State Space Discovery of Physical and Chemical Systems

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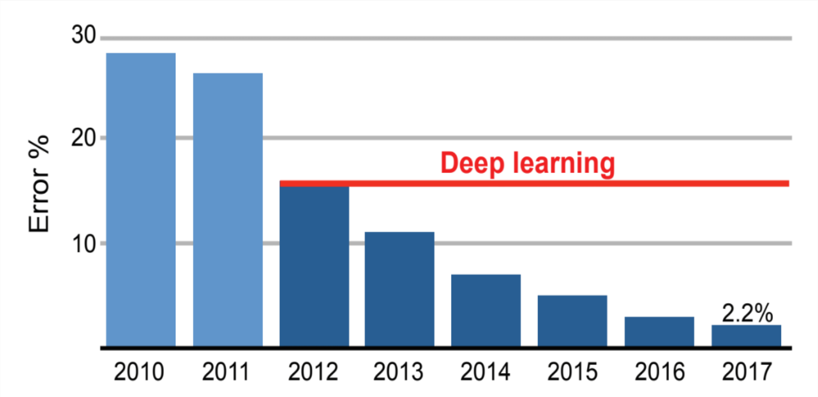
Scientific Machine Learning

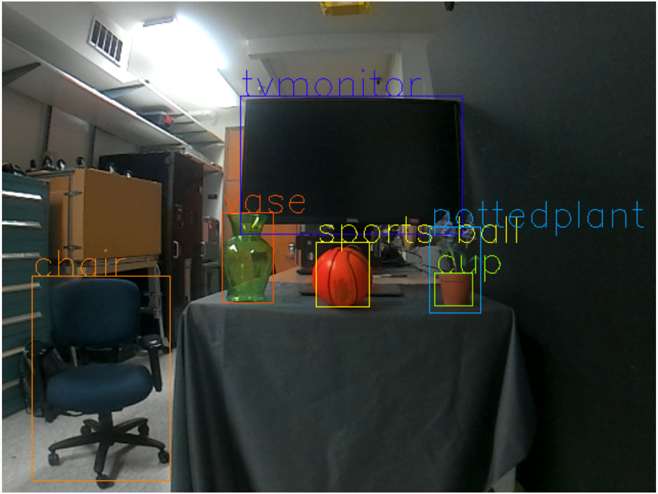
Era of Machine Learning: Image Recognition



Goal: Develop an algorithm to detect 1000 different classes of objects.
Human error is around 5%.

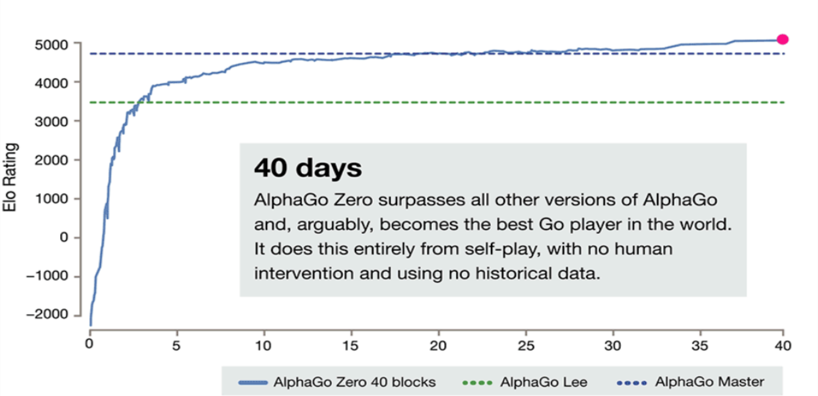
ImageNet Competition ILSVRC Challenge

Era of Machine Learning: Object Detectors



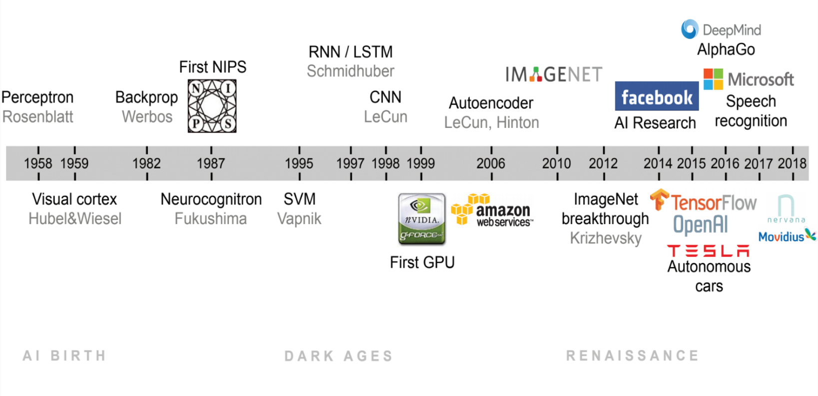
You **O**nly **L**ook **O**nce: https://pjreddie.com/darknet/yolo/

Era of Machine Learning: Reinforcement Learning



deepmind.com

History



geometricdeeplearning.com

Some issues: Big Data and Complex Models

	VGGNet	DeepVideo	GNMT
Used For	Identifying Image Category	Identifying Video Category	Translation
Input	Image	Video	English Text
Output	1000 Categories	47 Categories	French Text
Parameters	140M	~100M	380M
Data Size	1.2M Images with assigned Category	1.1M Videos with assigned Category	6M Sentence Pairs, 340M Words
Dataset	ILSVRC-2012	Sports-1M	WMT'14

https://medium.com/nanonets/nanonets-how-to-use-deep-learning-when-you-have-limited-data-f68c0b512cab

Era of Machine Learning... for Science!?

Relational inductive biases, deep learning, and graph networks

Peter W. Battaglia[1]*, Jessica B. Hamrick[1], Victor Bapst[1], Alvaro Sanchez-Gonzalez[1], Vinicius Zambaldi[1], Mateusz Malinowski[1], Andrea Tacchetti[1], David Raposo[1], Adam Santoro[1], Ryan Faulkner[1], Caglar Gulcehre[1], Francis Song[1], Andrew Ballard[1], Justin Gilmer[2], George Dahl[2], Ashish Vaswani[2], Kelsey Allen[3], Charles Nash[4], Victoria Langston[1], Chris Dyer[1], Nicolas Heess[1], Daan Wierstra[1], Pushmeet Kohli[1], Matt Botvinick[1], Oriol Vinyals[1], Yujia Li[1], Razvan Pascanu[1]

[1]DeepMind; [2]Google Brain; [3]MIT; [4]University of Edinburgh

"Despite deep learning's successes, however, important critiques have highlighted key challenges it faces in...reasoning about structured data, transferring learning beyond the training conditions, and learning from small amounts of experience."

"In general, a tension exist between the need for increased complexity of machine learning models to improve results and the need for users to interpret the models and derive new insights and conclusions."

What should machine learning look like in science?

There are a lot of mathematical challenges that accompany this question.

Scientific Machine Learning: Applied Math + ML

Machine Learning requirements:

- Data:

  Massive number of samples that represent your problem.
- Compute power:

  Special-purpose hardware to perform parallel computation.
- High-Capacity Models:

  Dense set of functions in the function space of your problem.

Scientific requirements:

- Domian-Aware:

  Leveraging and respecting scientific domain knowledge.
- Interpretable:

  Explainable and understandable results.
- Robust:

  Stable, well-posed, and reliable formulations.

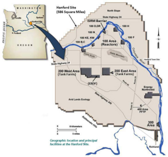
State Estimation of Porous Media

Hanford Site

The **Hanford Site** is a decommissioned **nuclear** production complex operated by the United States federal government on the Columbia River in Benton County in the U.S. state of **Washington**.

Hanford Site - Wikipedia
https://en.wikipedia.org › wiki › Hanford_Site

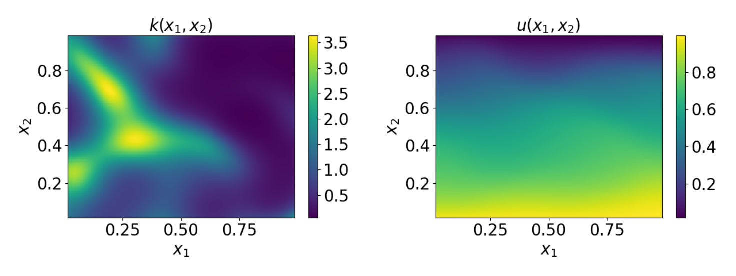
- In the 1980s, groundwater contamination totaled about 80 square miles. Today, about **60 square miles of groundwater remains contaminated above federal standards** — and the level of contamination has been greatly reduced for significant portions of that area.
- There are no active nuclear production facilities; however, the site contains some of **the nation's most complicated nuclear and mixed dangerous waste**, which must be cleaned up.



The U.S. Department of Energy is required to

google: hanford site nuclear waste doe
https://ecology.wa.gov/Waste-Toxics/Nuclear-waste/Hanford-cleanup

Predict the Hydraulic Conductivity and Pressure:



given a small number of measurements.

Diffusion Equation

These two quantities are related by the following differential equation,

$$\nabla \cdot (K(\mathbf{x})\nabla u(\mathbf{x})) = 0, \quad \mathbf{x} \equiv (x_1, x_2)^T \in (0,1) \times (0,1)$$

subject to the Dirichlet boundary conditions

$$u(\mathbf{x}) = 1, \quad x_2 = 0 \quad \text{and} \quad u(\mathbf{x}) = 0, \quad x_2 = 1$$

and the Neumann boundary conditions

$$\frac{\partial u(\mathbf{x})}{\partial x_1} = 0 \quad x_1 \in \{0, 1\}.$$

Physics Informed Neural Networks

Idea: Utilize the class of Deep Neural Networks to both fit the data and solve the PDE during training.

Formulation: Recast the problem of solving a general nonlinear partial differential equation (PDE) as a supervised learning problem with the PDE as a constraint and optimize over the weights of the neural network.

Solve: Approximate the solution by solving the lagrangian relaxation.

I. Lagaris et al. "Artificial neural networks for solving ordinary and partial differential equations" (1998)

M. Rassi et al. "Physics-informed Deep neural networks: A deep learning framework for solving forward and inverse problems" (2019)

Deep Learning Approach

Define the following deep neural networks:

- $\hat{K}(\mathbf{x};\gamma) = \mathcal{N}\mathcal{N}_K(\mathbf{x};\gamma)$
- $\hat{u}(\mathbf{x};\theta) = \mathcal{N}\mathcal{N}_u(\mathbf{x};\theta)$

together with the following two auxiliary functions,

- $f(\mathbf{x};\gamma,\theta) = \nabla \cdot [\mathcal{N}\mathcal{N}_K(\mathbf{x};\gamma)\nabla\mathcal{N}\mathcal{N}_u(\mathbf{x};\theta)] = \mathcal{N}\mathcal{N}_f(\mathbf{x};\theta,\gamma)$
- $f_N(\mathbf{x};\theta) = \partial\mathcal{N}\mathcal{N}_u(\mathbf{x};\theta)/\partial x_2 = \mathcal{N}\mathcal{N}_N(\mathbf{x};\theta)$

Loss Function

Next define the following loss function:

$$L(\theta, \gamma) = \frac{1}{N_K} \sum_{i=1}^{N_K} \left[\hat{K}(\mathbf{x}_i^K; \gamma) - K_i^* \right]^2 + \frac{1}{N_u} \sum_{i=1}^{N_u} [\hat{u}(\mathbf{x}_i^u; \theta) - u_i^*]^2$$
$$+ \frac{1}{N_D} \sum_{i=1}^{N_D} \left[\hat{u}(\mathbf{x}_i^D; \theta) - g_i^* \right]^2 + \frac{1}{N_N} \sum_{i=1}^{N_N} f_N(\mathbf{x}_i^N; \gamma, \theta)^2$$
$$+ \frac{1}{N_c} \sum_{i=1}^{N_c} f(\mathbf{x}_i^c; \gamma, \theta)^2.$$

for some know location observations $\{\mathbf{x}_i^K\}_{i=1}^{N_K}$ and $\{\mathbf{x}_i^u\}_{i=1}^{N_u}$ and collocation points $\{\mathbf{x}_i^D\}_{i=1}^{N_D}$ and $\{\mathbf{x}_i^N\}_{i=1}^{N_N}$.

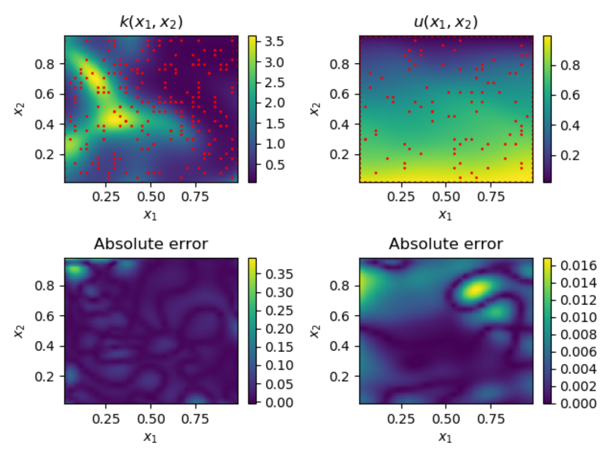
Training

Solve:

$$(\theta, \gamma) = \operatorname*{arg\,min}_{\theta,\gamma} L(\theta, \gamma)$$

using L-BFGS-B and some weight initialization scheme.

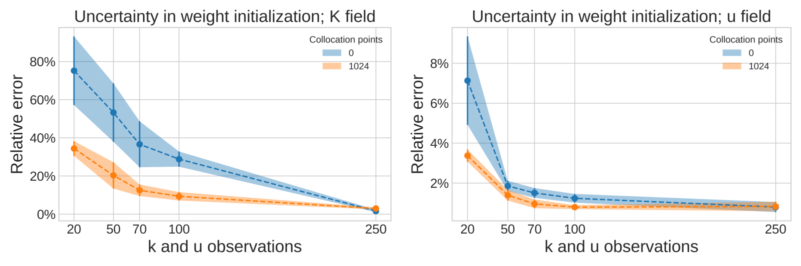
3-layered Network, 32x32 grid, $N_K = 250$, $N_u = 100$, $N_c = 1024$



Relative Error

$$\varepsilon_u = \frac{||u(\mathbf{x}) - \hat{u}(\mathbf{x})||_{L_2}^2}{||u(\mathbf{x})||_{L_2}^2}, \quad \varepsilon_K = \frac{||K(\mathbf{x}) - \hat{K}(\mathbf{x})||_{L_2}^2}{||K(\mathbf{x})||_{L_2}^2}$$

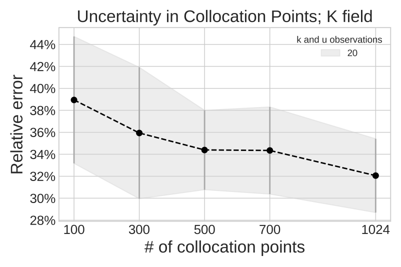
Uncertainty in Weight Initialization; $N_c = 1024$

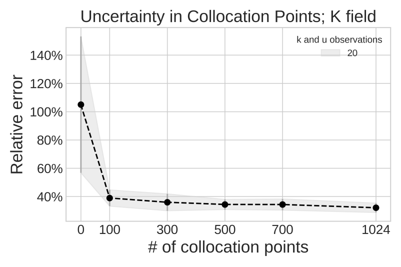


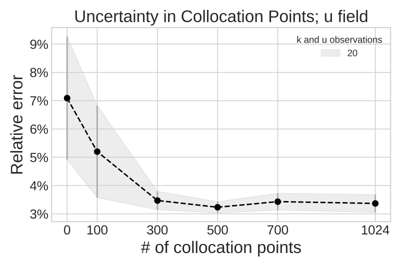
We initialized all our networks using Xavier's normal initialization* scheme.

*Glorot, Xavier and Yoshua Bengio. "Understanding the difficulty of training deep feedforward neural networks" (2010)

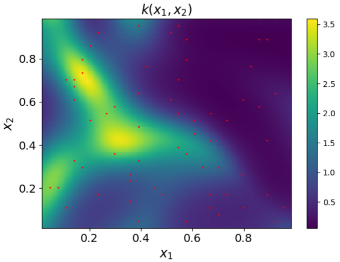
Uncertainty in Collocation Points; $N_K = N_u = 20$



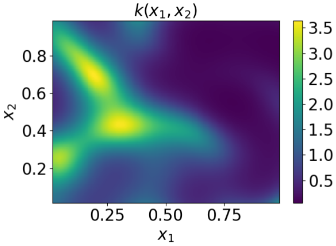




Results



$k(x_1, x_2)$
0.8
0.6
0.4
0.2
x_2
0.2
0.4
0.6
0.8
x_1
3.5
3.0
2.5
2.0
1.5
1.0
0.5

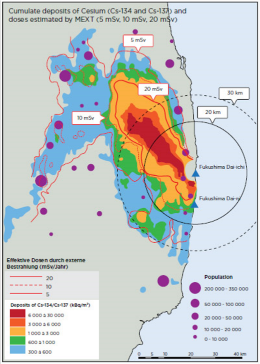


$k(x_1, x_2)$
0.8
0.6
0.4
0.2
x_2
0.25
0.50
0.75
x_1
3.5
3.0
2.5
2.0
1.5
1.0
0.5

Bonus: Forcasting the fate of Radioactive Iodine

We examine a subset of water radiolysis and subsequent iodine reactions to show proof-of-concept of the ability to forecast chemical evolutions using Recurrent Neural Networks i.e. learn the flow map of the underlying ODE.

Key: Neural Networks can capture dynamics of large dimensional data e.g. multiple chemical species.



ENSI Report on Fukushima IV: Radiological Effects **2012**.

Open Problems and Reference

- Theoretical Guarantees!?
- Better uncertainty quantification.
- Connections to universal approximation theorem.

Alexandre Tartakovsky, Carlos Ortiz Marrero, Paris Perdikaris, Guzel Tartakovsky, David Barajas-Solano, ***Learning Parameters and Constitutive Relationships with Physics Informed Deep Neural Networks*** (2018)

Jenna A. Bilbrey, Carlos Ortiz Marrero, Michel Sassi, Neil Henson, Malachi Schram, ***Tracking the chemical evolution of iodine species via recurrent neural networks*** (2019)

Scientific Machine Learning

Goal: Facilitate scientific discovery via automation.

Key ingredients for Scientific Machine Learning:

1. Proper mathematical formulation
2. Incorporate prior/domain knowledge
3. Acquire data