Dynamic System and Deep Learning[1]

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[1] **libookdynamic**.

Outline

Machine learning and deep learning

- Task: explore the information in data

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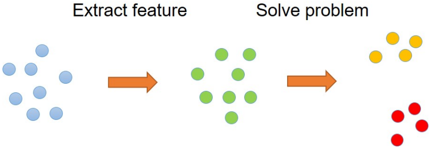
- A general scheme of machine learning: extract features from data and solve problem with features



Machine learning and deep learning

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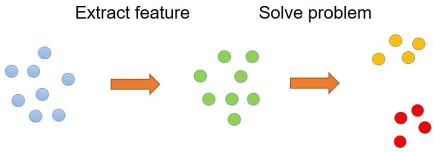
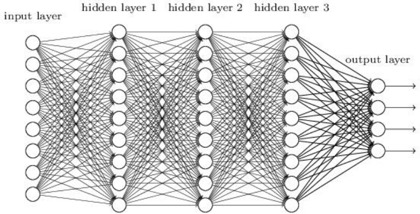


- Deep learning also follow the scheme, however in a deep way



Is deep learning explainable?

- Traditional machine learning models are explainable
  - meaningful features
  - less parameters
  - designable architecture

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We need an explainable model to model deep learning models!

ResNet is a typical deep learning model

- ResNet[2] is a milestone in deep learing

- A simple change on each block (layer) of DNN

$$x_{k+1} = v(x_k, \theta_k) \rightarrow x_{k+1} = x_k + v(x_k, \theta_k)$$

- ResNet can be really deep (more than 1000 layers) and is widely used in practice as a base model

[2]**he2016deep**.

The intuition to use dynamic system

The "model" we use is dynamic system

- Consider an ODE

$$\frac{dx}{dt} = F(x, t) \tag{1}$$

- Forward Euler method:

$$x_{t+h} = x_t + hF(x_t, t) \tag{2}$$

[3] **weinan2017proposal**.

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- Analogous to ResNet block

$$x_{k+1} = x_k + v(x_k, \theta_k) \tag{3}$$

- ResNet can be regarded as a numerical solution of an ODE by disretizing time[3]

[3] **weinan2017proposal**.

Connection to dynamic system

What can the connection of ResNet and dynamic system help?

- Formulize deep learning to optimal control problem
- Inspire new learning algorithms
- Inspire new architectures

Outline

The optimal control

Definition

Optimal control theory is a branch of mathematical optimization that deals with finding a control for a dynamical system over a period of time such that an objective function is optimized

- The dynamics

$$\dot{x}(t) = f(x(t), \theta(t)), \quad t \in [t_0, t_1], \quad x(t_0) = x_0$$

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- The cost function

$$J[\theta] = \int_{t_0}^{t_1} L(t, x(t), \theta(t))dt + \Phi\left(t_1, x\left(t_1\right)\right)$$

- L is called running cost and Φ is called terminal cost

Optimal control formulation

- The formulation of the optimal control problem is

$$\begin{aligned}
&\inf_{\theta} J[\theta] = \int_{t_0}^{t_1} L(t, x(t), \theta(t))dt + \Phi\left(t_1, x\left(t_1\right)\right) \\
&\text{subject to} \\
&\dot{x}(t) = f(t, x(t), \theta(t)), \quad t \in \left[t_0, t_1\right], \quad x\left(t_0\right) = x_0
\end{aligned} \tag{4}$$

- Based on the connection between dynamic system and deep learining, we can study the optimization of deep learning from the optimal control view

A mean-field optimal control formulation of deep learning

- Consider supervised learning with ResNet with K blocks (layers)
  - (x, y) is sampled from distribution μ
  - Let $\Phi(x_K, y)$ denote the loss function on data x and its label y
  - Let $L(x_k, \theta_k)$ denotes the regularizer of the k-th block (e.g., L_2 regularizer)

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  - Let $\Phi(x_K, y)$ denote the loss function on data x and its label y
  - Let $L(x_k, \theta_k)$ denotes the regularizer of the k-th block (e.g., L_2 regularizer)
- The supervised learning problem can be formulated as

$$\inf_{(\theta(0),\cdots,\theta(K-1))\in\Theta^K} \mathbb{E}_{(x,y)\sim\mu}\left[\Phi(x(K), y) + \sum_{k=0}^{K-1} L(x(k), \theta(k))\right]$$

subject to

$$x(k+1) = x(k) + f(x(k), \theta(k)), \quad k = 0, \cdots, K-1, \quad x(0) = x$$

A mean-field optimal control formulation of deep learning

- The continuous-time version of the supervised learning problem is

$$\begin{aligned} &\inf_{\theta \in L^{\infty}([0,T],\Theta)} \mathbb{E}_{(x,y)\sim\mu} \left[\Phi(x(T), y) + \int_0^T L(x(t), \theta(t))dt\right] \\ &\text{subject to} \\ &\dot{x}(t) = f(x(t), \theta(t)), \quad t \in [0, T], \quad x(0) = x \end{aligned} \tag{5}$$

- Mean-field: emphasize the fact that we seek an optimal control that is shared with all input-label pairs (x, y).
- They are jointly distributed according to μ

Optimality conditions

- Pontryagin's maximum principle (PMP) gives necessary condition for optimality for our problem[4]

[4] **li2017maximum**.

Optimality conditions

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- We first define the Hamiltonian

$$
\begin{aligned}
&H : \mathbb{R} \times \mathbb{R}^d \times \mathbb{R}^d \times \Theta \to \mathbb{R} \\
&H(t, x, p, \theta) = p^\top f(t, x, \theta) - L(t, x, \theta)
\end{aligned} \tag{6}
$$

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Pontryagin's maximum principle

If θ^* is optimal and x^* is the corresponding state trajectory, then there exists an absolutely continuous process p

$$\begin{aligned} &\dot{x}^*(t) = \nabla_p H\left(t, x^*(t), p^*(t), \theta^*(t)\right), \quad x^*\left(t_0\right) = x_0 \\ &\dot{p}^*(t) = -\nabla_x H\left(t, x^*(t), p^*(t), \theta^*(t)\right), \quad p^*\left(t_1\right) = -\nabla_x \Phi\left(x^*\left(t_1\right), y\right) \\ &H\left(t, x^*(t), p^*(t), \theta^*(t)\right) \geqslant H\left(t, x^*(t), p^*(t), \theta\right) \\ &\forall \theta \in \Theta \text{ and a.e. } t \in [t_0, t_1] \end{aligned} \tag{7}$$

[4] **li2017maximum**.

Understanding PMP from nonlinear program

- We can view the optimal control problem as a nonlinear program where the constraint is the ODE
- Co-state process p^* plays the role of a continuous-time analogue of Lagrange multipliers.
- The key difference between the PMP and KKT conditions is the Hamiltonian maximization condition, which is stronger than a typical first-order condition that assumes smoothness with respect to θ
- In particular, the PMP says that H is not only stationary, but globally maximized at an optimal control

Outline

Control inspired learning algorithm

Method of successive approximations (MSA)

start with an initial guess θ^0, at the n^{th} iteration we solve

$$\begin{aligned}
&\dot{x}^n(t) = f\left(x^n(t), \theta^n(t)\right) && x^n(0) = x \\
&\dot{p}^n(t) = -\nabla_x H\left(x^n(t), p^n(t), \theta^n(t)\right) && p^n(T) = -\nabla_x \Phi\left(x^n(T), y\right) \\
&\theta^{n+1}(t) = \arg\max_{\theta \in \Theta} H\left(x^n(t), p^n(t), \theta\right).
\end{aligned} \tag{8}$$

- if (x^n, p^n, θ^n) converges, then the limit must be a solution of the PMP

Connection between BP and MSA

- Recall
$$H(t,x,p,\theta) = p^\top f(t,x,\theta) - L(t,\theta) \tag{9}$$
Since
$$\dot{p}^n(t) = -\nabla_x H\left(x^n(t), p^n(t), \theta^n(t)\right), \quad p^n(T) = -\nabla_x \Phi\left(x^n(T), y\right) \tag{10}$$
It is easy to see
$$p^n(t) = -\nabla_{x^n(t)} \Phi\left(x^n(T), y\right) \tag{11}$$

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- Then we have

$$\begin{aligned} \nabla_{\theta(t)} J(\theta) &= \nabla_{x(t)} \Phi\left(x(T), y\right) \nabla_{\theta(t)} x(t) + \nabla_{\theta(t)} L(t, \theta) \\ &= -p(t) \nabla_{\theta(t)} f(x(t), \theta(t)) + \nabla_{\theta(t)} L(t, \theta) \\ &= \nabla_{\theta(t)} H \end{aligned} \tag{12}$$

Connection between BP and MSA

- For BP

$$\theta^{n+1}(t) = \theta^n(t) + \eta\nabla_\theta H\left(x^n(t), p^n(t), \theta\right) \tag{13}$$

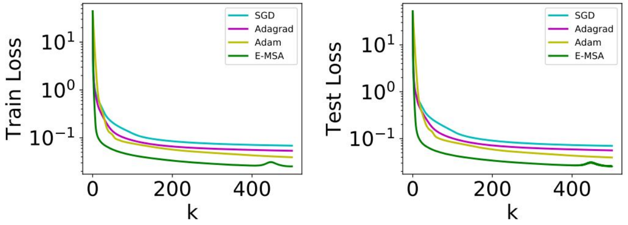
- For MSA

$$\theta^{n+1}(t) = \arg\max_{\theta\in\Theta} H\left(x^n(t), p^n(t), \theta\right) \tag{14}$$

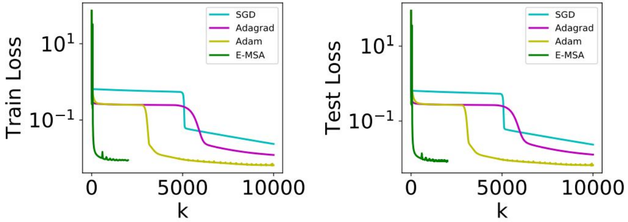
- MSA is a generalization of the back-propagation algorithm

Experiments of MSA

The target function is $F(x) = \sin(x)$
Line 1: good initialization; line 2: bad initialization



(a)



Layer parallel training algorithm[5]

- Note that the equation for x has a initial condition, the equation for p has a terminal condition

$$x(0) = x, \quad p(T) = -\nabla_x \Phi\left(x(T), y\right)$$

We can break it down to two sub-problems

[5] **parpas2019predict**.

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  We can break it down to two sub-problems
- Let $S = T/2$,
  - P1: $(t \in [0, S])$

$$\begin{aligned} \dot{p}^n(t) &= -\nabla_x H\left(x^{n-1}(t), p^n(t), \theta^n(t)\right) \quad p^n(S) = p^{n-1}(S) \\ \dot{x}^n(t) &= f\left(x^n(t), \theta^n(t)\right) \quad x^n(0) = x \end{aligned} \tag{15}$$

  - P2: $(t \in [S, T])$

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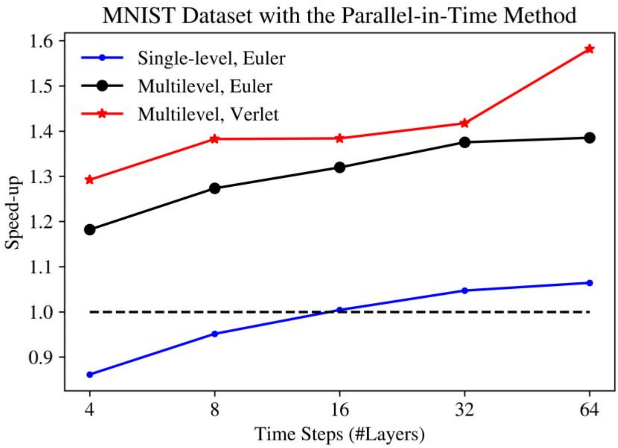
- P1 and P2 can be run in parallel

[5] **parpas2019predict**.

Layer-parallel vs data-parallel



Layer-parallel implementation has more merit when network is deep

Outline

Control inspired architecture

Stability of linear system

A simple linear ODE $\dot{x}(t) = Ax(t), \quad x(0) = x_0 \Rightarrow x(t) = e^{tA}x_0$
$\lambda_1, \cdots, \lambda_d \in \mathbb{C}$ are the eigenvalues of A. x_ϵ is a small perturbation of x.
Then 1) if $\mathcal{R}(\lambda_i) \leqslant 0 \Rightarrow \|x(t) - x_\epsilon(t)\|$ is bounded; 2) if $\mathcal{R}(\lambda_i) > 0$ for some $i \Rightarrow \|x(t) - x_\epsilon(t)\| \to \infty$ as $t \to \infty$

[6] **haber2017stable**.

Control inspired architecture

Stability of linear system

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- If A is anti symmetric,i.e., $A^T = -A$ then $\mathcal{R}(\lambda_i) = 0$
- Anti symmetric can be constructed by $A = B - B^T$
- One can reparameterize the neural network in a similar way[6]

$$\dot{x}(t) = \sigma(W(t)x(t)+b(t)) \rightarrow \quad \dot{x}(t) = \sigma\left(\left[V(t) - V(t)^\top\right] x(t) + b(t)\right) \tag{17}$$

[6] **haber2017stable**.

Experiments

Comparison of training error (TE) and validation error (VE)

	ResNet		anti symmetric ResNet		Hamiltonian Verlet	
layers	TE	VE	TE	VE	TE	VE
4	0.96%	1.71%	1.13%	1.70%	1.49%	2.29%
8	0.80%	1.59%	0.92%	1.46%	0.82%	1.60%
16	0.73%	1.53%	0.91%	1.38%	0.35%	1.58%

The antisymmetric ResNet giving slightly lower validation errors at each level

Backward Euler discretization[7]

- ResNet corresponds to the forward Euler discretization

[7] **lu2018beyond**.

Backward Euler discretization[7]

- ResNet corresponds to the forward Euler discretization
- The backward Euler is

$$\begin{aligned} \widehat{x}(k+1) &= \widehat{x}(k) + \Delta t f((k+1)\Delta t, \widehat{x}(k+1)) \\ &\Downarrow \\ \widehat{x}(k+1) &= (I - \Delta t f((k+1)\Delta t, \cdot))^{-1}(\widehat{x}(k)) \end{aligned} \tag{18}$$

- For linear f one can expand as

$$\widehat{x}(k+1) \approx \widehat{x}(k) + \Delta t f((k+1)\Delta t, \widehat{x}(k)) + \Delta t^2 \left[f((k+1) \ \ \Delta t, \cdot)^2\right](\widehat{x}(k)) \tag{19}$$

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- In numerical analysis, backward Euler enjoy better stability

[7] **lu2018beyond**.

Linear multi-step discretization

- Another family of networks based on linear multi-step discretization

$$\widehat{x}(k+1) = (1-\alpha_k)\,\widehat{x}(k) + \alpha_k \widehat{x}(k-1) + \Delta t f(k\Delta t, \widehat{x}(k)) \tag{20}$$

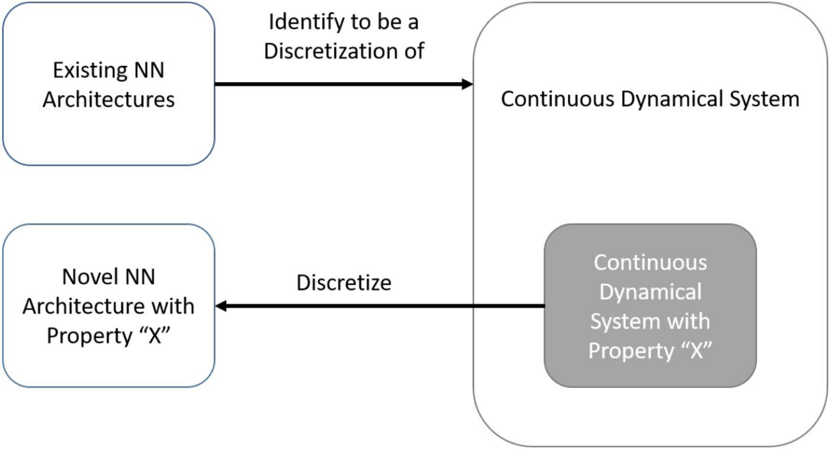
- The weight α_k as a trainable parameter

- DenseNet[8] can be thought of as an extreme case of such a multi-step method

[8] **huang2017densely**.

Architecture from PDE Theory

- Derive new models with better robustness or other good properties from PDE Theory



Connection to transport equation (TE)[9]

- For an ODE,

$$\frac{dx}{dt} = F(A(t), x), \;\; x(0) = x_0$$

  let $u(x, t)$ be a function that is constant along the trajectory defined by the ODE

- Then

$$\frac{du(x(t), t)}{dt} = \frac{\partial u(x, t)}{\partial t} + F(A(t), x)\frac{\partial u}{\partial x} = 0$$

- Enforce $u(x(1), 1) = f(x(0))$ and $u(x(0), 0) = y$

- Then training ResNet is to find u and $u(x(0), 0)$ is the classifier

[9] **li2017deep**.

TE view of ResNet

- The formulization is

$$\begin{cases} \frac{\partial u(x,t)}{\partial t} + F(A(t),x)\frac{\partial u}{\partial x} = 0 \\ u(x(1),1) = f(x(0)) \\ u(x(0),0) = y \end{cases} \tag{21}$$

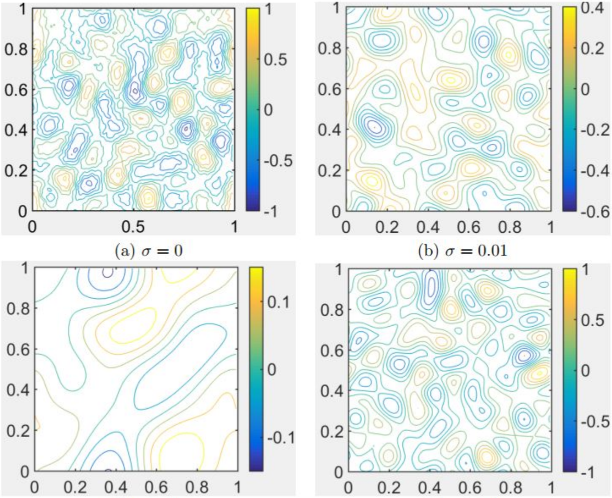
- When F is complex, $u(x,0)$ may be highly irregular
- TE more regular $\rightarrow$ ResNet more robust
- Solve the convection diffusion equation

$$\frac{\partial u(x,t)}{\partial t} + F(A(t),x)\frac{\partial u}{\partial x} + \frac{1}{2}\sigma^2 \Delta u(x,t) = 0 \tag{22}$$

instead

Regularity of convection diffusion equation

Terminal condition of convection diffusion equation with different σ



(a) $\sigma = 0$ (b) $\sigma = 0.01$

(c) $\sigma = 0.1$ (d) $u(\mathbf{x}, 1)$

ResNets Ensemble via the Feynman-Kac Formula

- The convection-diffusion equation can be solved using the Feynman-Kac formula in high dimensional space

$$dx(t) = F(A(t), x)dt + \sigma dB_t \tag{23}$$

- The term σdB_t in the Itô process that can be approximated by adding a specially designed Gaussian noise, $\sigma N(0, I)$

- Idea: approximate the Feynman-Kac formula by an ensemble of modified ResNets

Results of experiment

Model	dataset	$\mathcal{A}_{\text{nat}}$	$\mathcal{A}_{\text{rob}}$ (FGSM)	$\mathcal{A}_{\text{rob}}$ (IFGSM^{20})	$\mathcal{A}_{\text{rob}}$ (C&W)
ResNet20	CIFAR10	75.11	50.89	46.03	58.73
En_1ResNet20	CIFAR10	77.21	55.35	49.06	65.69
En_2ResNet20	CIFAR10	80.34	57.23	50.06	66.47
En_5ResNet20	CIFAR10	82.52	58.92	51.48	67.73
ResNet44	CIFAR10	78.89	54.54	48.85	61.33
En_1ResNet44	CIFAR10	82.03	57.80	51.83	66.00
En_2ResNet44	CIFAR10	82.91	58.29	51.86	66.89
ResNet110	CIFAR10	82.19	57.61	52.02	62.92
En_2ResNet110	CIFAR10	82.43	59.24	53.03	68.67
En_1WideResNet34-10	CIFAR10	**86.19**	**61.82**	**56.60**	**69.32**

Ensemble of ResNets is more robust to different attacks (FGSM, IFGSM and C&W)