

Neural Ordinary Differential Equations

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Presented by
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Convention

Number of layers are referred to as time (or t) in the following slides except in the case of RNNs

Resnets

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Where $h=1$

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OR

```
def f(z, t, θ):  
    return nnet(z, θ[t])
```

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

If time was continuous?

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```
def f(z, t, θ):  
    return nnet([z, t], θ)
```

```
def ODEnet(z, θ):  
    return ODEsolve(f, z, 0, 1, θ)
```

$$\mathbf{z}(t_1) = \mathbf{z}(t_0) + \int_{t_0}^{t_1} f(\mathbf{z}(t), t, \theta) dt$$

Training

$$L(\mathbf{z}(t_1)) = L\left(\mathbf{z}(t_0) + \int_{t_0}^{t_1} f(\mathbf{z}(t), t, \theta) dt\right) = L(\text{ODESolve}(\mathbf{z}(t_0), f, t_0, t_1, \theta))$$

- 1) This seems familiar. We can probably backprob through the ODESolver.

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Not a good idea. ODESolvers are not perfect. Backprob will take accumulate more losses over epochs

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Adjoint sensitivity method (Pontryagin et al., 1962)

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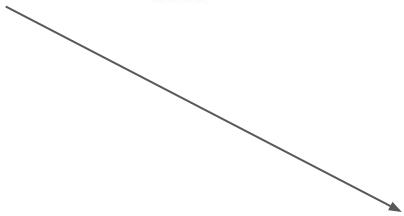
$$\mathbf{a}(t) = \partial L / \partial \mathbf{z}(t) \qquad \frac{d\mathbf{a}(t)}{dt} = -\mathbf{a}(t)^\top \frac{\partial f(\mathbf{z}(t), t, \theta)}{\partial \mathbf{z}}$$

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$$\frac{dL}{d\theta} = - \int_{t_1}^{t_0} \mathbf{a}(t)^\top \frac{\partial f(\mathbf{z}(t), t, \theta)}{\partial \theta} dt$$

Used to update
parameters of \mathbf{f}

Can be solved
using an ODE
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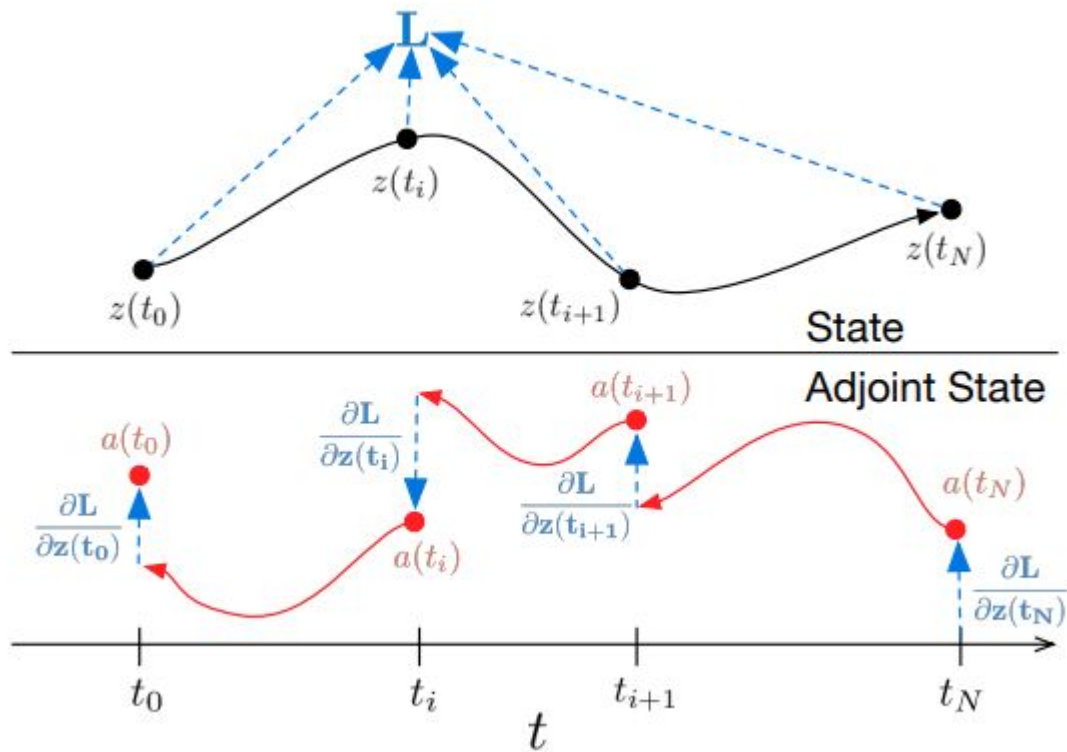
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Advantages

- $O(1)$ Memory gradients: as the activations are not stored at each layer, instead the dynamics are run backwards from the output to input

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- $O(1)$ Mem instead of $O(N)$



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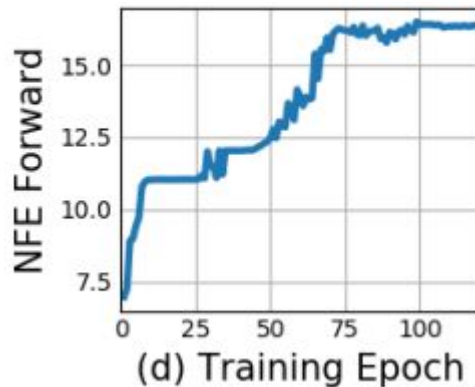
Table 1: Performance on MNIST. †From LeCun et al. (1998).

	Test Error	# Params	Memory	Time
1-Layer MLP†	1.60%	0.24 M	-	-
ResNet	0.41%	0.60 M	$\mathcal{O}(L)$	$\mathcal{O}(L)$
RK-Net	0.47%	0.22 M	$\mathcal{O}(\tilde{L})$	$\mathcal{O}(\tilde{L})$
ODE-Net	0.42%	0.22 M	$\mathcal{O}(1)$	$\mathcal{O}(\tilde{L})$

Advantages

Depth of ODEs

- It is left to the ODE solver. Hence it can change during training
- Approximately 2-4x the depth of resnet architectures - (shown empirically)

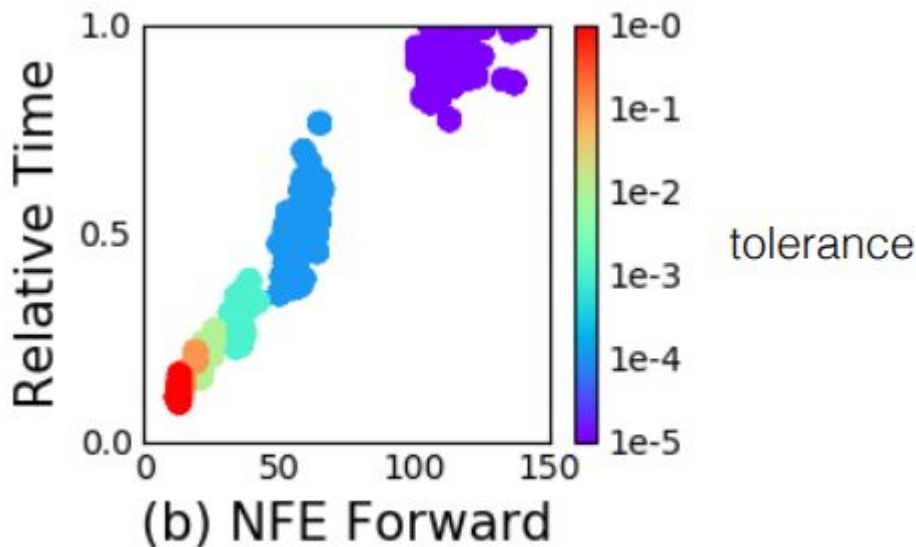


NFE- Number of forward evaluations

Advantages

Explicit Error Control.

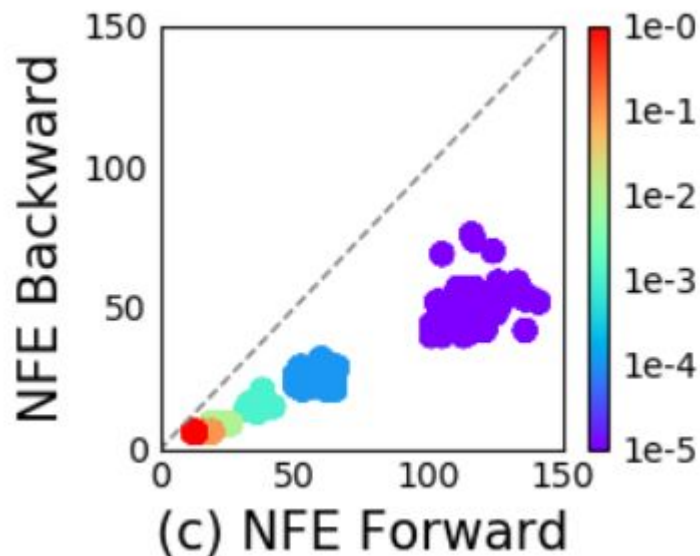
ODEsolver's error can be explicitly controlled. Hence trade-off between speed and error is in the user's hand



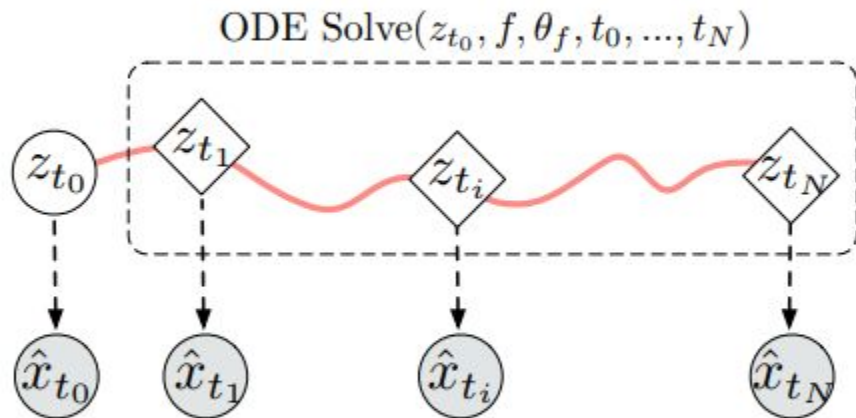
Advantages

Cost of evaluation (Forward pass vs Backward Pass)

Unlike, SGD based training methods for neural networks, NeuralODEs have a faster backward pass



Continuous-time models



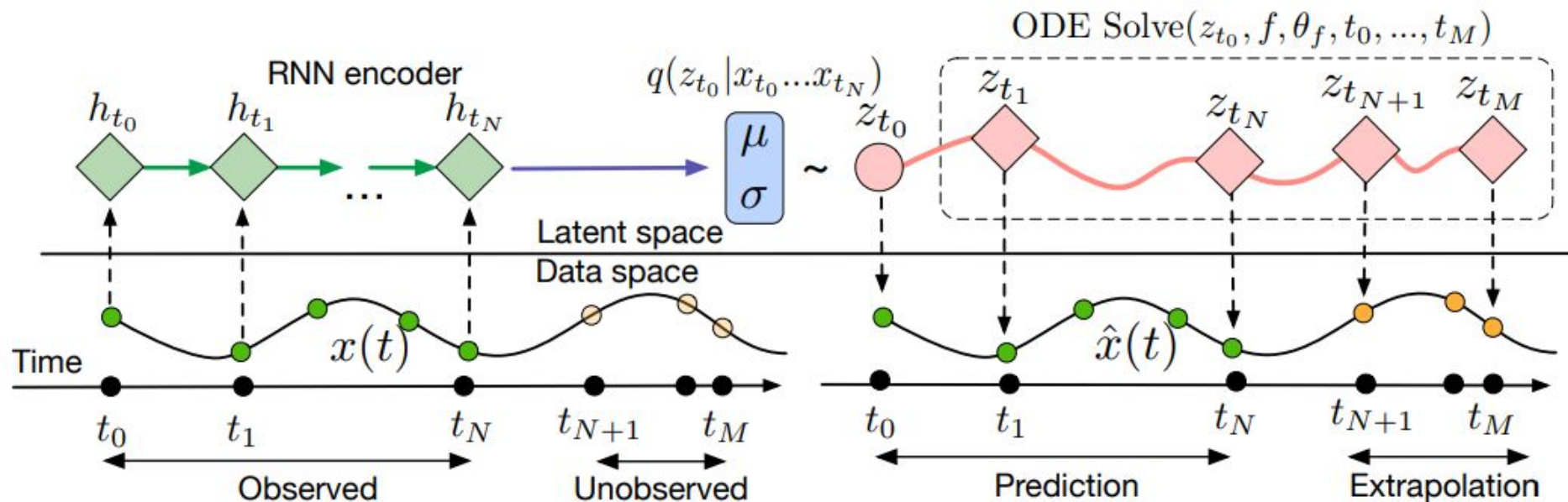
- Well-defined state at all times
- Dynamics separate from inference
- Irregularly-timed observations.

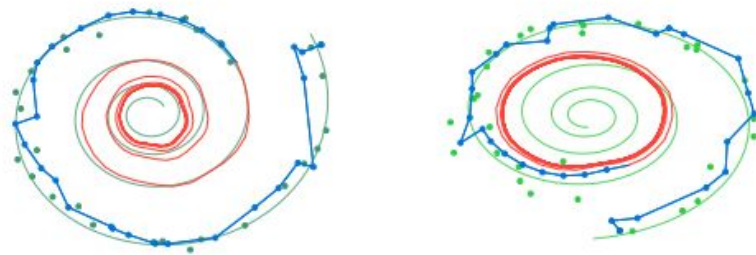
$$z_{t_0} \sim p(z_{t_0})$$

$$z_{t_1}, z_{t_2}, \dots, z_{t_N} = \text{ODESolve}(z_{t_0}, f, \theta_f, t_0, \dots, t_N)$$

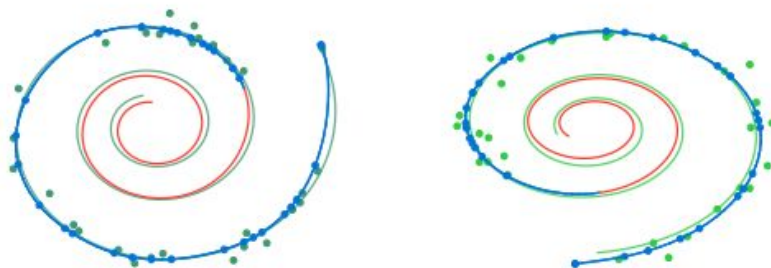
$$\text{each } x_{t_i} \sim p(x|z_{t_i}, \theta_x)$$

Handles unobserved variables and can extrapolate





(a) Recurrent Neural Network



(b) Latent Neural Ordinary Differential Equation

- Ground Truth
- Observation
- Prediction
- Extrapolation

