. ……



Euler's method and residual neural networks

$$h_{t+1} = h_t + f(h_t)$$

Euler's method and residual neural networks

$$h_{t+1} = h_t + f(h_t)$$
$$= h_t + \frac{\Delta t}{\Delta t} f(h_t)$$

Euler's method and residual neural networks

$$
\begin{aligned}
h_{t+1} &= h_t + f(h_t) \\
&= h_t + \frac{\Delta t}{\Delta t} f(h_t) \\
&= h_t + \Delta t \; G(h_t)
\end{aligned}
$$

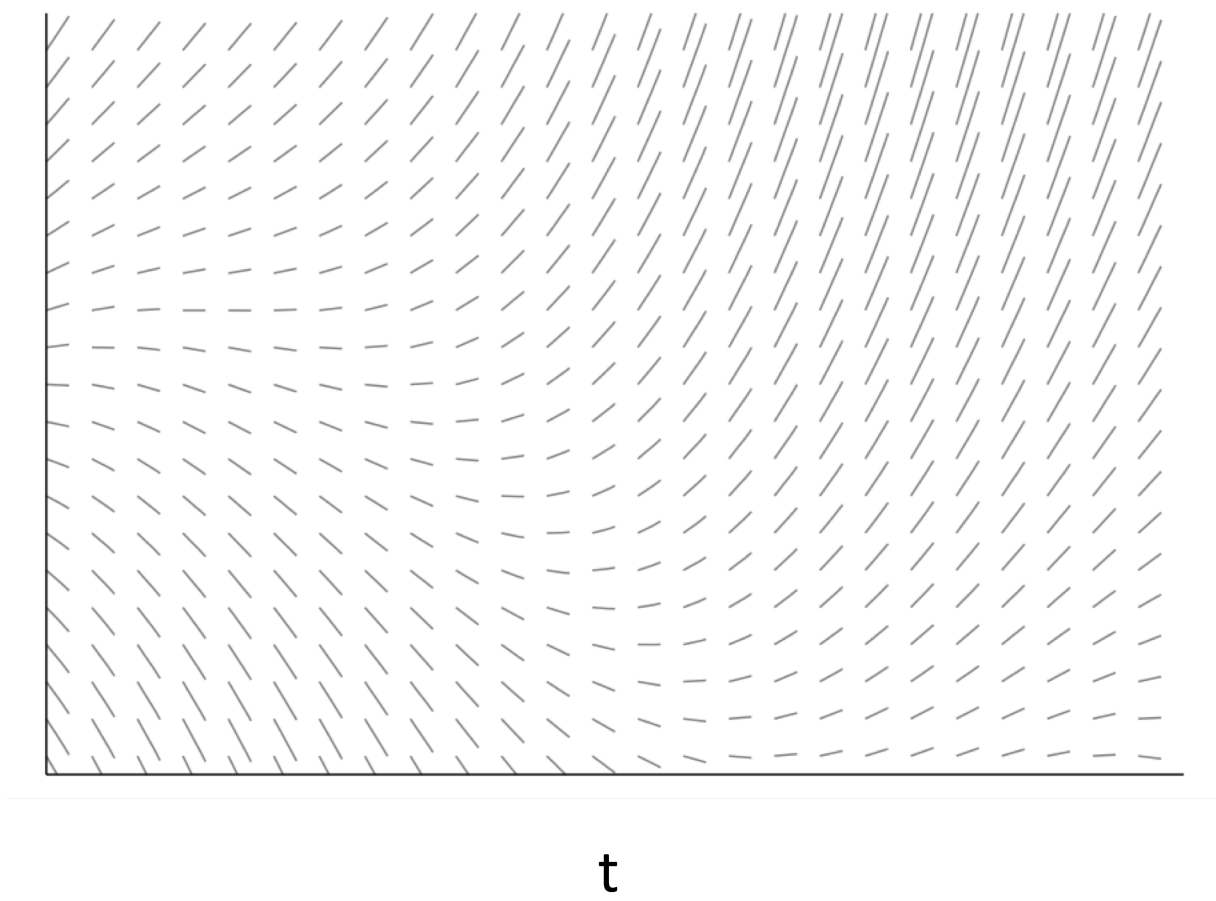
Euler's method and residual neural networks

$$h_{t+1} = h_t + f(h_t)$$
$$= h_t + \frac{\Delta t}{\Delta t} f(h_t)$$
$$= h_t + \Delta t\, G(h_t)$$

A single step of Euler's method for solving ODE

Background: ODE solvers

- State h changes with depth
- Depth-derivative: $\frac{dh}{dt} = G(h(t), t)$



Source: https://en.wikipedia.org/wiki/Euler_method

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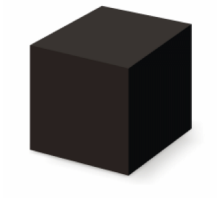
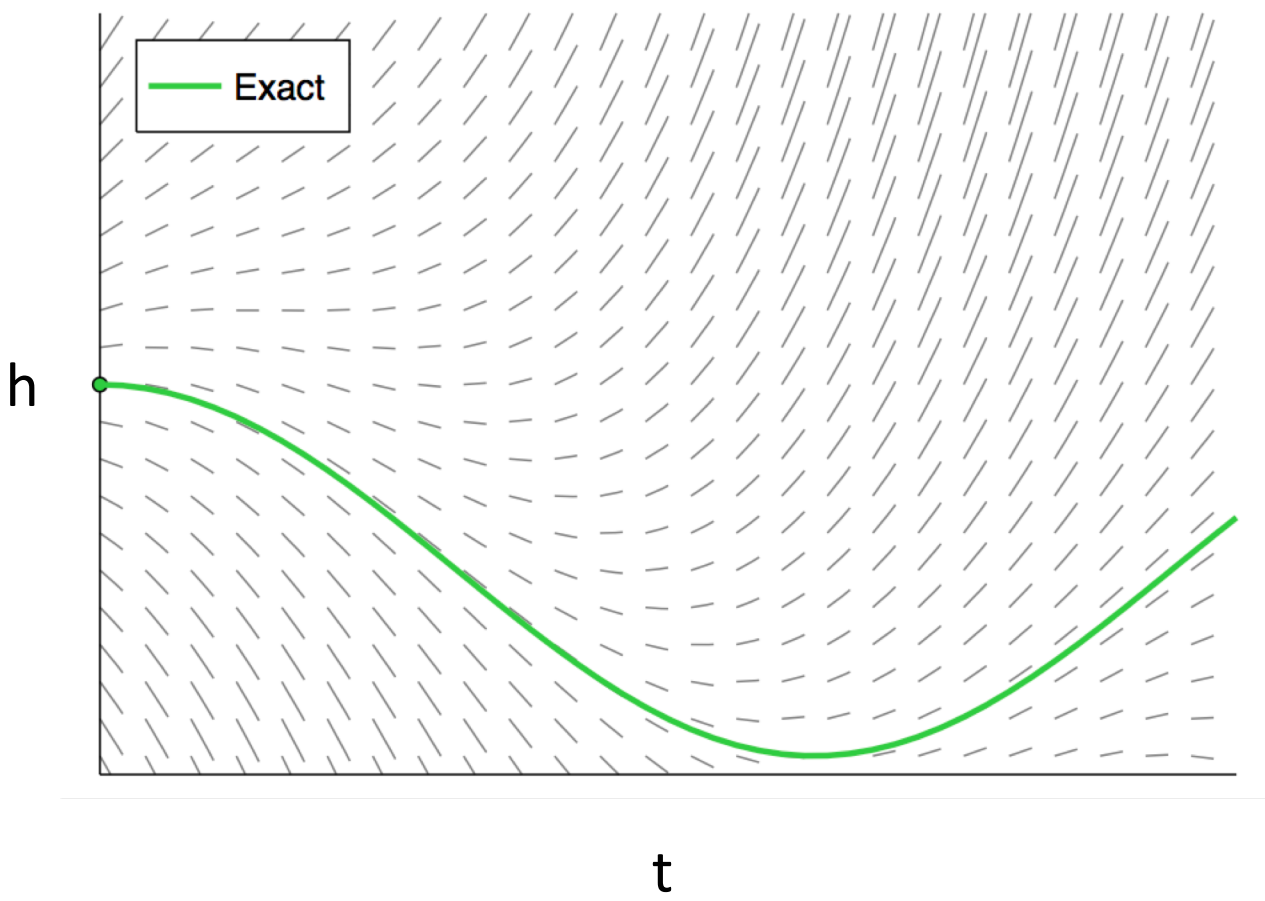
- Initial-value problem: given $\mathrm{h}(t_0)$, find

$$h(t_1) = h(t_0) + \int_{t_0}^{t_1} G(h(t), t, \theta)dt$$
$$= ODESolver(h(t_o), G, t0, t1, \theta)$$





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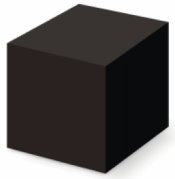
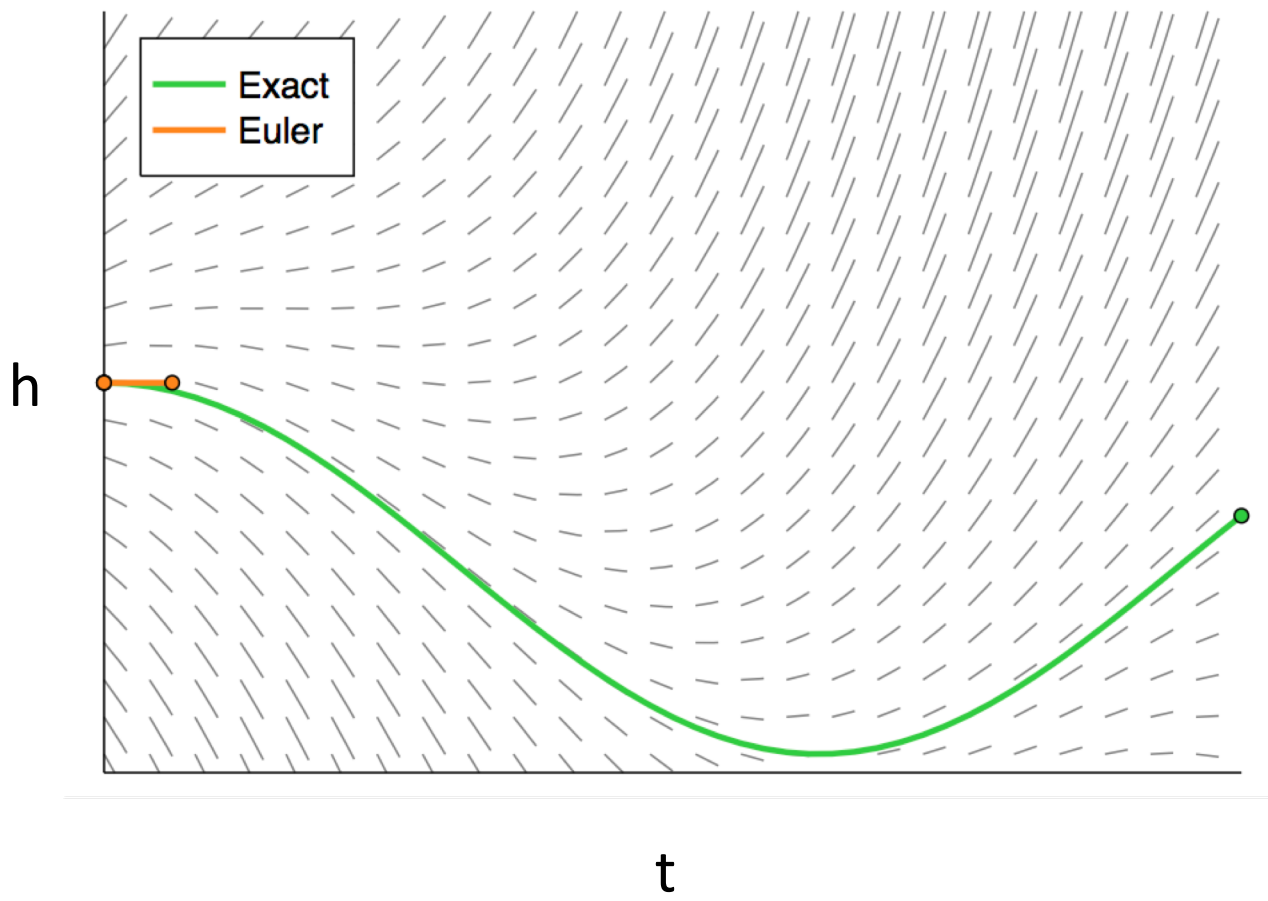


- Euler approximates with small steps:
  $h(t_1) = h(t_0) + (t_1 - t_0)G(h(t_0), t_0)$



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Background: ODE solvers

- Vector-valued h changes with depth
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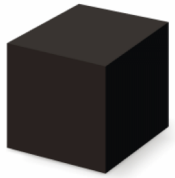

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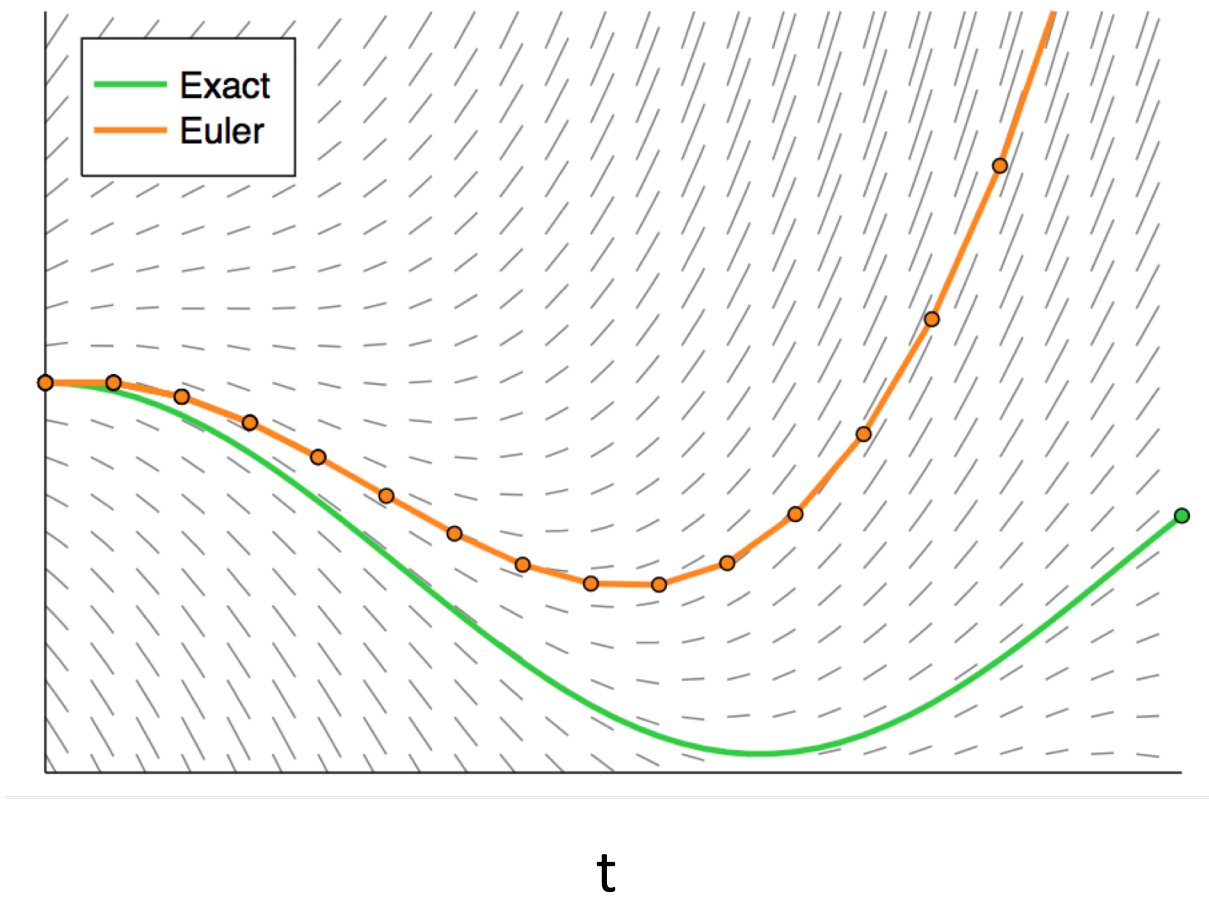

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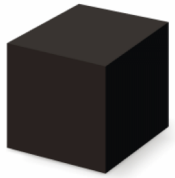

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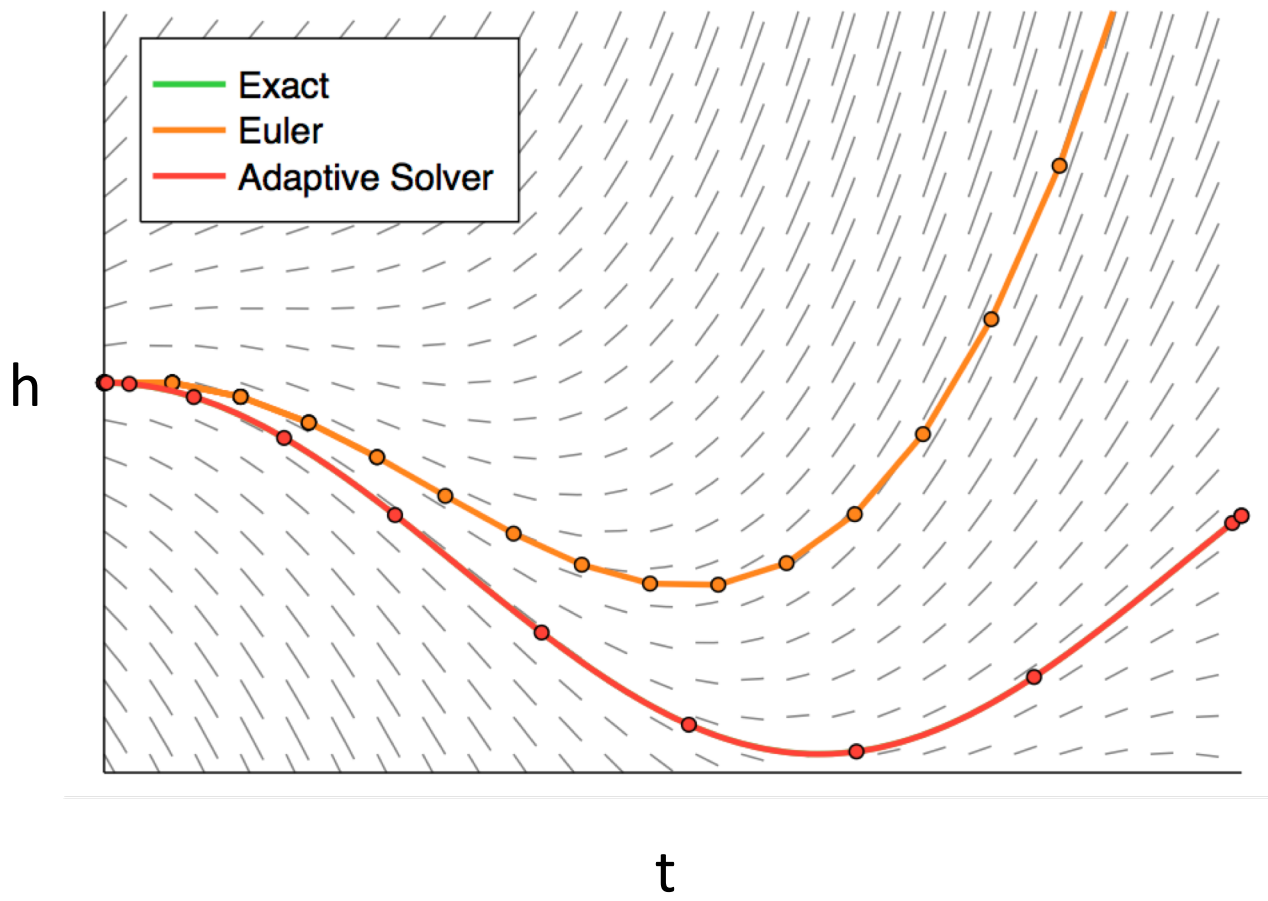
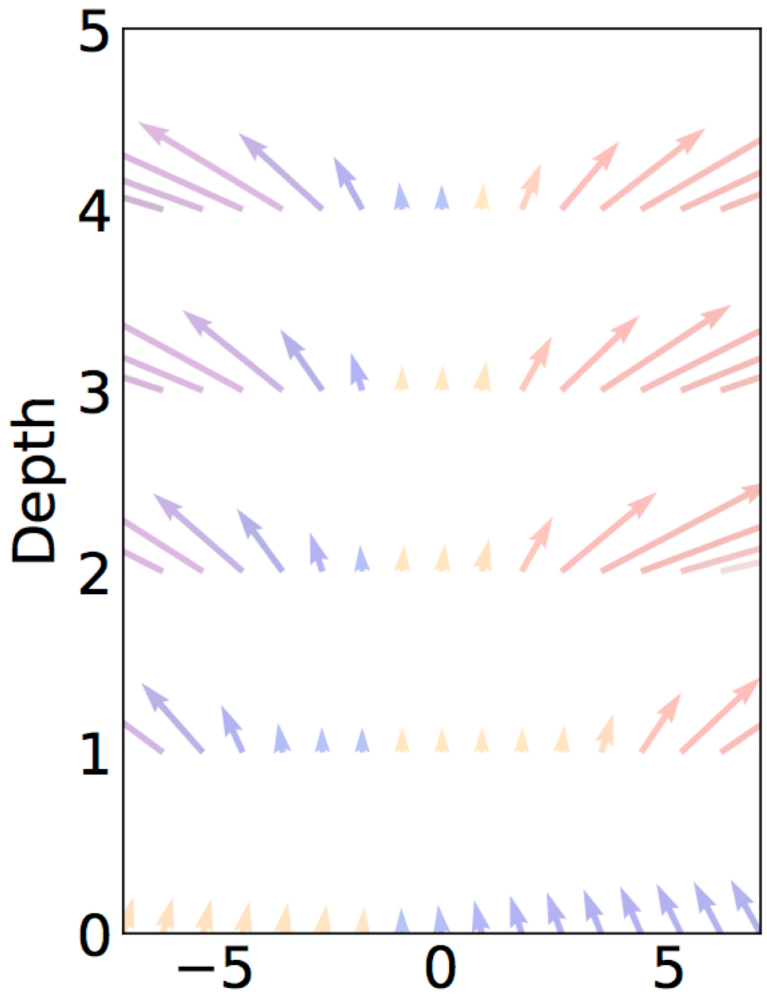


Source: https://en.wikipedia.org/wiki/Euler_method

ResNet

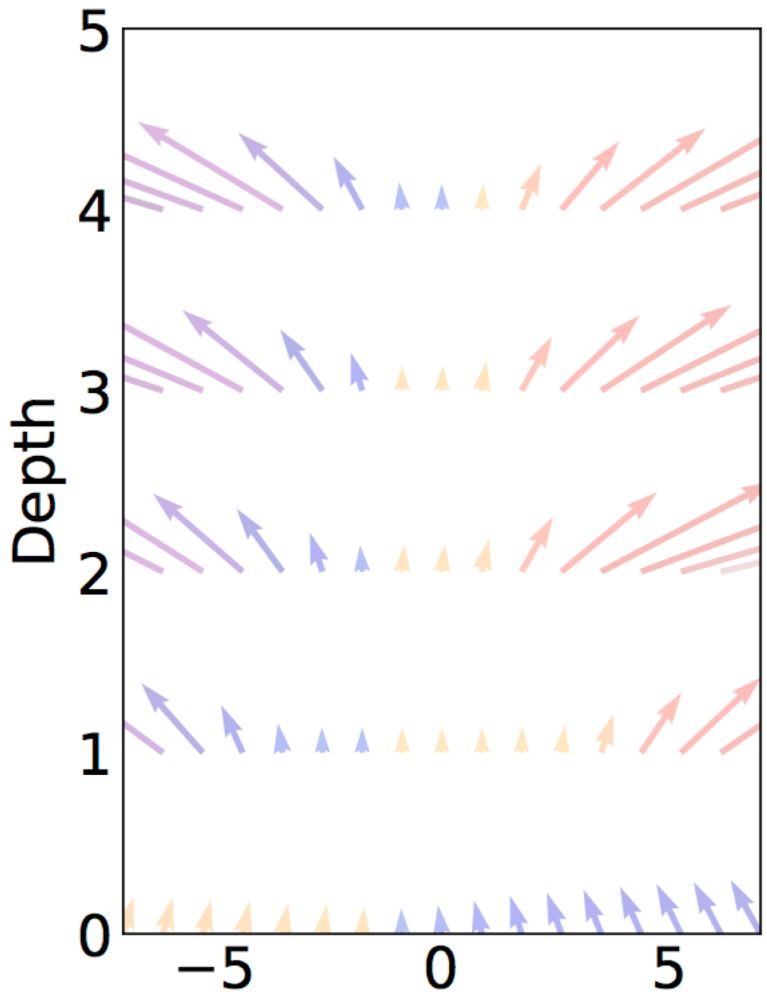
```
def G(h, t, θ):
  return nnet(h, θ[t])
```



ResNet

```
def G(h, t, θ):
  return nnet(h, θ[t])

def resnet(h):
  for t in [1:T]:
    h = h + G(h, t, θ)
  return h
```



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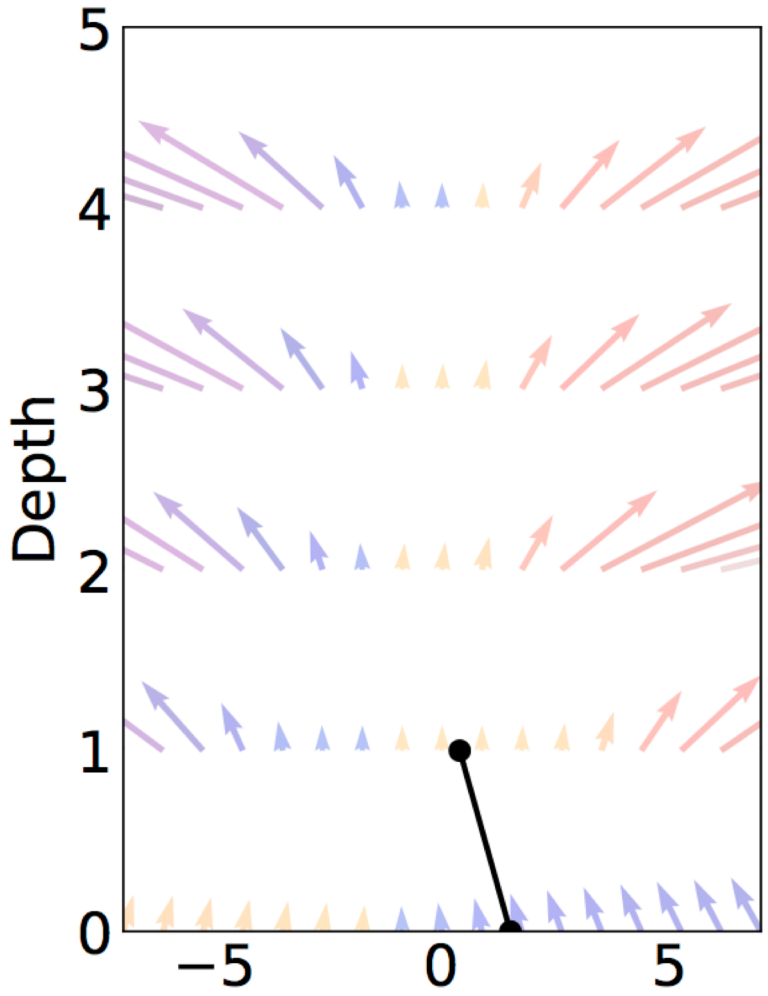

ResNet

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def resnet(h):
  for t in [1:T]:
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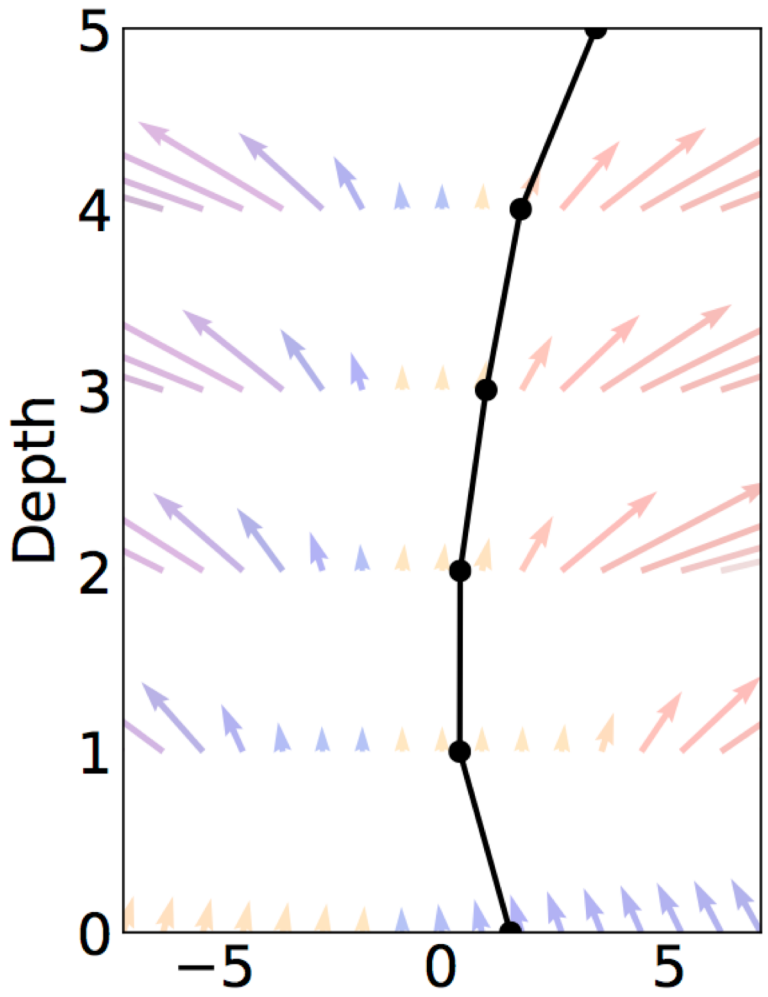
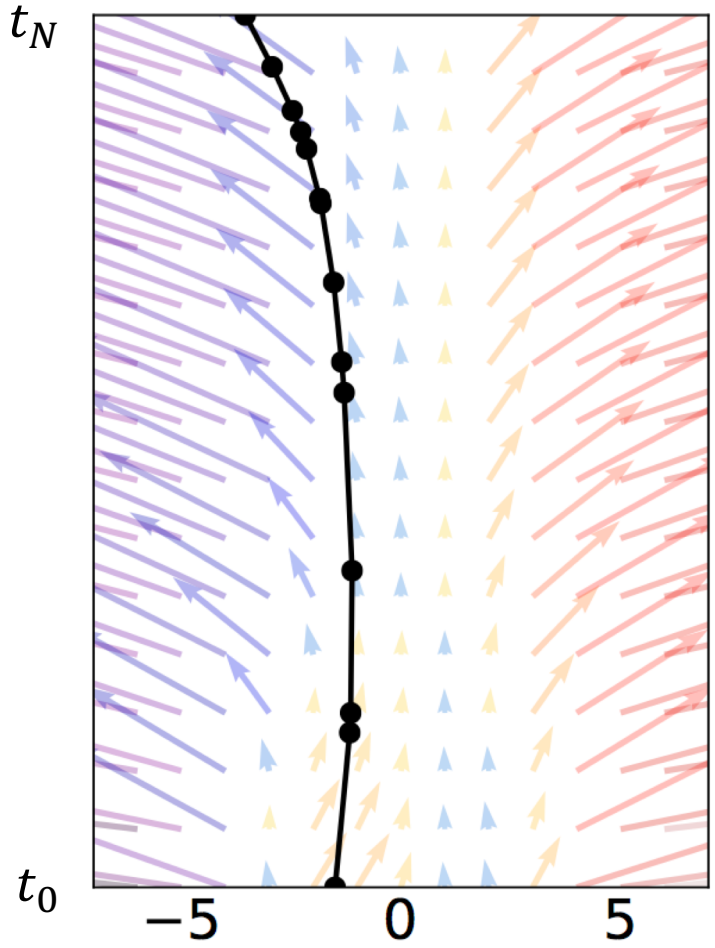
```



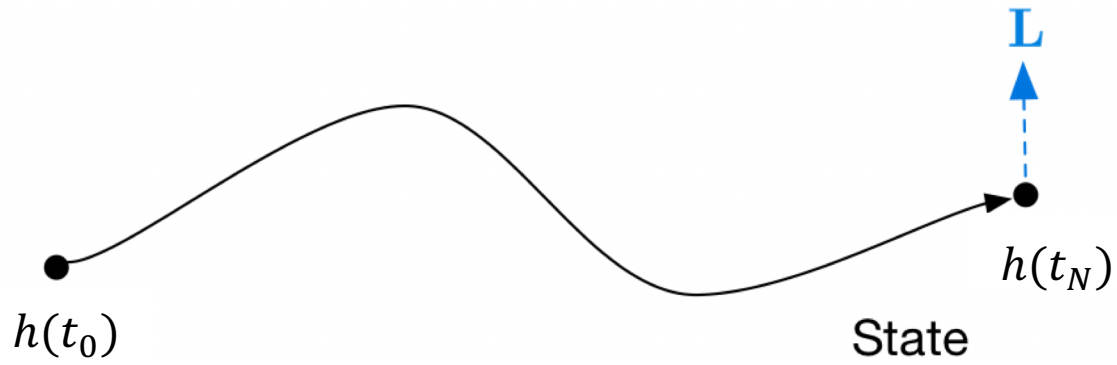
ODE-net

```
def G(h, t, θ):
  return nnet([h,t], θ)

def ODEnet(h, θ):
  return ODESolve(G, h, 0, 1, θ)
```



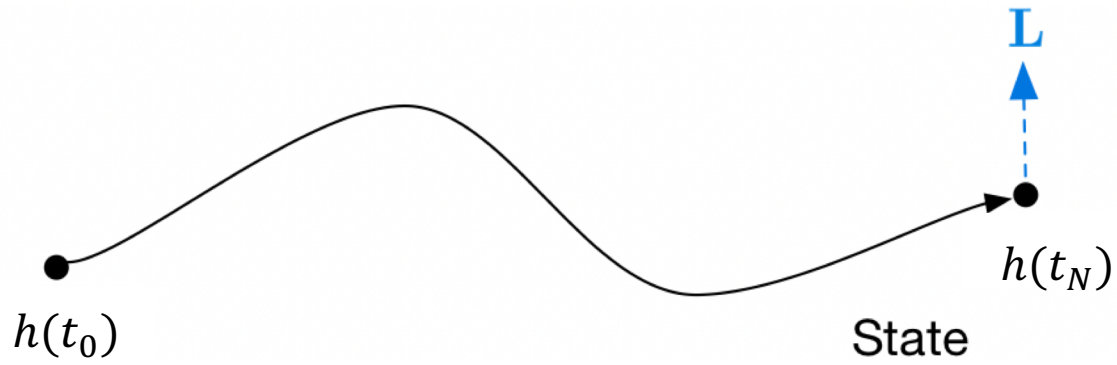
Training the beast



Loss function:

$$L(h(t_N)) = L(ODESolver(h(t_o), G, t_0, t_N, \theta))$$

Training the beast



Loss function:

$$L(h(t_N)) = L(ODESolver(h(t_o), G, t_0, t_N, \theta))$$

$$\frac{\partial L}{\partial h(t_0)}, \frac{\partial L}{\partial \theta}, \frac{\partial L}{\partial t_0}, \frac{\partial L}{\partial t_N} = ???$$

- Don't backprop through solver: High memory cost, extra numerical error
- Approximate the derivative, don't differentiate the approximation!

Backprop

Standard Backprop:

$$\frac{\partial \mathrm{h}_t}{\partial h_{t+1}} = \frac{\partial L}{\partial h_{t+1}} \frac{\partial G(h_t, \theta)}{\partial h_t}$$

$$\frac{\partial L}{\partial \theta_t} = \frac{\partial L}{\partial h_t} \frac{\partial G(h_t, \theta)}{\partial \theta_t}$$

Backprop

Standard Backprop:

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$$\frac{\partial L}{\partial \theta_t} = \frac{\partial L}{\partial h_t} \frac{\partial G(h_t, \theta)}{\partial \theta_t}$$

Adjoint sensitivity equations:

$$\mathrm{a(t)} = \frac{\partial L}{\partial h(t)}$$

Backprop

Standard Backprop:

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Adjoint sensitivity equations:

$$\mathrm{a(t)} = \frac{\partial L}{\partial h(t)}$$

Adjoint sensitivity:

$$\mathrm{a(t)} = \frac{\partial L}{\partial h(t)}$$

$$\frac{\partial a(t)}{\partial t} = a(t) \frac{\partial G(h(t), t, \theta)}{\partial h(t)}$$

$$\frac{\partial L}{\partial \theta_t} = \int_{t_N}^{t_0} a(t) \frac{\partial G(h(t), t, \theta)}{\partial \theta} dt$$

Backprop

Standard Backprop:

$$\frac{\partial \mathrm{h}_t}{\partial h_{t+1}} = \frac{\partial L}{\partial h_{t+1}} \frac{\partial G(h_t, \theta)}{\partial h_t}$$

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Adjoint sensitivity equations:

$$\mathrm{a(t)} = \frac{\partial L}{\partial h(t)}$$

Adjoint sensitivity:

Use autodiff to define it!

$$\mathrm{a(t)} = \frac{\partial L}{\partial h(t)}$$

$$\frac{\partial a(t)}{\partial t} = a(t) \frac{\partial G(h(t), t, \theta)}{\partial h(t)}$$

$$\frac{\partial L}{\partial \theta_t} = \int_{t_N}^{t_0} a(t) \frac{\partial G(h(t), t, \theta)}{\partial \theta} dt$$

Training the beast

- Define this quantity as an adjoint state: $\mathrm{a(t)} = \frac{\partial L}{\partial h(t)}$
- Its dynamics are given by another ODE:

  Given $\mathrm{a}(t_N)$, find $a(t_0) = \int_{t_N}^{t_0} a(t) \frac{\partial G(h(t),t,\theta)}{\partial h(t)} dt$

$$\frac{\partial L}{\partial h(t_0)}$$

Training the beast

- Define this quantity as an adjoint state: $\mathrm{a}(\mathrm{t}) = \frac{\partial L}{\partial h(t)}$
- Its dynamics are given by another ODE:

  Given $\mathrm{a}(t_N)$, find $a(t_0) = \int_{t_N}^{t_0} a(t) \frac{\partial G(h(t),t,\theta)}{\partial h(t)} dt$

$$\frac{\partial L}{\partial h(t_0)}, \frac{\partial L}{\partial \theta}, \frac{\partial L}{\partial t_0}, \frac{\partial L}{\partial t_n} = ???$$

$$\frac{dL}{d\theta} = \int_{t_N}^{t_0} a(t) \frac{\partial G(h(t),t,\theta)}{\partial \theta} dt$$

$$\frac{dL}{dt_0} = \int_{t_N}^{t_0} a(t) \frac{\partial G(h(t),t,\theta)}{\partial t} dt$$

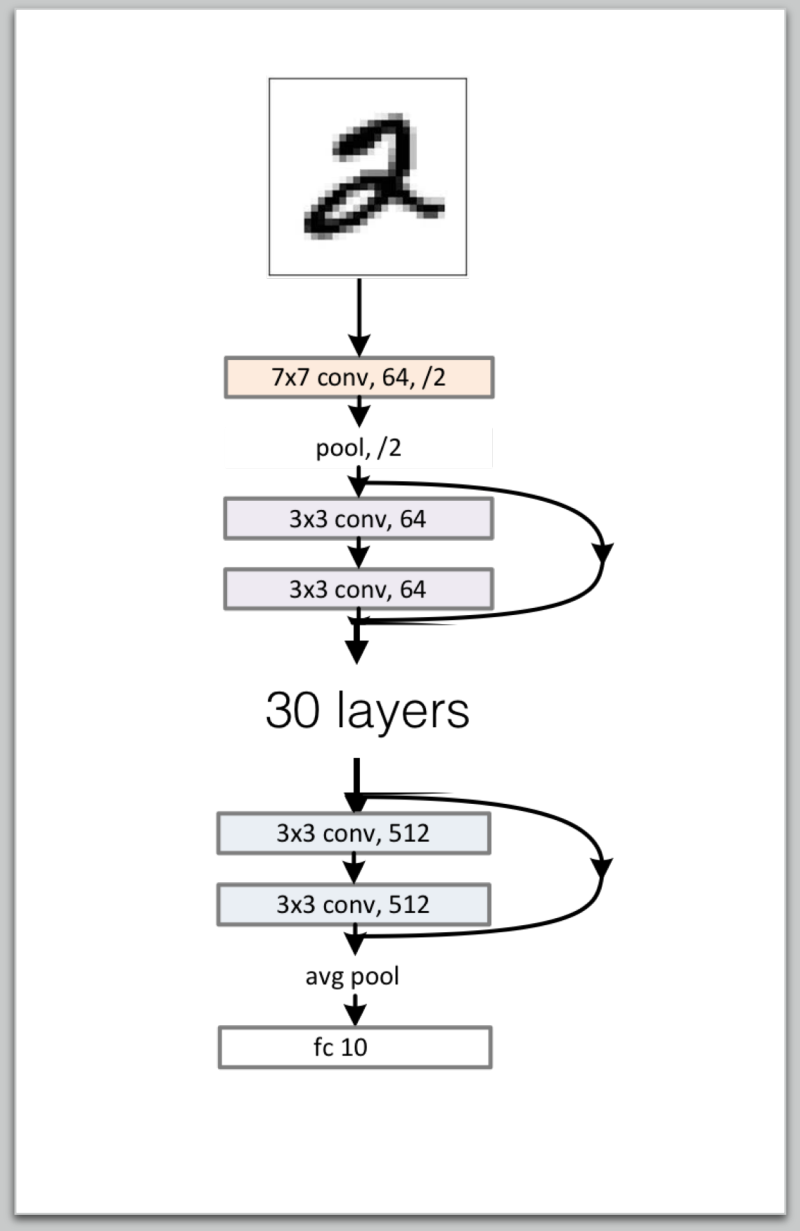
$$\frac{dL}{dt_N} = -a(t_N) \frac{\partial G(h(t),t,\theta)}{\partial t_N}$$

Break

Drop-in replacement for ResNet

	Test Error	# Params	Memory
1-Layer MLP	1.60%	0.24 M	-
ResNet	0.41%	0.60 M	O(L)

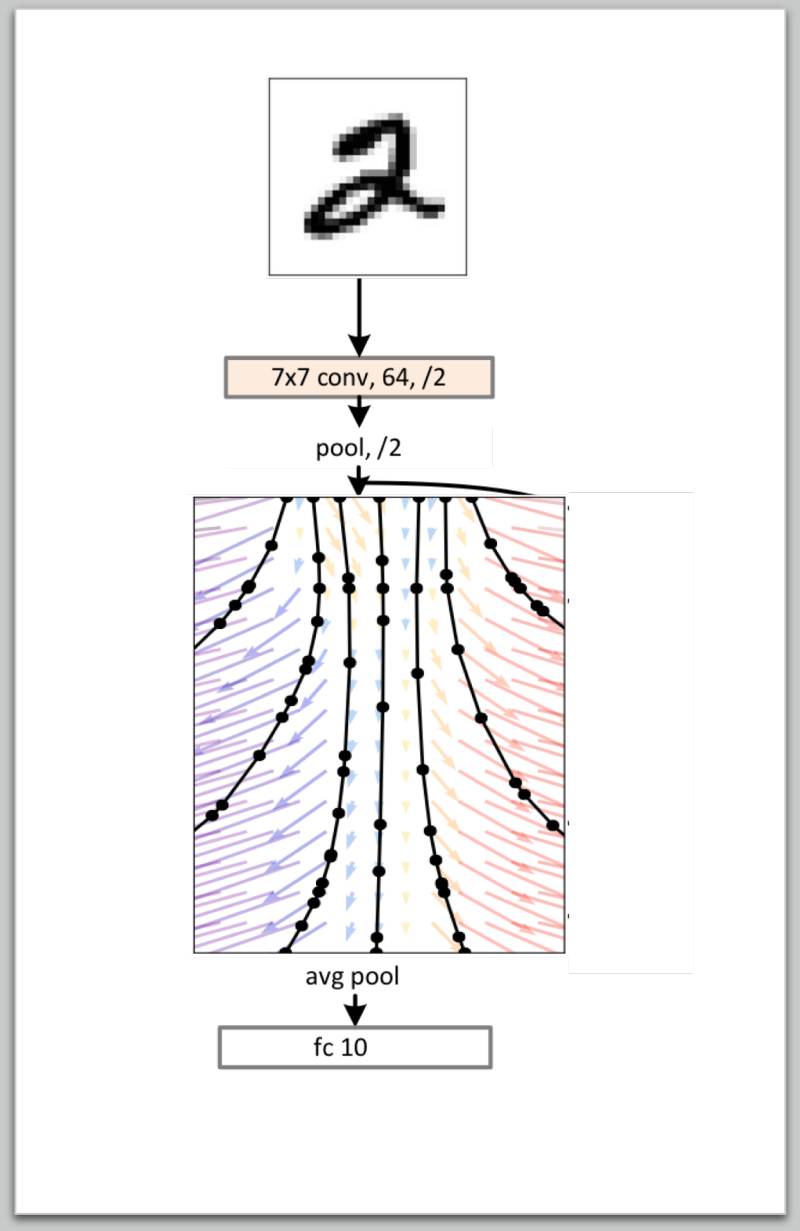
L: number of layers in ResNet



Drop-in replacement for ResNet

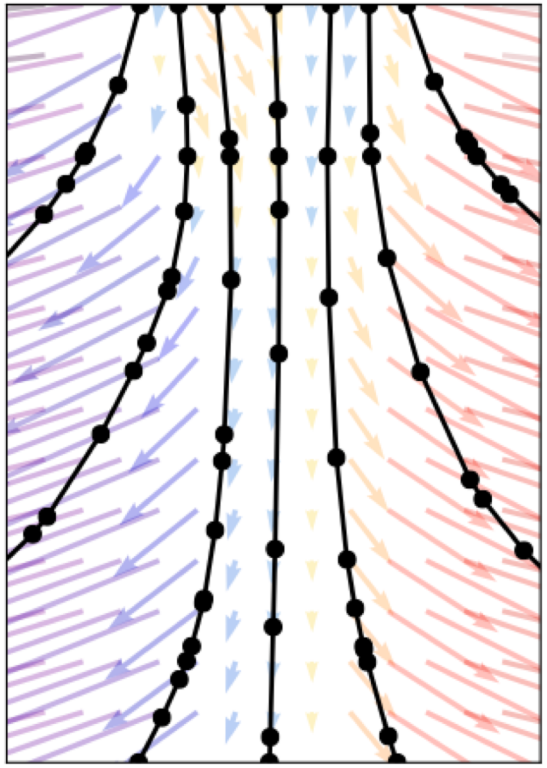
	Test Error	# Params	Memory
1-Layer MLP	1.60%	0.24 M	-
ResNet	0.41%	0.60 M	O(L)
ODE-Net	0.42%	0.22 M	O(1)

L: number of layers in ResNet



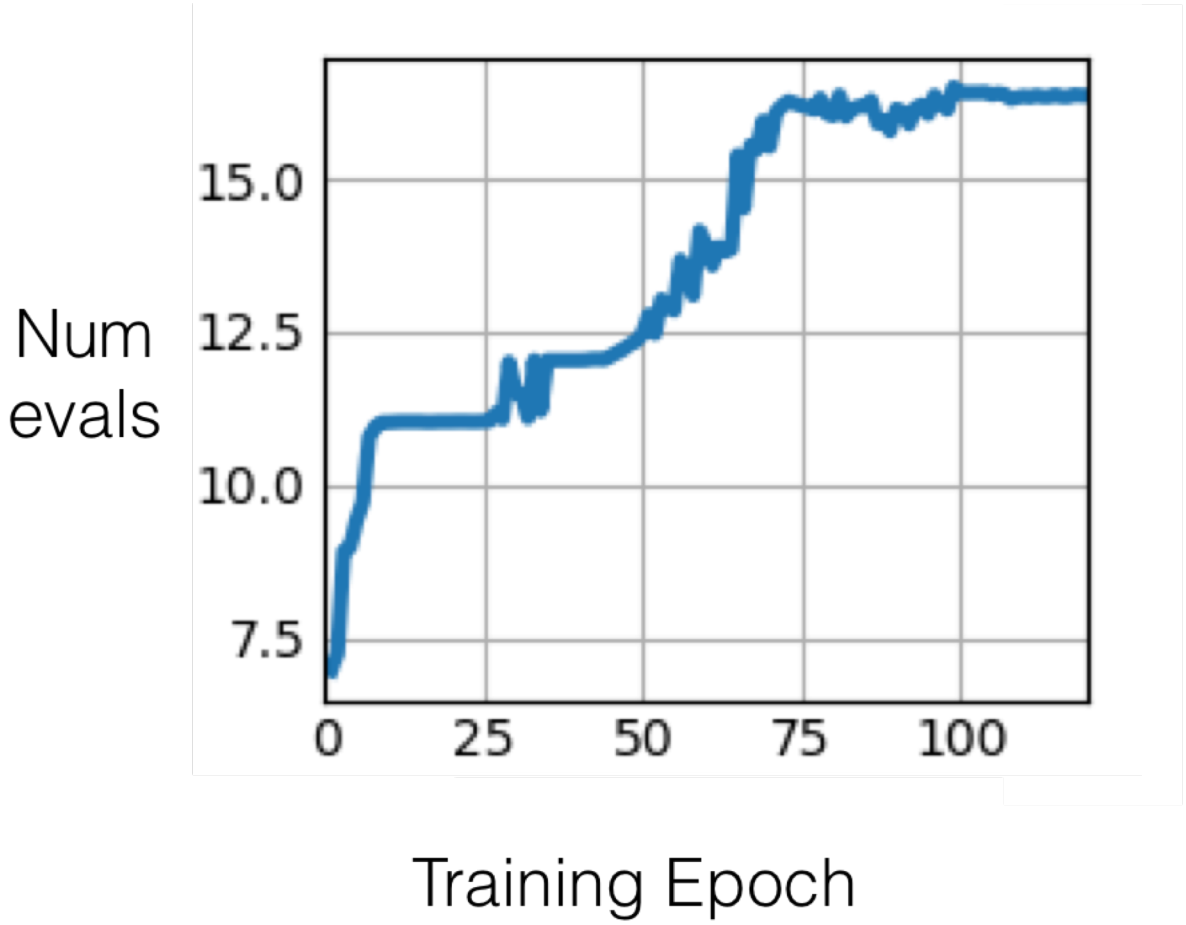
How deep are ODE-nets?

- No fixed number of layers
- Number of evaluations in ODE-nets ≈ Depth in ResNets



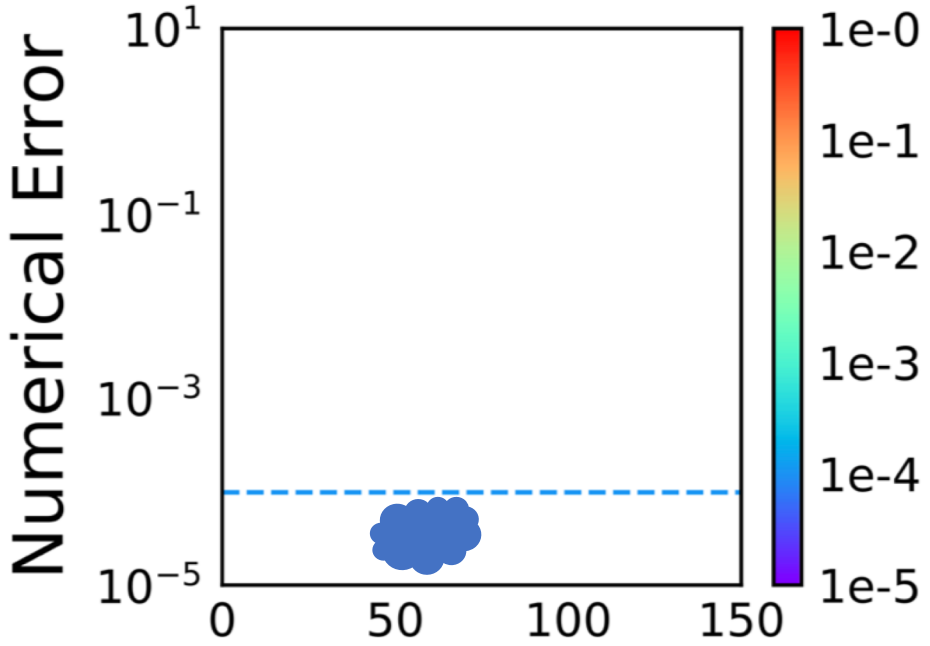
How deep are ODE-nets?

- No fixed number of layers
- Number of evaluations in ODE-nets ≈ Depth in ResNets
- Dynamics become more demanding to compute during training
- Downside: can't directly control the time-cost of the model during training



Explicit Error Control

ODESolver(h, x, t0, t1, θ, error)

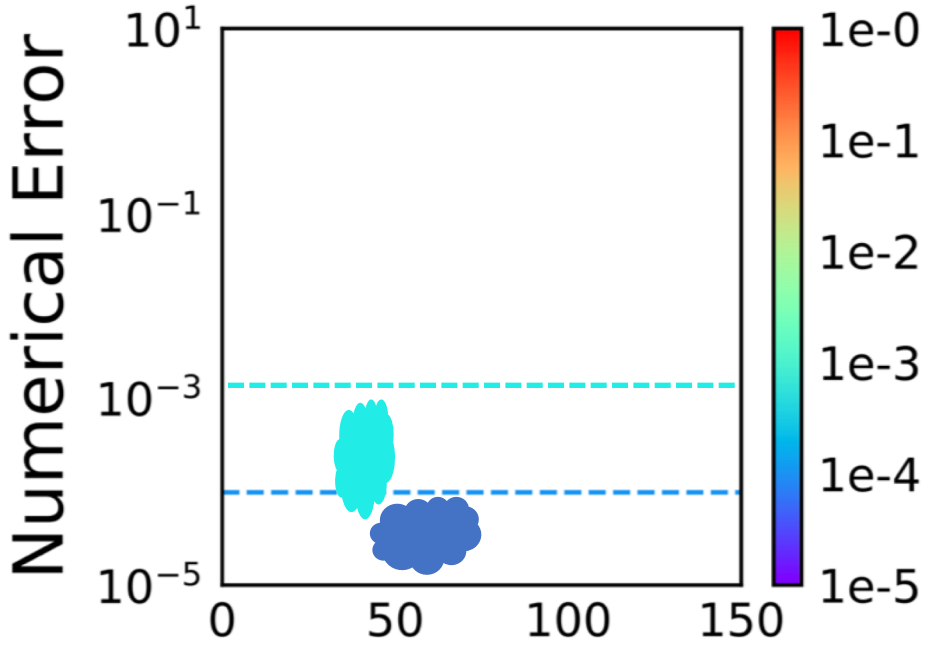


Number of dynamics evaluations

- Although we can't control the time cost of the model during training, we can control the time-cost at test time!!!!

Explicit Error Control

ODESolver(h, x, t0, t1, θ, error)



Number of dynamics evaluations

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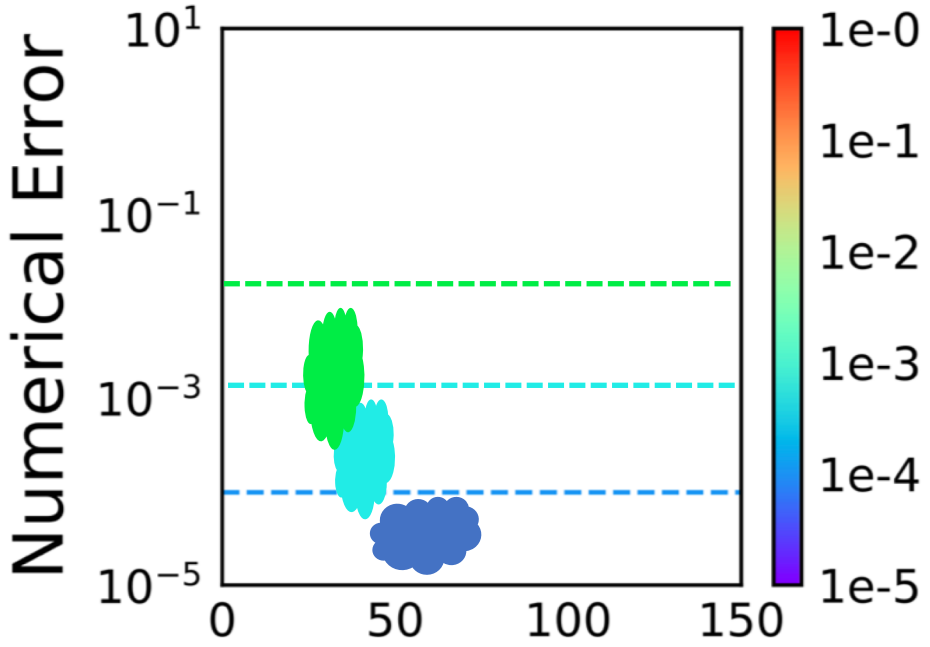

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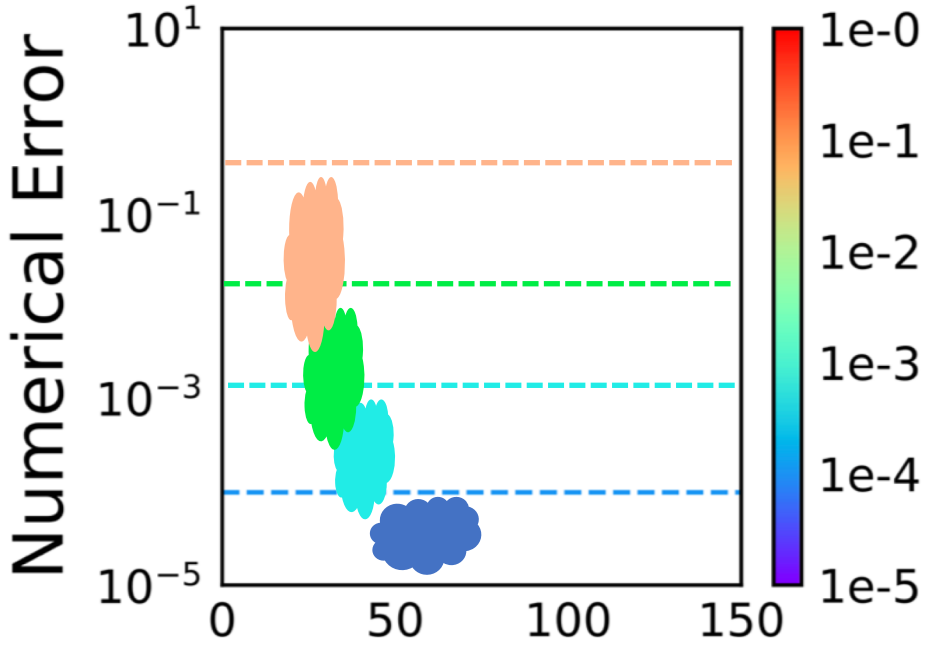

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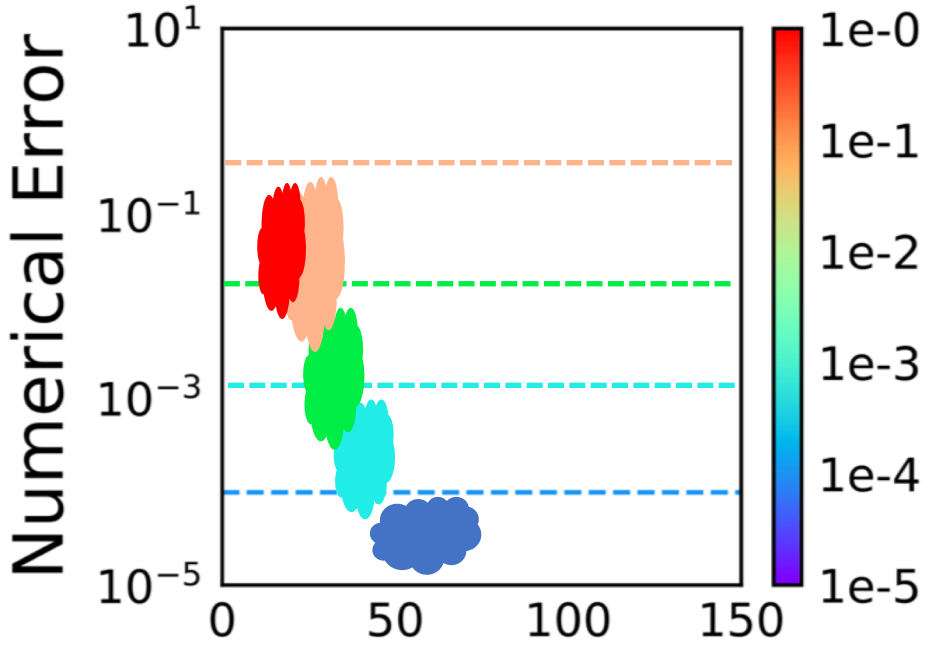
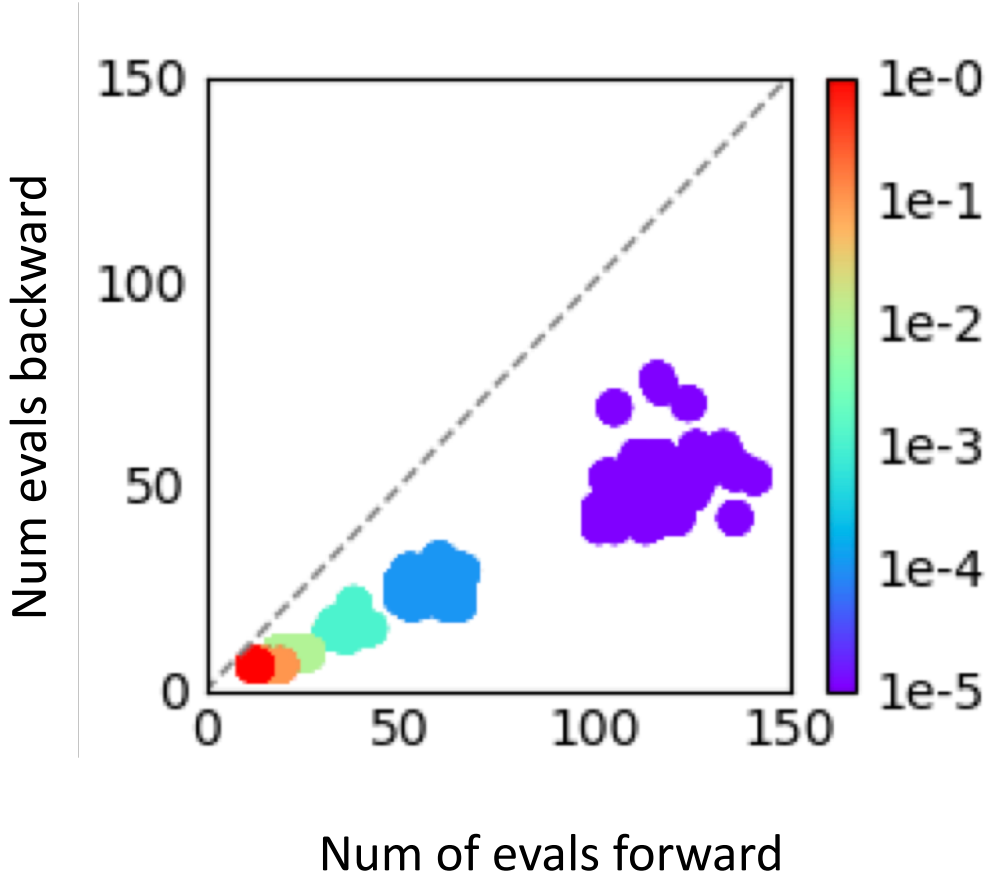


Number of dynamics evaluations

Reverse vs forward cost

Number of evaluations in the backward pass is roughly half of the forward (credit to adjoint sensitivity)



Major contributions

- New family of continuous-depth architectures (e.g. ResNets)
    1. No need to specific # of layers beforehand, just specific accuracy and it will train itself
    2. Adaptive computation
    3. Constant memory cost
- Other applications:

    Irregular time series data (medical history recorded at random time)

Discussions

- How to regularize the dynamics to need fewer evaluations?
- What basis for comparison would makes sense for the assessment of its utility generally?