Machine Learning

for Quantum Application

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박찬신 수석연구원

포스코홀딩스 미래기술연구원

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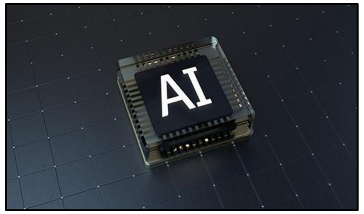
포스코홀딩스 미래기술연구원 전경

AI 연구소



이차전지소재 연구소

수소저탄소 연구소

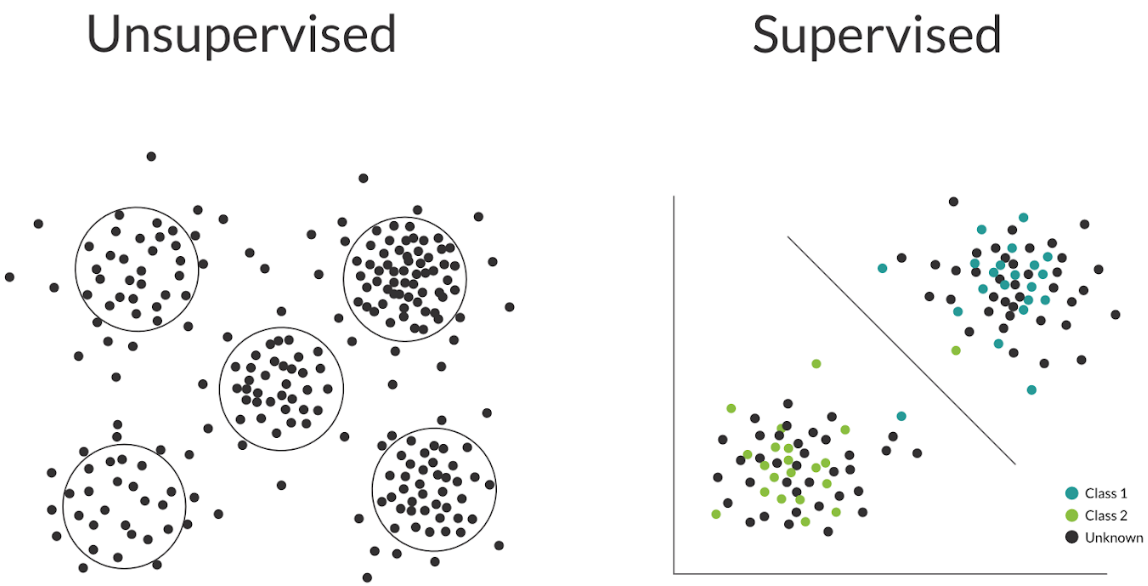
포스코그룹 새로운 50년 친환경 미래기술을 선도하는 Global Top Tier 연구소

Overview Machine Learning

Machine Learning

: Machine learning consists in extracting information from data and using it to predict trends and behaviour patterns.

- **Supervised learning (i.e. classification / regression):** The machine learning task of learning a function that maps an input to an output based on example input-output pairs.
- **Unsupervised learning (i.e. clustering):** a type of machine learning that looks for previously undetected patterns in a data set with no pre-existing labels.

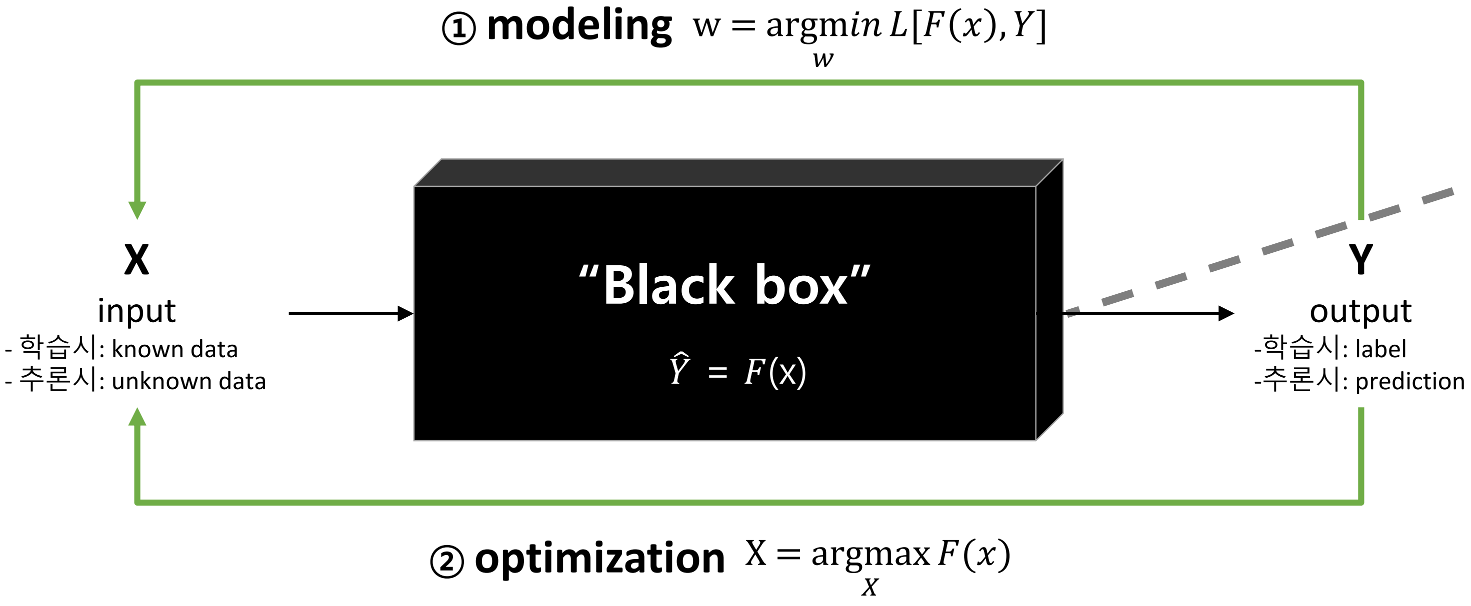


출처: https://www.extrahop.com/company/blog/2019/supervised-vs-unsupervised-machine-learning-for-network-threat-detection/

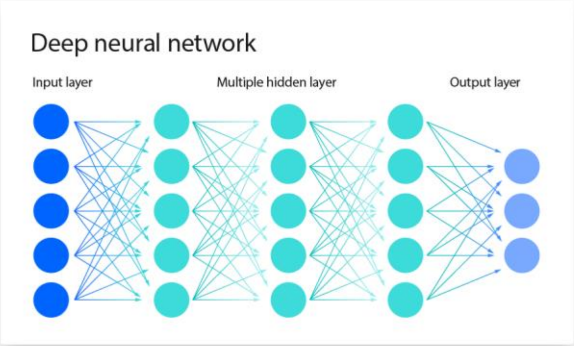
Overview Learning Method

Machine Learning 방법(Machine Learning/Quantum Circuit Learning)

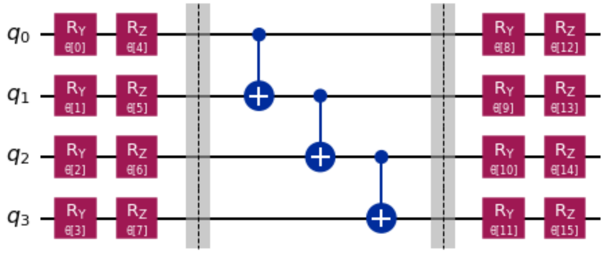
- **Black box**(기계학습모델): 입력값과 출력값 간의 관계를 학습 (Universal Function Approximator)
    a. **머신러닝모델**(Neural-Net): Multi-layer, Activation Function, Optimizer, Backpropagation(Gradient Descent)
    b. **양자머신러닝**(Quantum Circuit Learning[1]): Multi-layer, Unitary Operator/Entanglement, Optimizer, Variational Method



<Learning Machine>



<Neural Network[2]>



<Quantum Circuit[3]>

[1] Mitarai, Kosuke, et al. "Quantum circuit learning." *Physical Review A* 98.3 (2018): 032309.
[2] https://www.ibm.com/topics/neural-networks
[3] https://qiskit.org/ecosystem/nature/tutorials/07_leveraging_qiskit_runtime.html

ML-based DE solver: PINNs damped oscilliation

고전적인 해석기법

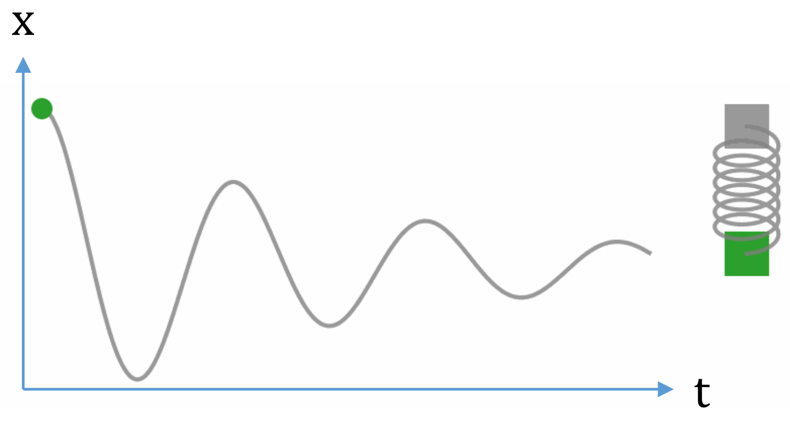
- 감쇠 진동(damped oscilliation): 진동자의 속도에 비례하는 마찰력이 존재할 경우 (m: 진동자의 질량, μ: 마찰계수, k는 용수철 상수, x는 거리, t는 시간)

$$m\frac{d^2u}{dt^2} + \mu\frac{dx}{dt} + kx = 0$$

Second order differential equation

Initial Condition: $X(0) = 1, \frac{dx}{dt} = 0$

Solution: $x(t) = e^{-\delta t}(2A\cos(\phi + \omega t))\ ,\quad \text{with}\ \omega = \sqrt{\omega_0^2 - \delta^2}$

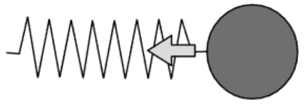


관성 = 탄성력 + 마찰력

$F = m\frac{d^2u}{dt^2}$

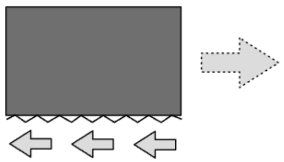
<관성>

$F_f = -kx$



<탄성력>

$F_r = -\mu\frac{dx}{dt}$



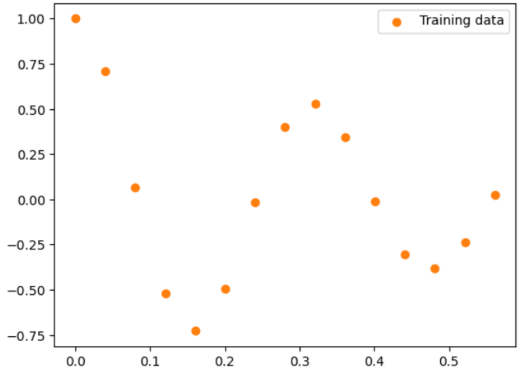
<마찰력>

참조: https://benmoseley.blog/my-research/so-what-is-a-physics-informed-neural-network/

ML-based DE solver vanilla ML

머신러닝(Supervised Learning) 기반 해석 (Regression)

- **데이터 확보**: 시간에 따른 감쇄진동자의 움직임을 측정
- **Model Discovery**: Neural-network기반의 모델링을 진행



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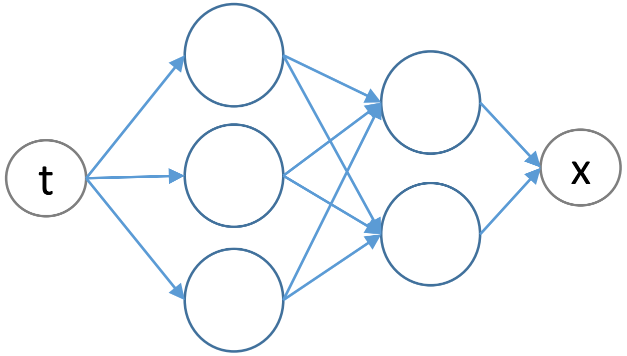
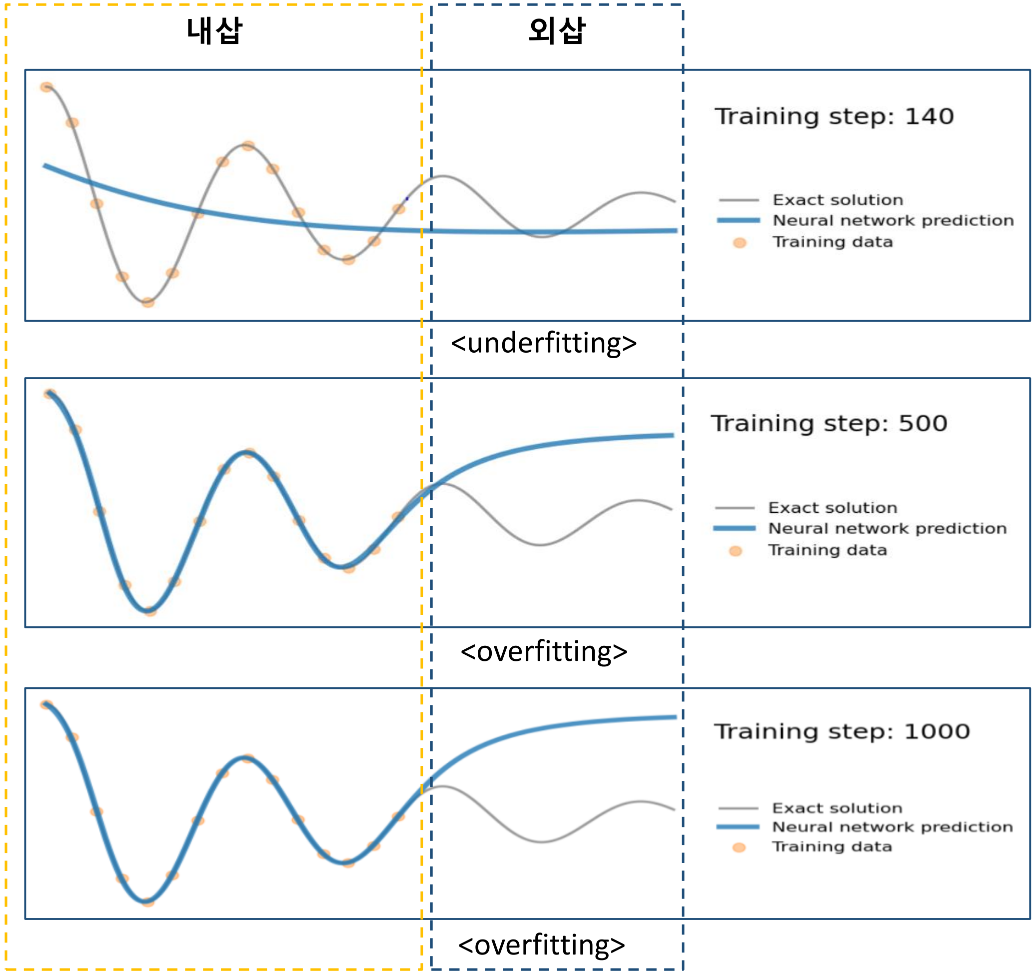


<Neural Network>



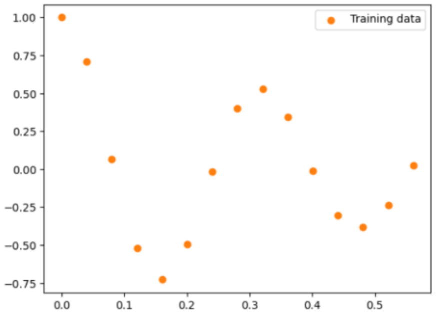
https://benmoseley.blog/my-research/so-what-is-a-physics-informed-neural-network/

ML-based DE solver PINN

물리신경망(Physics-informed Neural Network) 기반 해석

- **오류함수 추가**: 기존 신경망 오류(Neural-Network Loss)에 물리방정식 기반 오류(Physical Loss)를 추가하여 모델 적합(Fitting)

$$Loss = Loss_{prediction} + Loss_{physical} \ (+ Loss_{Boundary\ Condition})$$



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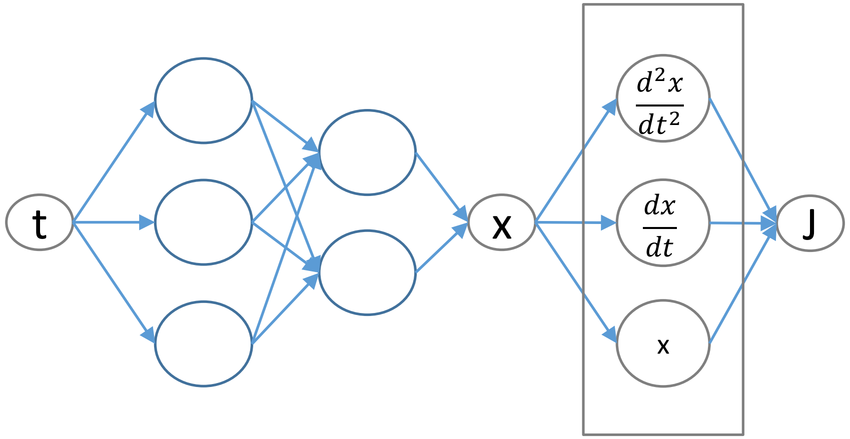
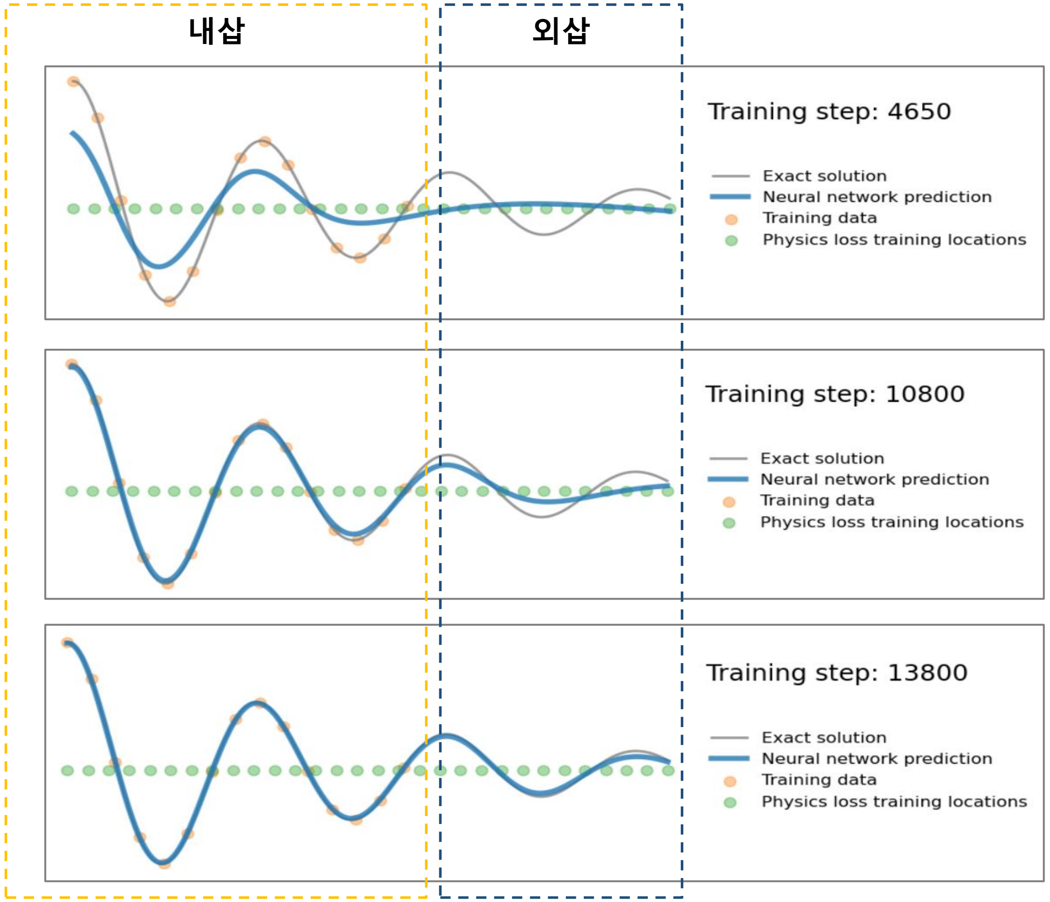


<neural network> <Physics>



https://benmoseley.blog/my-research/so-what-is-a-physics-informed-neural-network/

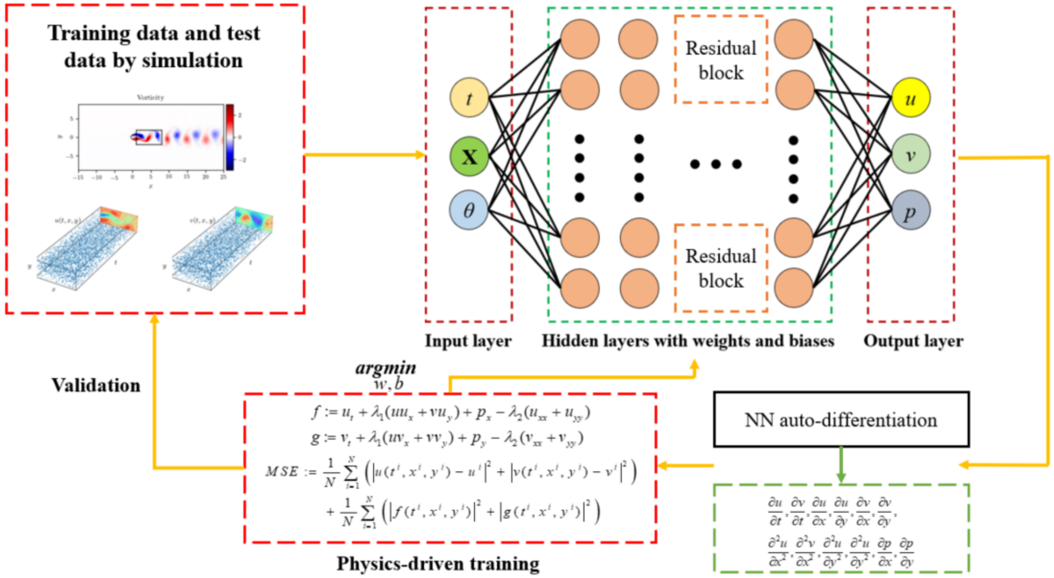
New Approach(Classical/ML) PINNs

Physics-informed Neural Networks

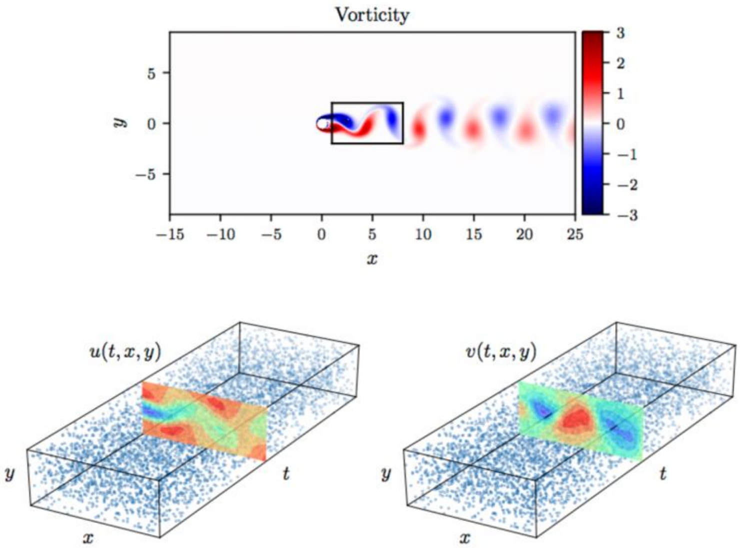
- 기존의 전통적인 수치해석적 방법과 달리 메쉬가 필요없는 mesh-free기법으로 복잡한 형상에도 효과적으로 적용 가능하고, 비교적 빠른 시간에 정확한 PDE해를 도출할 수 있다.
- 기존의 신경망이 데이터 중심 접근 방식인데 비해 PINN은 PDE(편미분방정식)에 내재되어 있는 물리 정보를 신경망에 도입함으로 학습 데이터를 줄여 학습 속도를 빠르게 한다.

  ※ 기존 FEM 방법에 비해 Nonlinear Dynamics를 정확히 계산할 수 있음이 Bifurcation Theory 연구에서 보고됨[1].

  ※ Paremeter가 충분하다면 Universal Approximation Theorem[2]과 Universal Differential Equation Theorem[3]에 의해서 복잡한 Geometry도 학습 가능



<PINN with Resnet Block for solving Fluid Flow Problems[5]>



<Navier-Stokes equation4)>

1) Sandor Beregi et al., Using scientific machine learning for experimental bifurcation analysis of dynamic systems, *arXiv*. 2110.11854, 2022
2) Hornik Kurt et al., Multilayer Feedforward Networks are Universal Approximators, Neural Networks, 2, 359–366
3) Christopher Rackauckas et al., Universal Differential Equations for Scientific Machine Learning, arXiv. 2001.04385, 2020
4) M. Raissi, P. Perdikaris, G.E. Karniadakis, Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations, Journal of Computational Physics, Volume 378, 2019
5) Cheng, C.; Zhang, G.-T. Deep Learning Method Based on Physics Informed Neural Network with Resnet Block for Solving Fluid Flow Problems. Water 2021