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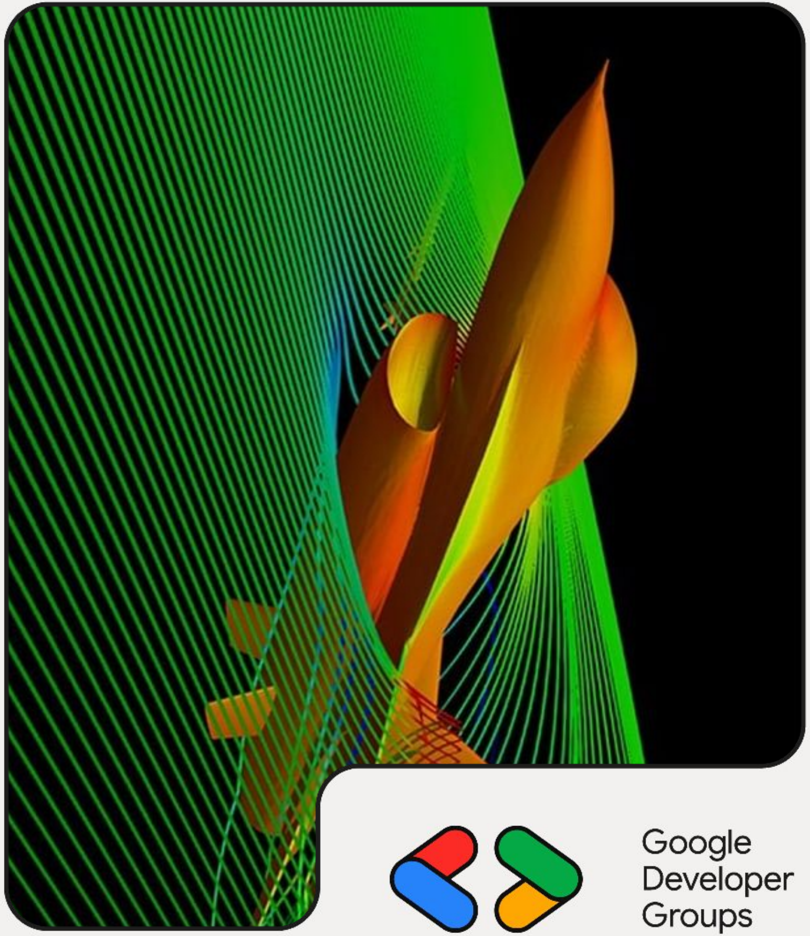
Baku

Merging Physics and Data: The SciML Approach



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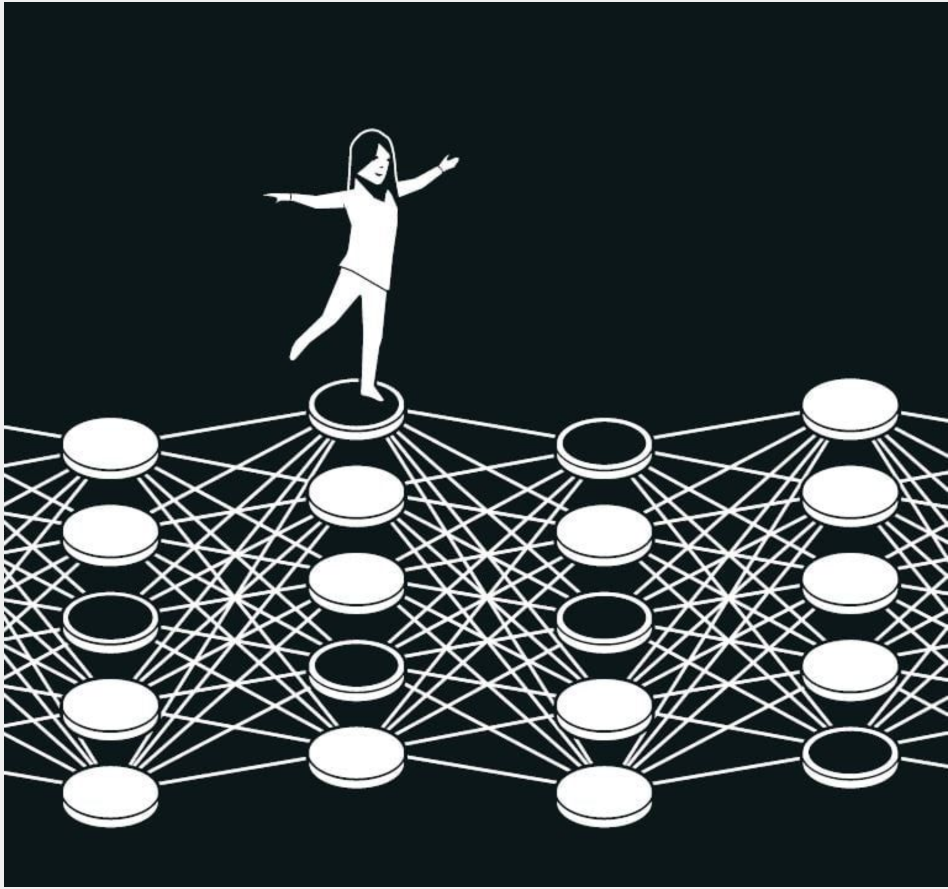
Evolution of Deep Learning
by Geoff Hinton
2024 Nobel Prize Winner

Hand drawing
by Tom Yeh



They used physics to find patterns in information: Bridging Physics and Machine Learning in Scientific Discovery

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John Hopfield

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Professor, Princeton University
Verified email at princeton.edu - Homepage

Neural Networks · AI · Neuroscience · Systems Biology · Semiconductor Physics

TITLE	CITED BY	YEAR
Neural networks and physical systems with emergent collective computational abilities. JJ Hopfield Proceedings of the national academy of sciences 79 (8), 2554-2558	27909	1982
Neurons with graded response have collective computational properties like those of two-state neurons. JJ Hopfield Proceedings of the national academy of sciences 81 (10), 3088-3092	9584	1984
“Neural” computation of decisions in optimization problems JJ Hopfield, DW Tank Biological cybernetics 52 (3), 141-152	8972	1985

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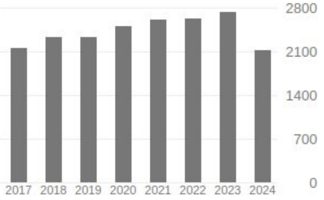
Citations	91241	14959
h-index	94	33
i10-index	176	75



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Geoffrey Hinton

FOLLOW

Emeritus Prof. Computer Science, University of Toronto
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machine learning · psychology · artificial intelligence · cognitive science · computer science

TITLE	CITED BY	YEAR
Imagenet classification with deep convolutional neural networks A Krizhevsky, I Sutskever, GE Hinton Advances in neural information processing systems 25	163698 *	2012
Deep learning Y LeCun, Y Bengio, G Hinton Nature 521 (7553), 436-44	85196	2015
Learning internal representations by error-propagation DE Rumelhart, GE Hinton, RJ Williams Parallel Distributed Processing: Explorations in the Microstructure of ...	54924 *	1986
Dropout: a simple way to prevent neural networks from overfitting N Srivastava, G Hinton, A Krizhevsky, I Sutskever, R Salakhutdinov The journal of machine learning research 15 (1), 1929-1958	53007	2014

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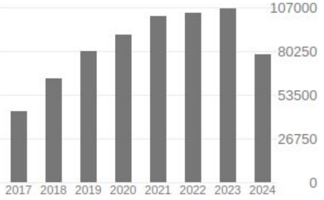
Citations	855997	562445
h-index	187	137
i10-index	481	365



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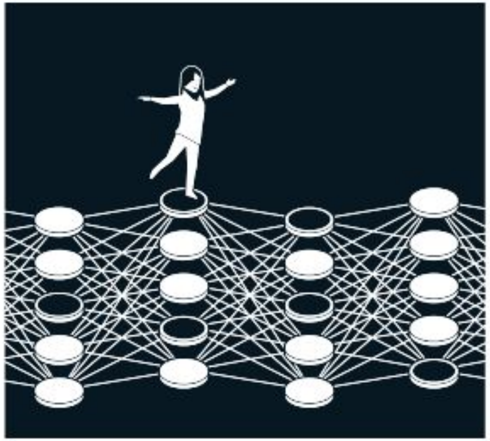
Go

They used physics to find patterns in information

This year's laureates used tools from physics to construct methods that helped lay the foundation for today's powerful machine learning. ***John Hopfield*** *created a structure that can store and reconstruct information.* ***Geoffrey Hinton*** *invented a method that can independently discover properties in data and which has become important for the large artificial neural networks now in use.*



Many people have experienced how computers can translate between languages, interpret images and even conduct reasonable conversations. What is perhaps less well known is that this type of technology has long been important for research, including the sorting and analysis of vast amounts of data. The development of machine learning has exploded over the past fifteen to twenty years and utilises a structure called an artificial neural network. Nowadays, when we talk about *artificial intelligence*, this is often the type of technology we mean.

Although computers cannot think, machines can now mimic functions such as memory and learning. This year's laureates in physics have helped make this possible. Using fundamental concepts and methods from physics, they have developed technologies that use structures in networks to process information.

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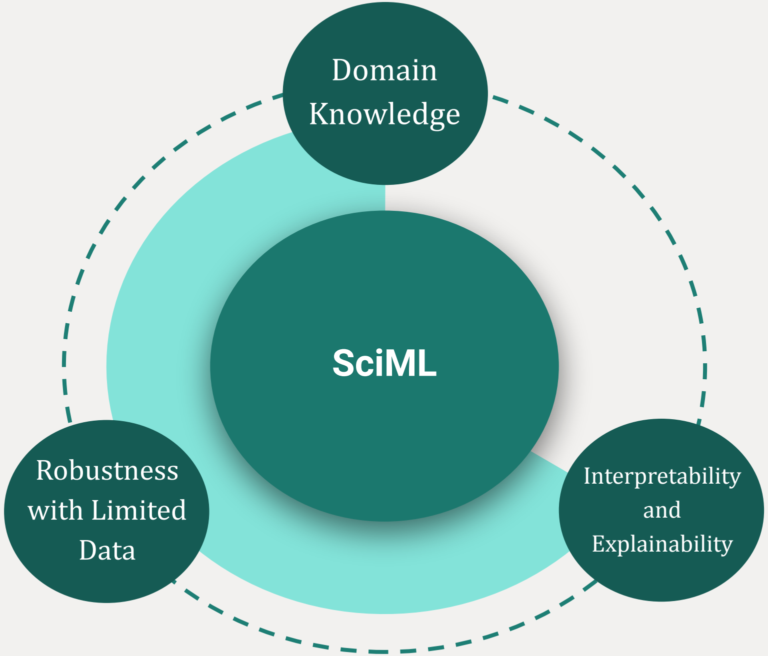
Scientific machine learning (SciML) is a rapidly growing field that combines machine learning techniques with physical knowledge to solve scientific problems.



Well-known SciML Applications

1. Bioinformatics and Computational Biology
2. Materials Science
3. Geosciences
4. Climate and Environmental Sciences
5. Mechanical Engineering

Traditional physics-based modeling (equations, assumptions)

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What are Partial Differential Equation (PDE) ?

- Mathematical descriptions of how things change in space and time

- Nature's way of "programming" physical phenomena

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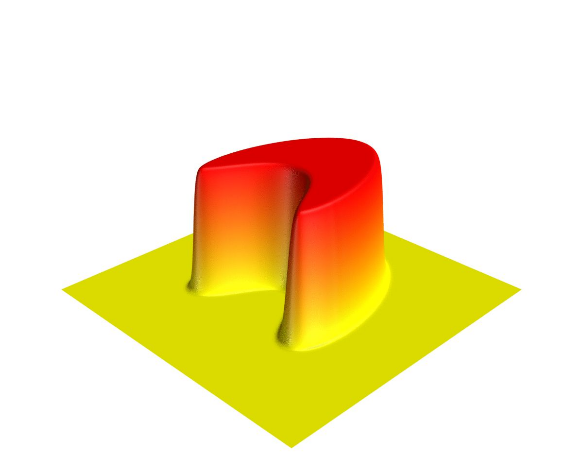
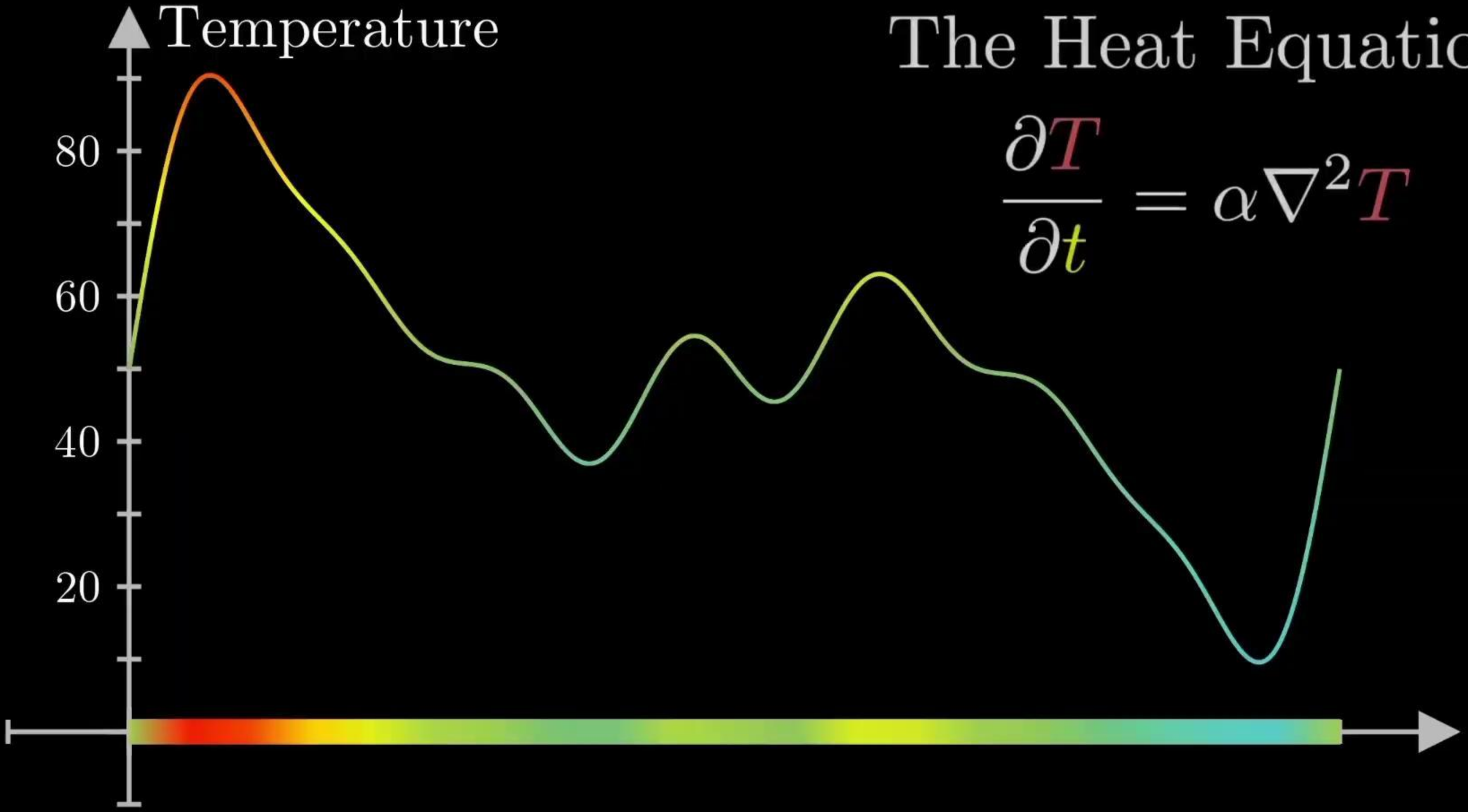


A visualisation of a solution to the two-dimensional heat equation with temperature represented by the vertical direction and color. (Wikipedia)

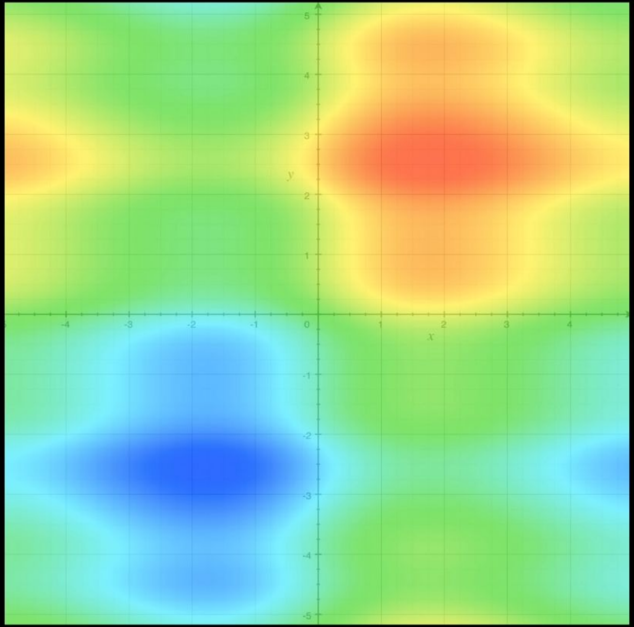
The Heat Equation

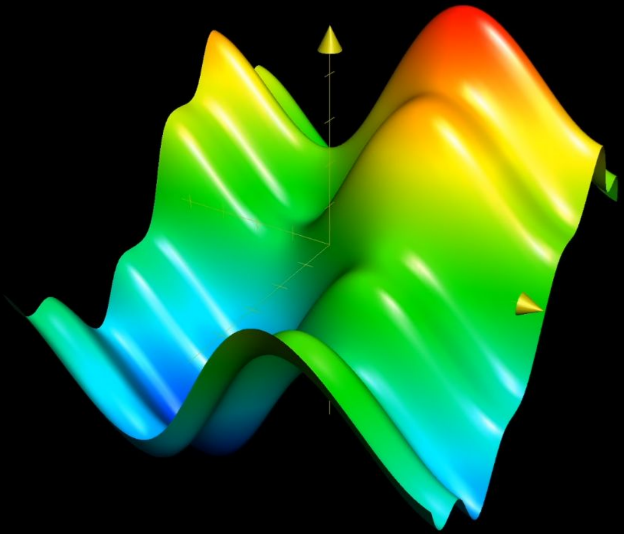
$$\frac{\partial T}{\partial t} = \alpha \nabla^2 T$$

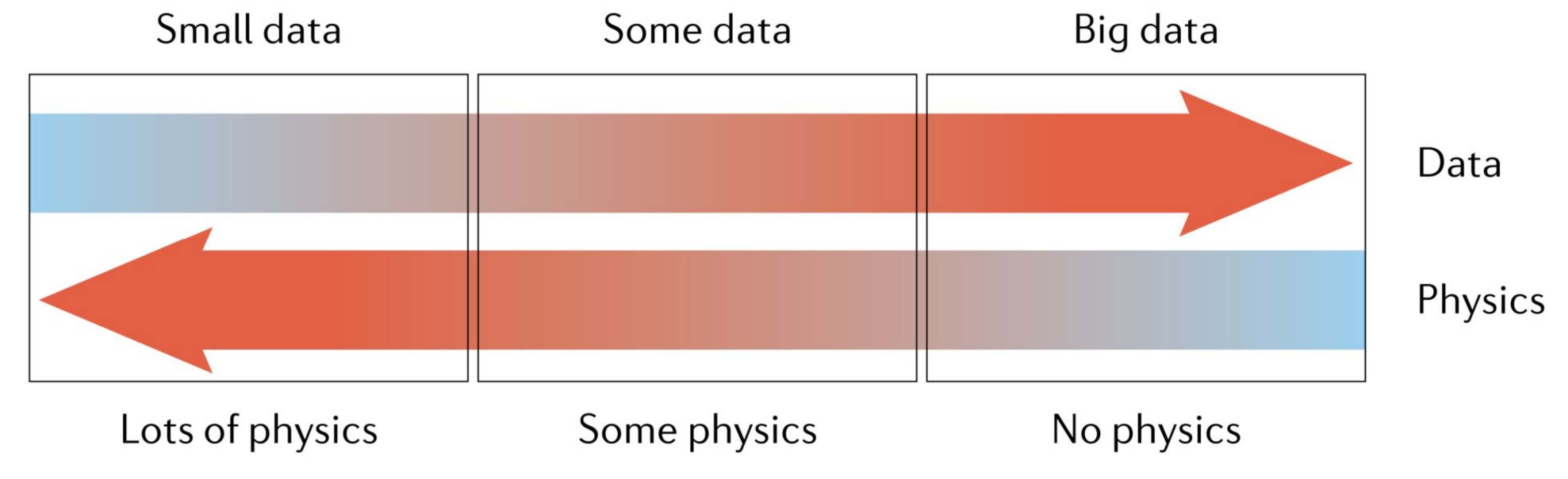


The Heat Equation

$$\frac{\partial T}{\partial t} = \alpha \nabla^2 T$$







"Physics-informed machine learning" by Karniadakist et al. (2021, Nature Reviews in Physics).

Why Physics-based models fails?

- Physics-based models can be extremely computationally intensive, especially for complex systems. This can make real-time predictions or large-scale simulations impractical.

- We don't always have a complete grasp of the underlying physics for all systems. Some phenomena are too complex to model accurately with current theories. Certain systems may involve unknown parameters or relationships.

1. Computational Complexity
2. Incomplete Physical Understanding

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Data-driven approaches (machine learning, big data)

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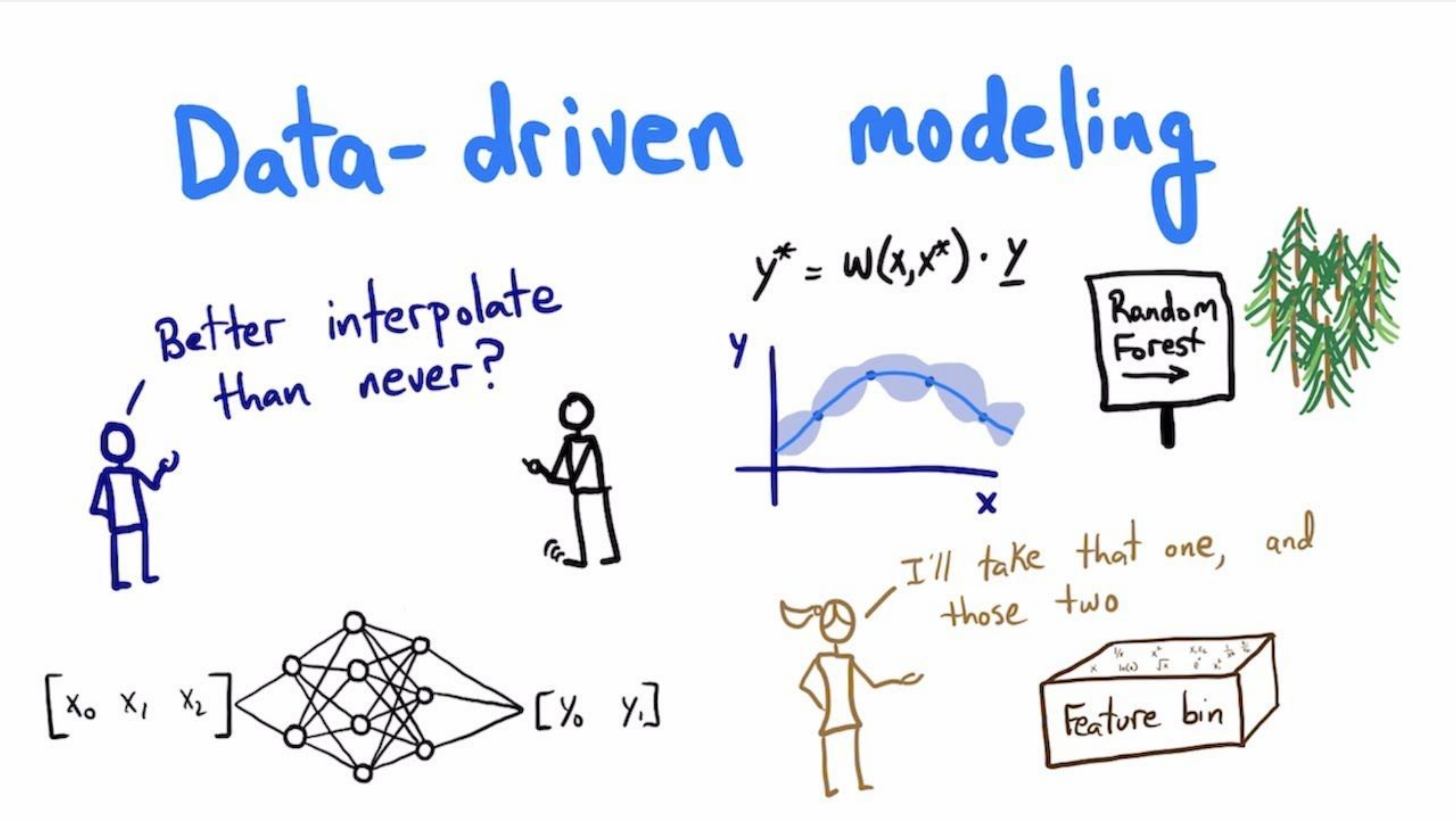
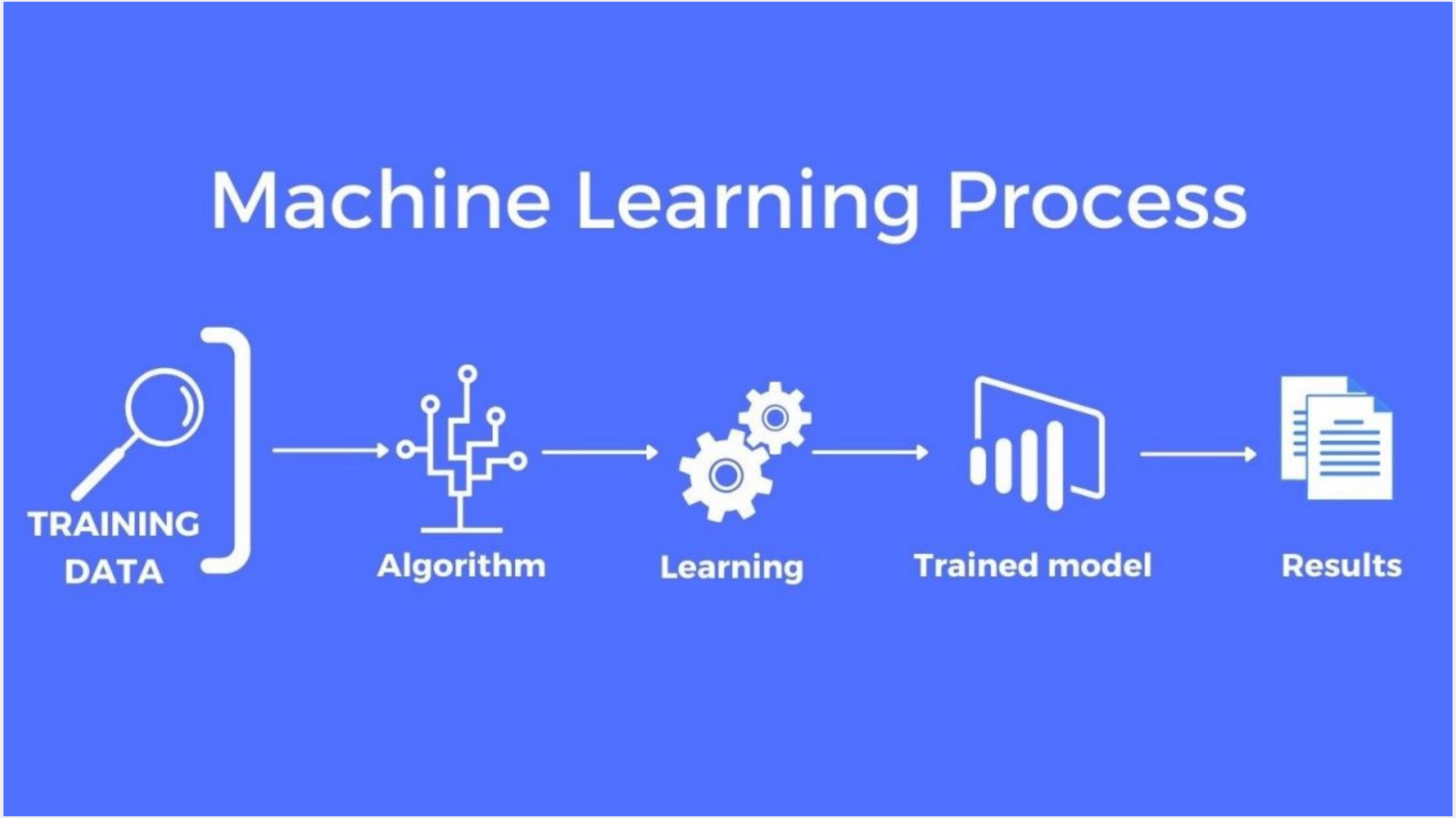

Data-driven modeling
Better interpolate than never?
$y^* = w(x, x^*) \cdot \underline{y}$
y
x
Random Forest
I'll take that one, and those two
Feature bin
$[x_0 \quad x_1 \quad x_2]$
$[y_0 \quad y_1]$


Machine Learning Process
TRAINING
DATA
Algorithm
Learning
Trained model
Results

Why data-driven models fail?

- ML models can produce physically impossible results. E.g: Predicting negative masses or faster-than-light speeds

- Models perform poorly on scenarios not seen in training. Physics-related data-driven models are highly prone to underfit.

- Require vast amounts of data and processing power.Training a large model can take days or weeks

1. May violate physical laws if not constrained
2. Struggle with extrapolation beyond training data
3. Computationally expensive and data-hungry

İdea: Merging physics-based knowledge with data-driven techniques

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Physics-informed neural networks (PINNs)

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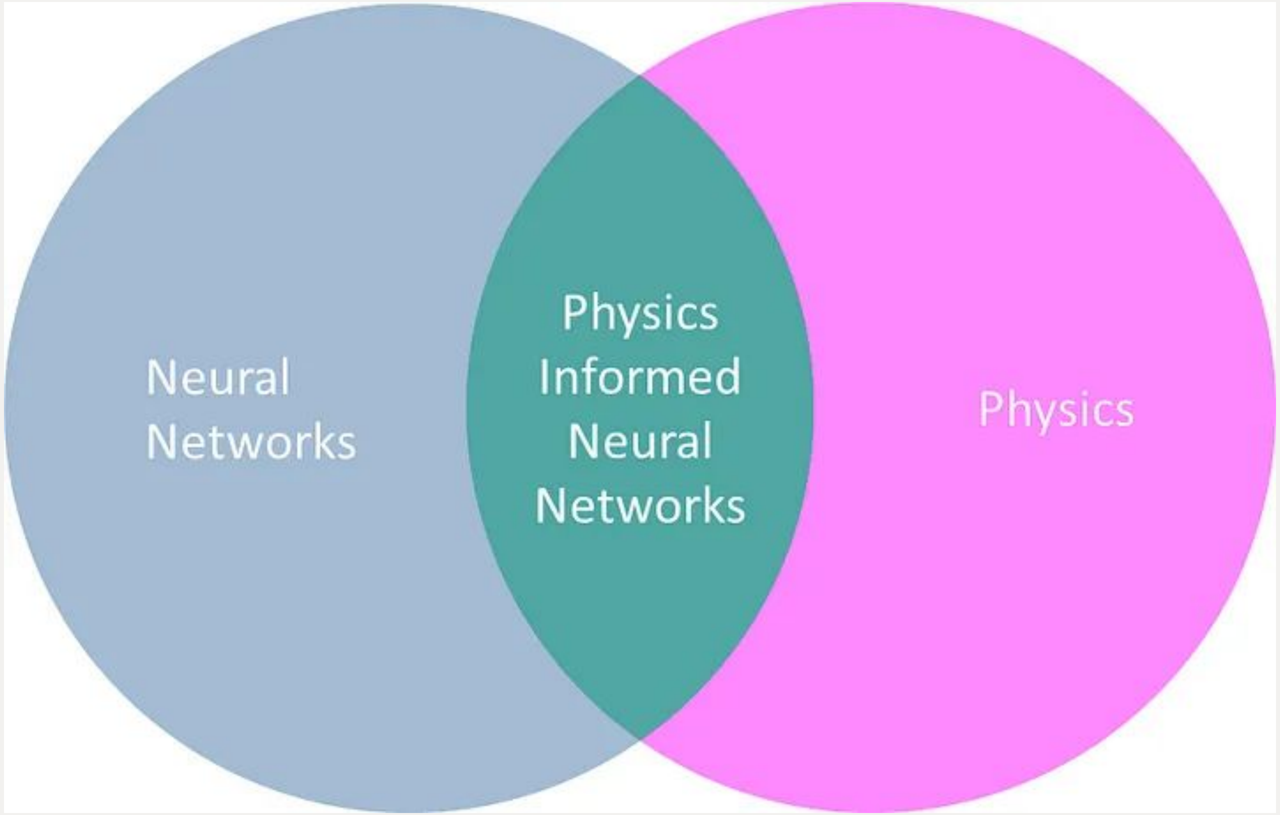
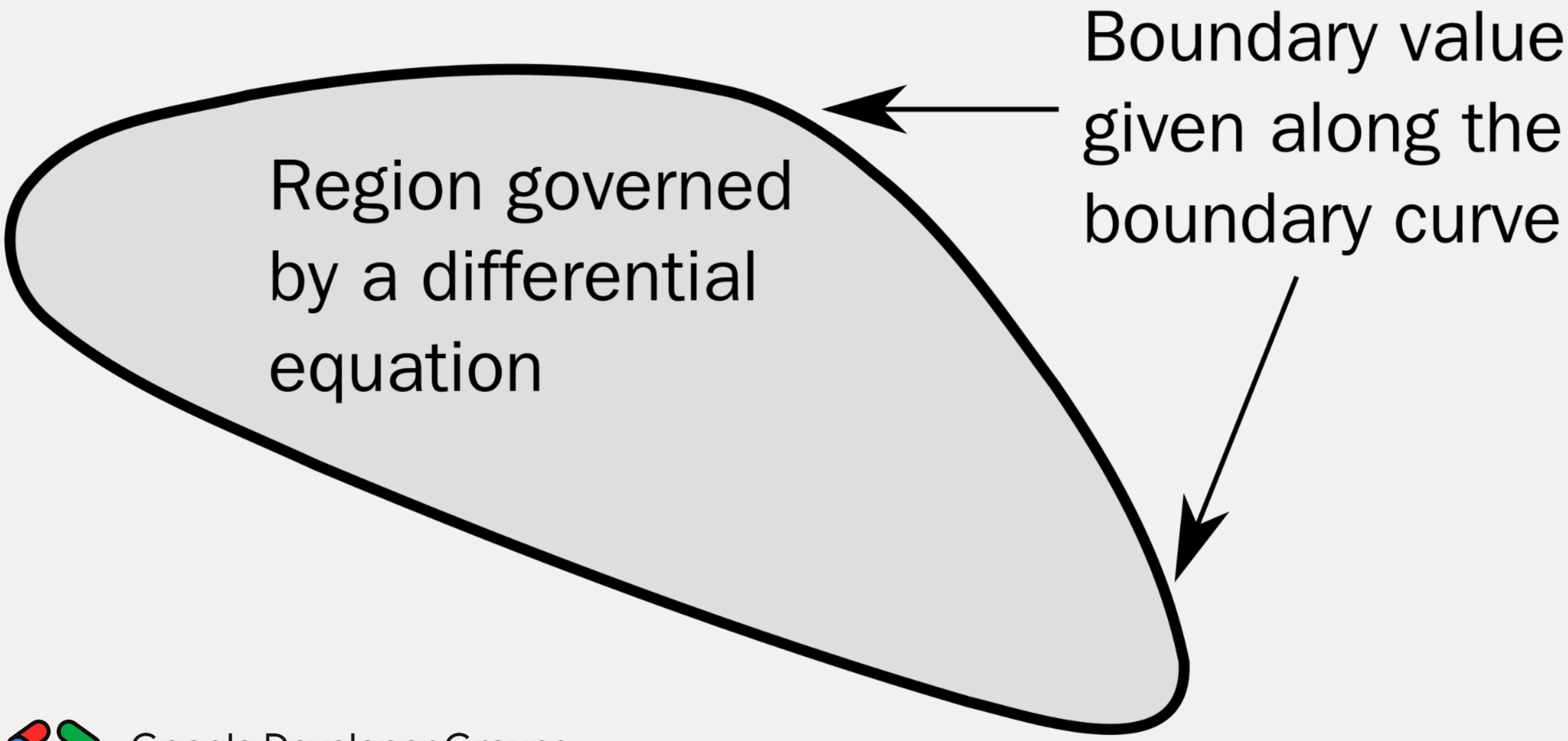

Neural
Networks
Physics
Informed
Neural
Networks
Physics



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PINN Loss Function Components for Heat Equation

1. Data Loss (L_{data})

$$L_{\text{data}} = \text{MSE}(u_{\text{pred}}, u_{\text{true}}) \tag{1}$$

Explanation: This term measures how well the neural network's predictions (u_{pred}) match the known data points (u_{true}). It ensures the model fits the available data.

- MSE stands for Mean Squared Error.
- Minimizing this loss improves the accuracy of the model's predictions at known data points.
- This is similar to loss functions in traditional machine learning.

2. PDE Loss (L_{pde})

$$L_{\text{pde}} = \text{MSE}\left(\frac{\partial u}{\partial t} - \alpha \frac{\partial^2 u}{\partial x^2}, 0\right) \tag{2}$$

Explanation: This term enforces the heat equation ($\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}$) throughout the domain.

- $\frac{\partial u}{\partial t}$ is the partial derivative of u with respect to time.
- $\frac{\partial^2 u}{\partial x^2}$ is the second partial derivative of u with respect to space.
- α is the thermal diffusivity coefficient.
- This loss encourages the neural network to learn solutions that satisfy the heat equation.
- It allows the model to generalize to areas where no data is available.

3. Boundary Condition Loss (L_{bc})

$$L_{\text{bc}} = \text{MSE}(u_{\text{pred}}(x = 0, t) - u_{\text{left}}, 0) + \text{MSE}(u_{\text{pred}}(x = L, t) - u_{\text{right}}, 0) \quad (3)$$

Explanation: This term ensures that the solution satisfies the boundary conditions of the problem.

- $u_{\text{pred}}(x = 0, t)$ is the predicted value at the left boundary.
- $u_{\text{pred}}(x = L, t)$ is the predicted value at the right boundary.
- u_{left} and u_{right} are the specified boundary conditions.
- This loss ensures that the neural network learns to respect the physical constraints at the boundaries.

$$\mathrm{L}_{\mathrm{data}} = \mathrm{MSE}(u_{\mathrm{pred}}, u_{\mathrm{true}})$$

$$\mathrm{L}_{\mathrm{pde}} = \mathrm{MSE}\,(ut - \alpha[2]ux, 0)$$

$$\mathrm{L}_{\mathrm{bc}} = \mathrm{MSE}(u_{\mathrm{pred}}(x = 0, t) - u_{\mathrm{left}}, 0) + \mathrm{MSE}(u_{\mathrm{pred}}(x = L, t) - u_{\mathrm{right}}, 0)$$

$$\mathrm{L}_{\mathrm{total}} = \lambda_1 L_{\mathrm{data}} + \lambda_2 L_{\mathrm{pde}} + \lambda_3 L_{\mathrm{bc}}$$

4. Total Loss (L_{total})

$$L_{\text{total}} = \lambda_1 L_{\text{data}} + \lambda_2 L_{\text{pde}} + \lambda_3 L_{\text{bc}} \tag{4}$$

Explanation: This is the overall loss function that the neural network aims to minimize.

- λ_1, λ_2, and λ_3 are weighting factors for each loss component.
- These weights balance the importance of fitting data, satisfying the PDE, and meeting boundary conditions.
- Adjusting these weights can prioritize different aspects of the solution based on the specific problem and available data.

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Is there data-driven but still Physics-informed approaches?

- Hopefully yes:)

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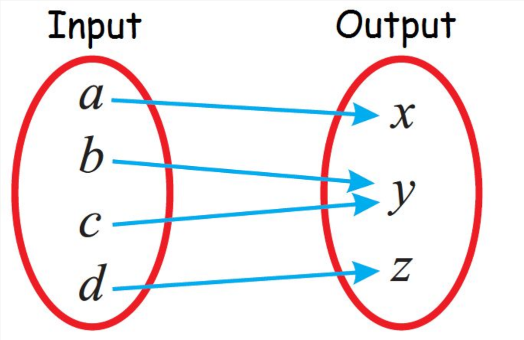
Operator learning

- Operators are mathematical entities that perform transformations or mappings between input and output spaces.
  - e.g integration or differentiation
  - Operator learning is continuous (Not discrete, like Conventional NN)



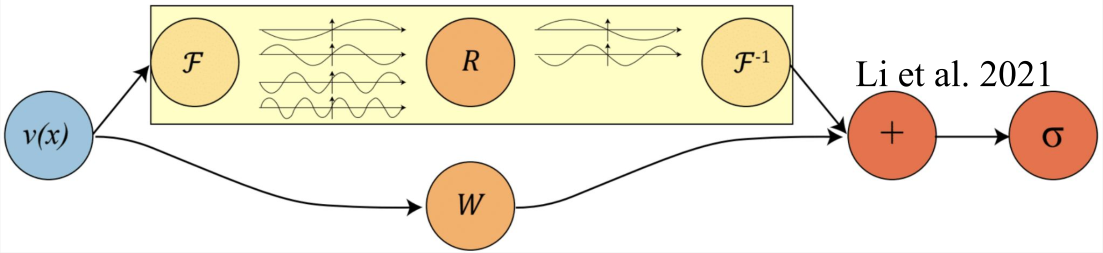
onlinemath4all.com

- Fourier neural operator (FNO) is a neural network that learns to represent the solution operator of a partial differential equation (PDE).

Neural differential equations

Fourier Neural Operators (FNOs)

- FNOs are composed of two parts: a Fourier layer and a neural network. The Fourier layer decomposes the input function into its constituent frequencies. The neural network then learns how to transform these frequencies into the desired output function.



Fourier Transform

$$x(t) * h(t) \overset{\mathcal{F}}{\longleftrightarrow} X(j\omega)H(j\omega)$$

Programming Languages and frameworks to perform SciML

PyTorch

flux

julia

DifferentialEquations.jl

SciML community, opportunities, well-known researchers

- Huge companies are investing in SciML
  - NVIDIA & Google
- Each year there are huge number of PhD positions in SciML in EU and US mainly
  - Colorado School Of Mines, Georgia Tech, Stanford, MIT (US)
  - TuDelft, almost all Norwegian and UK universities
  - KFUPM, KAUST (Saudi Arabia)
- Prestigious professors, researchers in SciML:
  - George Em Karniadakis
  - Karen Willcox
  - Anima Anandkumar
  - Umair Bin Waheed
  - Tariq Alkhalifah
  - Maziar Raissi
  - And other hundreds of brilliant minds

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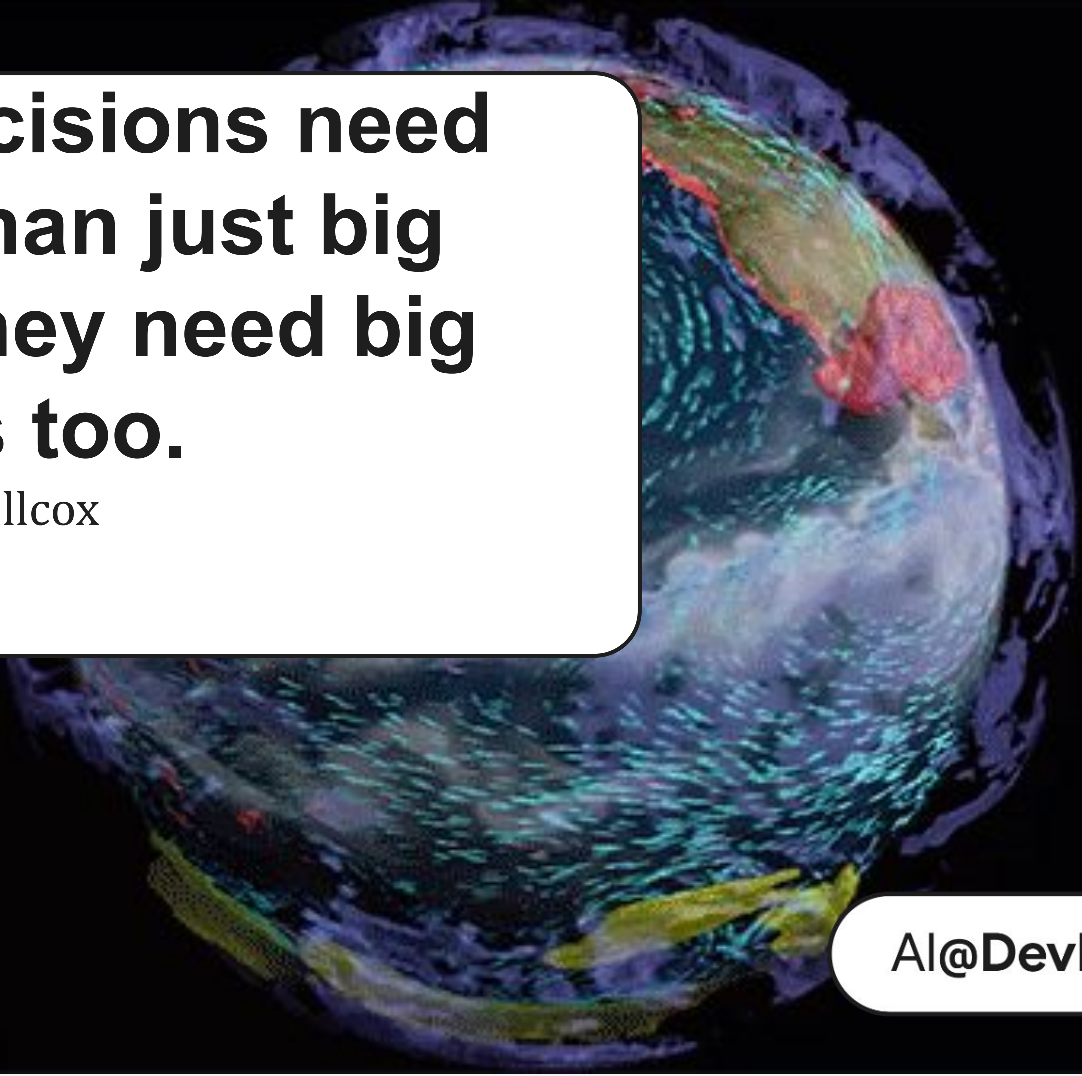
Scan the QR code for the relevant materials:



Big Decisions need more than just big data, they need big models too.

- Karen Willcox

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