Title: Lecture - Machine Learning, PHYS 777

Speakers: Mohamed Hibat Allah

Collection/Series: Machine Learning (Elective), PHYS 777, February 24 - March 28, 2025

Subject: Condensed Matter, Other

Date: February 25, 2025 - 9:00 AM

URL: https://pirsa.org/25020015

Machine Learning for many-body Physics

Feb 25 - Mar 28, 2025

PERIMETER INSTITUTE

UNIVERSITY OF WATERLOO

Course Outline

PERIMETER SCHOLARS INTERNATIONAL

Machine Learning for Many-Body Physics
Feb 25 - March 28, 2025
Course Outline

Objective: This course is designed to introduce machine learning techniques for studying classical and quantum many-body problems encountered in quantum matter, quantum information, and related fields of physics. Lectures will emphasize relationships between statistical physics and machine learning. Tutorials and homework assignments will focus on developing programming skills for machine learning using Python.

PSI Fellow: Subhayan Sahu
Email: `ssahu@perimeterinstitute.ca`
How to address me: Subhayan
How to get in touch with me: Just come with your question to my office. If I am not there, just send me an email and we can work out a schedule.

Lecturer: Mohamed Hibat-Allah
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How to get in touch with me: just send me an email and we can work out a schedule.

Teaching assistant: Cole Coughlin
Email: `ccoughlin@perimeterinstitute.ca`
How to address me: Cole
How to get in touch with me: by email

Subhayan Sahu

Cole Coughlin

Schedule

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Tutorials 0/1

Homework assignments 0/1

	Monday	Tuesday	Wednesday	Thursday	Friday
Week 1 (Feb 24 - 28)		Lecture 1 (Mohamed) 9:00 am - 10:00am	Lecture 2 (Mohamed) 9:00 am - 10:00am		Lecture 3 (Mohamed) 9:00 - 10:00am
Week 2 (Mar 3 - 7)		Lecture 4 (Mohamed) 9:00 - 10:00am	Lecture 5 (Mohamed) 9:00 - 10:00am		Lecture 6 (Mohamed) 9:00 - 10:00am
	Tutorial 1 - Linear regression 3:45 - 5:00pm			Tutorial 2 - Supervised Learning with Feedforward NNs 2:00 - 3:30 pm	
Week 3 (Mar 10 - 14)	**Homework 1 will be posted**	Lecture 7 (Mohamed) 9:00 - 10:00am		Lecture 8 (Mohamed) 9:00 - 10:00am	
				Tutorial 3 - Supervised Learning with Convolutional NNs 2:00 - 3:30pm	
Week 4 (Mar 17 - 21)	**Homework 2 will be posted**	Lecture 9 (Mohamed) 9:00 - 10:00am			Lecture 10 (Mohamed) 9:00 - 10:00am
				Tutorial 4 - Unsupervised learning 2:00 - 3:30pm	**Homework 1 and Presentation topic deadlines.**
Week 5 (Mar 24 - 28)		Lecture 11 (Mohamed) 9:00 - 10:00am	Lecture 12 (Mohamed) 9:00 - 10:00am		Lecture 13 (Mohamed) 9:00 - 10:00am
	Tutorial 5 - Quantum Machine Learning 3:45 - 5:15pm			Tutorial 6 - Neural Quantum States 2:00 - 3:30pm	

References

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Course outline
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References
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Schedule
PDF

Lecture notes 0/1

Tutorials 0/1

Homework assignments 0/1

Machine Learning for Many-Body Physics

Useful References

Books and review articles:

- Nielsen, "Neural Networks and Deep Learning"
- Goodfellow, Bengio and Courville, "Deep Learning", MIT Press (2016)
- Liu, Li and Wang, "Lecture Note on Deep Learning and Quantum Many-Body Computation" (2018)
- Mehta, Bukov, Wang, Day, Richardson, Fisher and Schwab, "A high-bias, low-variance introduction to Machine Learning for physicists", Physics Reports **810** 1-124 (2019), arXiv:1803.08823
- Carleo, Cirac, Cranmer, Daudet, Schuld, Tishby, Vogt-Maranto and Zdeborová, "Machine learning and the physical sciences", Rev. Mod. Phys. **91**, 045002 (2019), arXiv:1903.10563
- Carrasquilla and Torlai, "Neural networks in quantum many-body physics: a hands-on tutorial", arXiv:2101.11099
- Schuld and Petruccione, "Machine Learning with Quantum Computers", Second edition (2021)
- Dawid et al., "Modern applications of machine learning in quantum sciences", https://arxiv.org/ftp/arxiv/papers/2204/2204.04198.pdf (2022)
- **Monte Carlo methods:** Newman and Barkema, "Monte Carlo Methods in Statistical Physics" (1999)

Lecture notes

General course information 0/2

Lecture notes 0/1

Lecture Notes (last update Feb 24th)

PDF

Tutorials 0/2

Homework assignments 0/1

1 LECTURE 1 4

1 Lecture 1: Motivation, Goals, Definitions of Supervised, Unsupervised, and Reinforcement Learning

1.1 Background

Interest in machine learning has grown substantially in the last few years. In this course, we focus on many-body physics, but first, let us look at some exciting examples from other areas.

- Image classification (a neural network won a competition in 2012). Can play with this at `https://github.com/tensorflow/models`
- In 2016, AlphaGo won a Go competition against the world champion.
- Technology for self-driving cars uses reinforcement learning.
- Google Language Translation uses machine learning.

Machine Learning for many-body Physics 5

Quizzes

- General course information 0/3
- Lecture notes 0/1
- Tutorials 0/1
- Homework assignments 0/1
- Quizzes 0/1
  - Quiz 1: Machine Learning for Many-body physics
    QUIZ · 7 QUESTIONS

QUESTION 1 OF 7

Machine Learning (ML) is the equivalent as artificial intelligence (AI)

Choose only ONE best answer.

A Yes

B No

CONFIRM

What is Machine Learning (ML)?

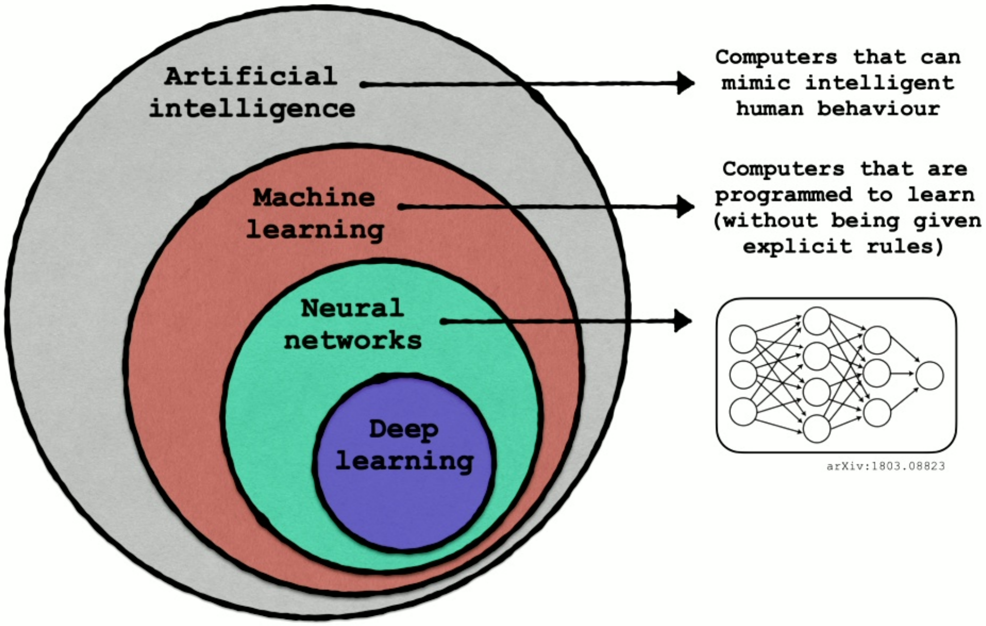
"Machine learning is a field of computer science that uses statistical techniques to give computer systems the ability to "learn" (i.e., progressively improve performance on a specific task) with data, without being explicitly programmed."

https://en.wikipedia.org

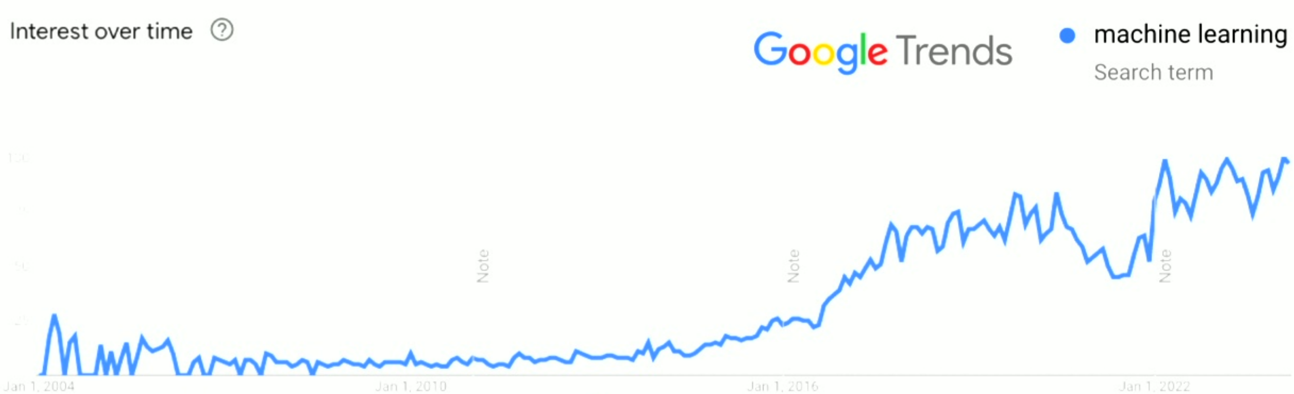
"[Machine learning] is about finding out regularities in data and making use of them for fun and profit."

L.-G. Liu, S.-H. Li and L. Wang, http://wangleiphy.github.io

Important remark to make



Machine learning popularity



2004 **2012** **2018** **2024**

Image Classification (2012)

ImageNet Classification with Deep Convolutional Neural Networks

Alex Krizhevsky
University of Toronto
kriz@cs.utoronto.ca

Ilya Sutskever
University of Toronto
ilya@cs.utoronto.ca

Geoffrey E. Hinton
University of Toronto
hinton@cs.utoronto.ca

Abstract

We trained a large, deep convolutional neural network to classify the 1.2 million high-resolution images in the ImageNet LSVRC-2010 contest into the 1000 different classes. On the test data, we achieved top-1 and top-5 error rates of 37.5% and 17.0% which is considerably better than the previous state-of-the-art. The neural network, which has 60 million parameters and 650,000 neurons, consists of five convolutional layers, some of which are followed by max-pooling layers, and three fully-connected layers with a final 1000-way softmax. To make training faster, we used non-saturating neurons and a very efficient GPU implementation of the convolution operation. To reduce overfitting in the fully-connected layers we employed a recently-developed regularization method called "dropout" that proved to be very effective. We also entered a variant of this model in the ILSVRC-2012 competition and achieved a winning top-5 test error rate of 15.3%, compared to 26.2% achieved by the second-best entry.

AlphaGo (2016)

nature
International journal of science

Altmetric: 3193 Citations: 569 More detail »

Article

Mastering the game of Go with deep neural networks and tree search

David Silver, Aja Huang, Chris J. Maddison, Arthur Guez, Laurent Sifre, George van den Driessche, Julian Schrittwieser, Ioannis Antonoglou, Veda Panneershelvam, Marc Lanctot, Sander Dieleman, Dominik Grewe, John Nham, Nal Kalchbrenner, Ilya Sutskever, Timothy Lillicrap, Madeleine Leach, Koray Kavukcuoglu, Thore Graepel & Demis Hassabis

Nature **529**, 484–489 (28 January 2016)
doi:10.1038/nature16961
Download Citation

Received: 11 November 2015
Accepted: 05 January 2016
Published: 27 January 2016

AlphaGo seals 4-1 victory over Go grandmaster Lee Sedol

DeepMind's artificial intelligence astonishes fans to defeat human opponent and offers evidence computer software has mastered a major challenge

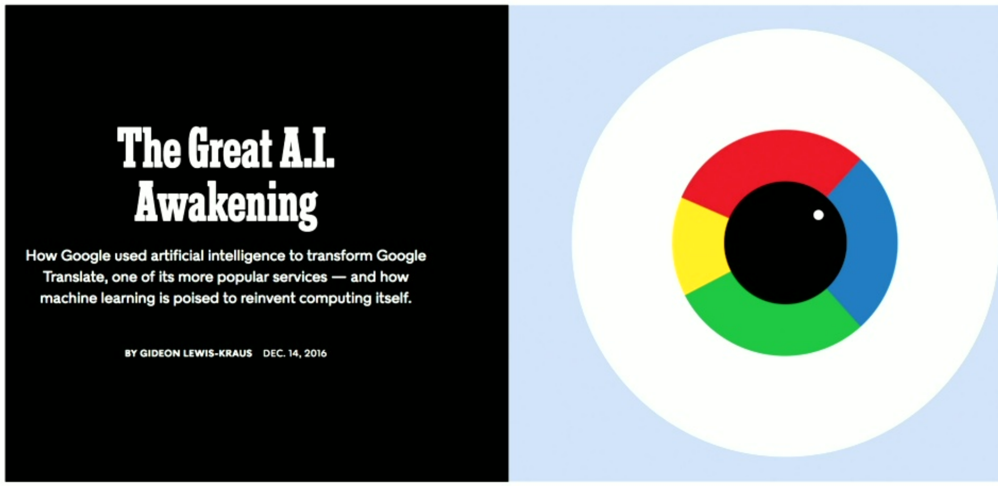
Steven Borowiec

Tue 15 Mar 2016 10.13 GMT

https://www.theguardian.com

You can learn about that on the AlphaGo (documentary movie) 2017

Language translation (2016)



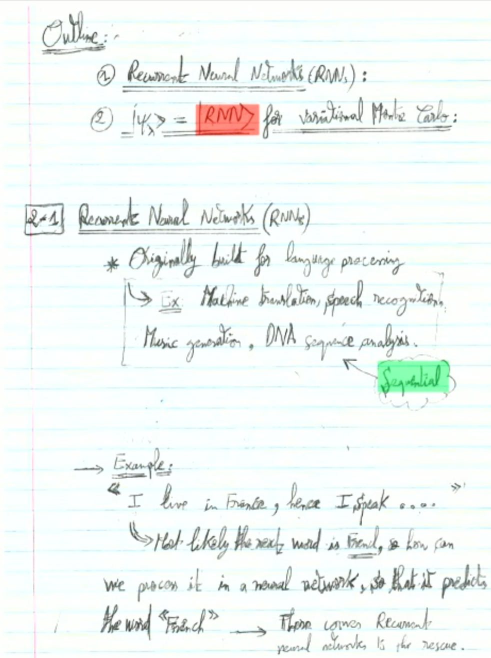
The New York Times

Large Language Models

M **You**
Explain quantum physics in 30 words exactly?

ChatGPT
Quantum physics describes the behavior of subatomic particles, emphasizing wave-particle duality, superposition, and entanglement. It challenges classical notions, revealing a probabilistic nature where particles exist in multiple states simultaneously.

GPT4o – Handwritten Notes to Latex


Outline:
① Recurrent Neural Networks (RNNs):
② $|\Psi\rangle$ = RNN for variational Monte Carlo:

2.1 Recurrent Neural Networks (RNNs)
* Originally built for language processing
↳ Ex. Machine translation, speech recognition, Music generation, DNA sequence analysis.
Sequential

→ Example:
"I live in France, hence I speak ...."
↳ Most likely the next word is French, so how can we process it in a neural network, so that it predicts the word "French" → There comes Recurrent neural networks to the rescue.

Prompt:

Can you convert the following handwritten notes to latex?

Outline

1. Recurrent Neural Networks (RNNs)
2. $|\Psi\rangle =$ RNN for variational Monte Carlo.

2.1 Recurrent Neural Networks (RNNs)

Originally built for language processing.
Examples:

- Machine translation
- Speech recognition
- Music generation
- DNA sequence analysis

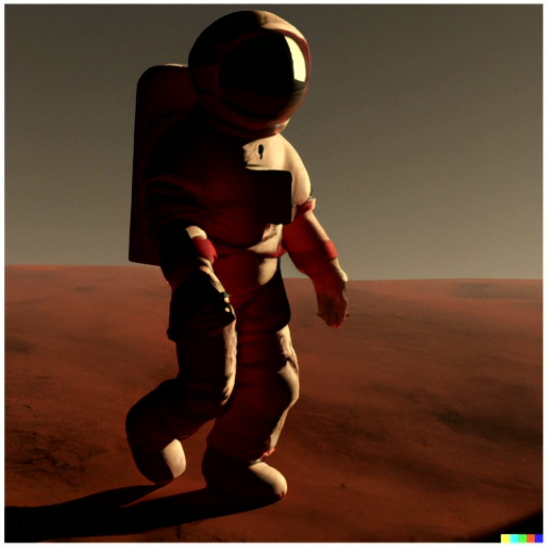
Note: These tasks involve **sequential** data.

Example

"I live in France, hence I speak ...."

It is highly likely that the next word is *French*. So, how can we process this in a neural network to predict the word *French*?
Here comes Recurrent Neural Networks to the rescue.

Dall-E



A 3d realistic render of an astronaut walking on Mars

https://labs.openai.com

AlphaProof and AlphaGeometry

RESEARCH

AI achieves silver-medal standard solving International Mathematical Olympiad problems

25 JULY 2024

AlphaProof and AlphaGeometry teams

Google DeepMind

Discovery of Physical Laws

ScienceAdvances

AI Feynman: A physics-inspired method for symbolic regression

SILVIU-MARIAN UDRESCU AND MAX TEGMARK Authors Info & Affiliations

SCIENCE ADVANCES · 15 Apr 2020 · Vol 6, Issue 16 · DOI: 10.1126/sciadv.aay2631

Abstract

A core challenge for both physics and artificial intelligence (AI) is symbolic regression: finding a symbolic expression that matches data from an unknown function. Although this problem is likely to be NP-hard in principle, functions of practical interest often exhibit symmetries, separability, compositionality, and other simplifying properties. In this spirit, we develop a recursive multidimensional symbolic regression algorithm that combines neural network fitting with a suite of physics-inspired techniques. We apply it to 100 equations from the *Feynman Lectures on Physics*, and it discovers all of them, while previous publicly available software cracks only 71; for a more difficult physics-based test set, we improve the state-of-the-art success rate from 15 to 90%.

Example: the neural network was able to find the energy of a particle in special relativity.

Predicting research trends

RESEARCH ARTICLE PHYSICAL SCIENCES

Predicting research trends with semantic and neural networks with an application in quantum physics

Mario Krenn and Anton Zeilinger Authors Info & Affiliations

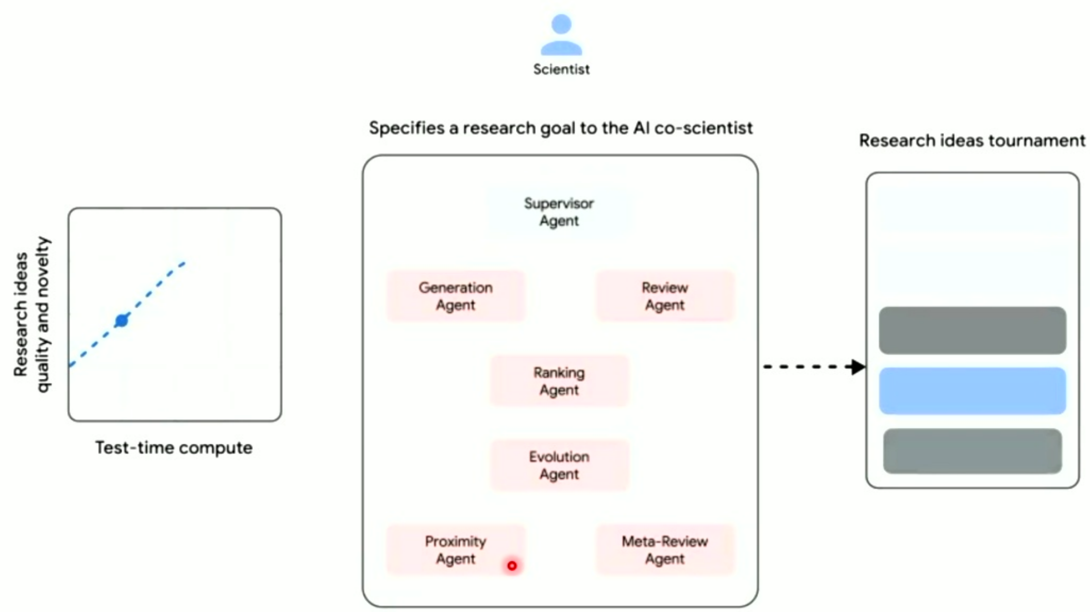
Contributed by Anton Zeilinger, October 24, 2019 (sent for review August 19, 2019; reviewed by Ebrahim Karimi and Terry Rudolph)

January 14, 2020 117 (4) 1910-1916 https://doi.org/10.1073/pnas.1914370116

Significance

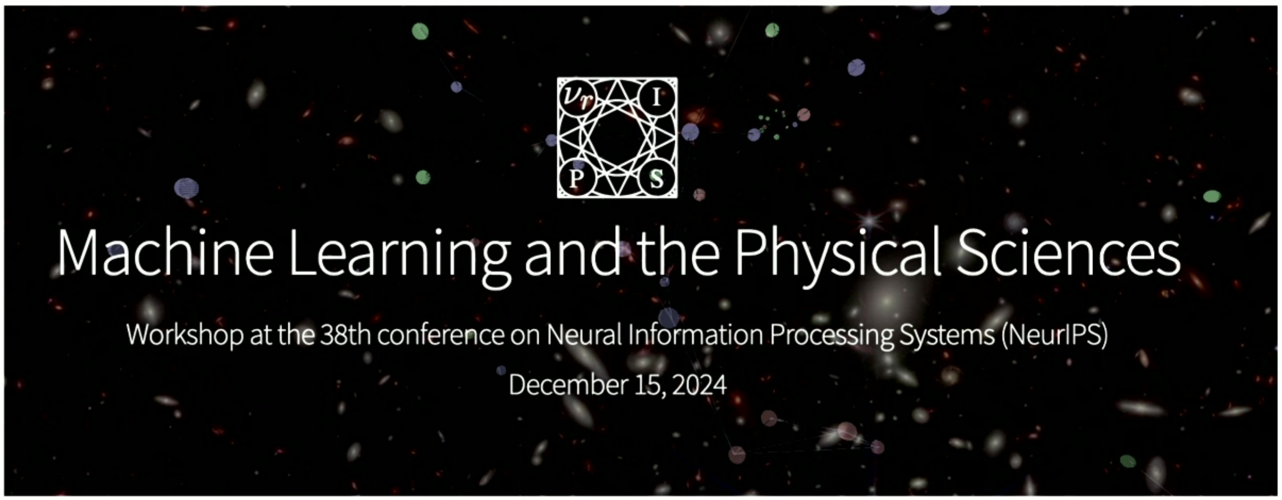
The corpus of scientific literature grows at an ever increasing speed. While this poses a severe challenge for human researchers, computer algorithms with access to a large body of knowledge could help make important contributions to science. Here, we demonstrate the development of a semantic network for quantum physics, denoted SemNet, using 750,000 scientific papers and knowledge from books and Wikipedia. We use it in conjunction with an artificial neural network for predicting future research trends. Individual scientists can use SemNet for suggesting and inspiring personalized, out-of-the-box ideas. Computer-inspired scientific ideas will play a significant role in accelerating scientific progress, and we hope that our work directly contributes to that important goal.

AI co-scientist



https://research.google/blog/accelerating-scientific-breakthroughs-with-an-ai-co-scientist/

< ML | Physics >


Machine Learning and the Physical Sciences
Workshop at the 38th conference on Neural Information Processing Systems (NeurIPS)
December 15, 2024

Nobel prize in Physics 2024

Ill. Niklas Elmehed © Nobel Prize Outreach

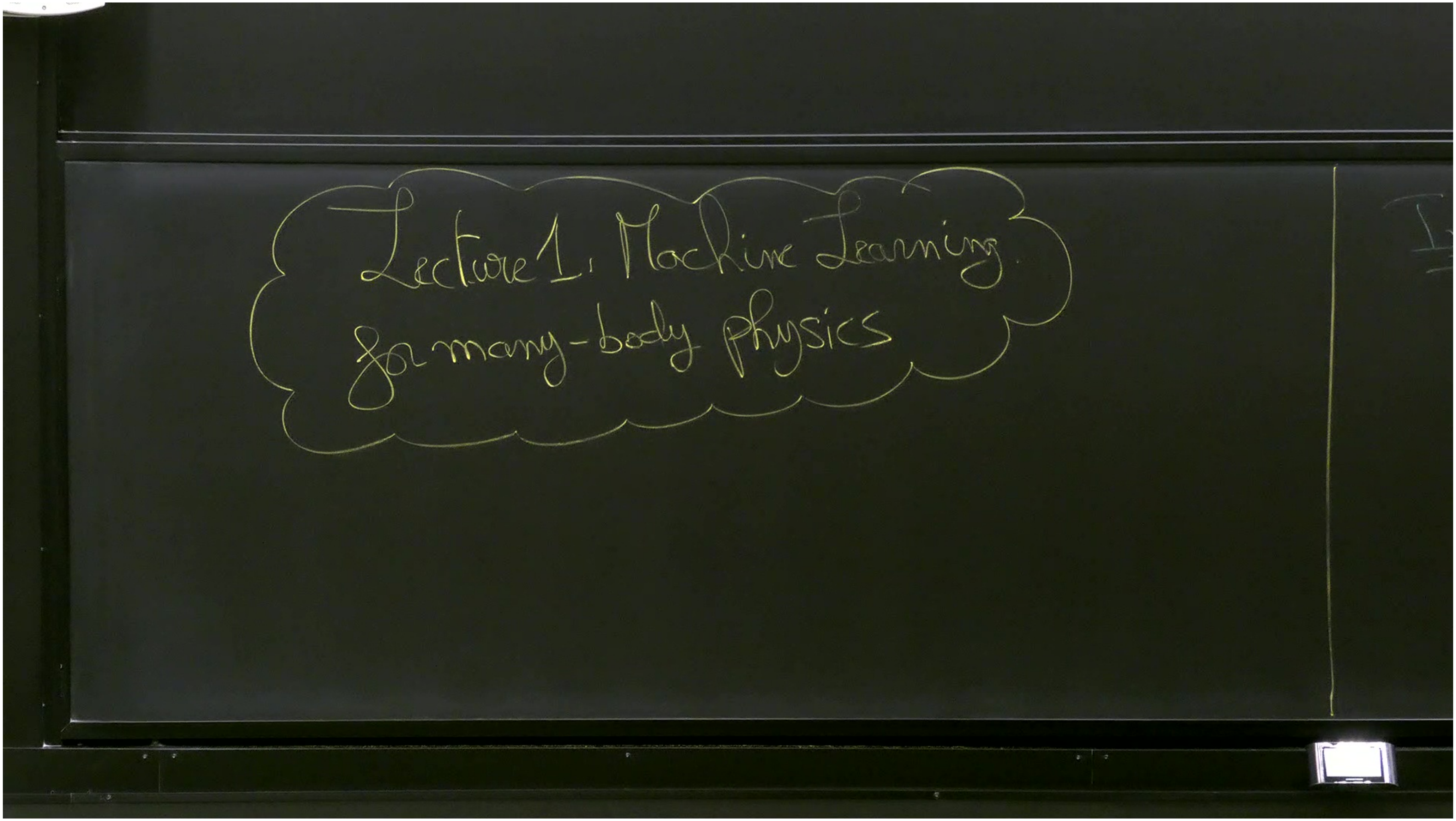
John J. Hopfield

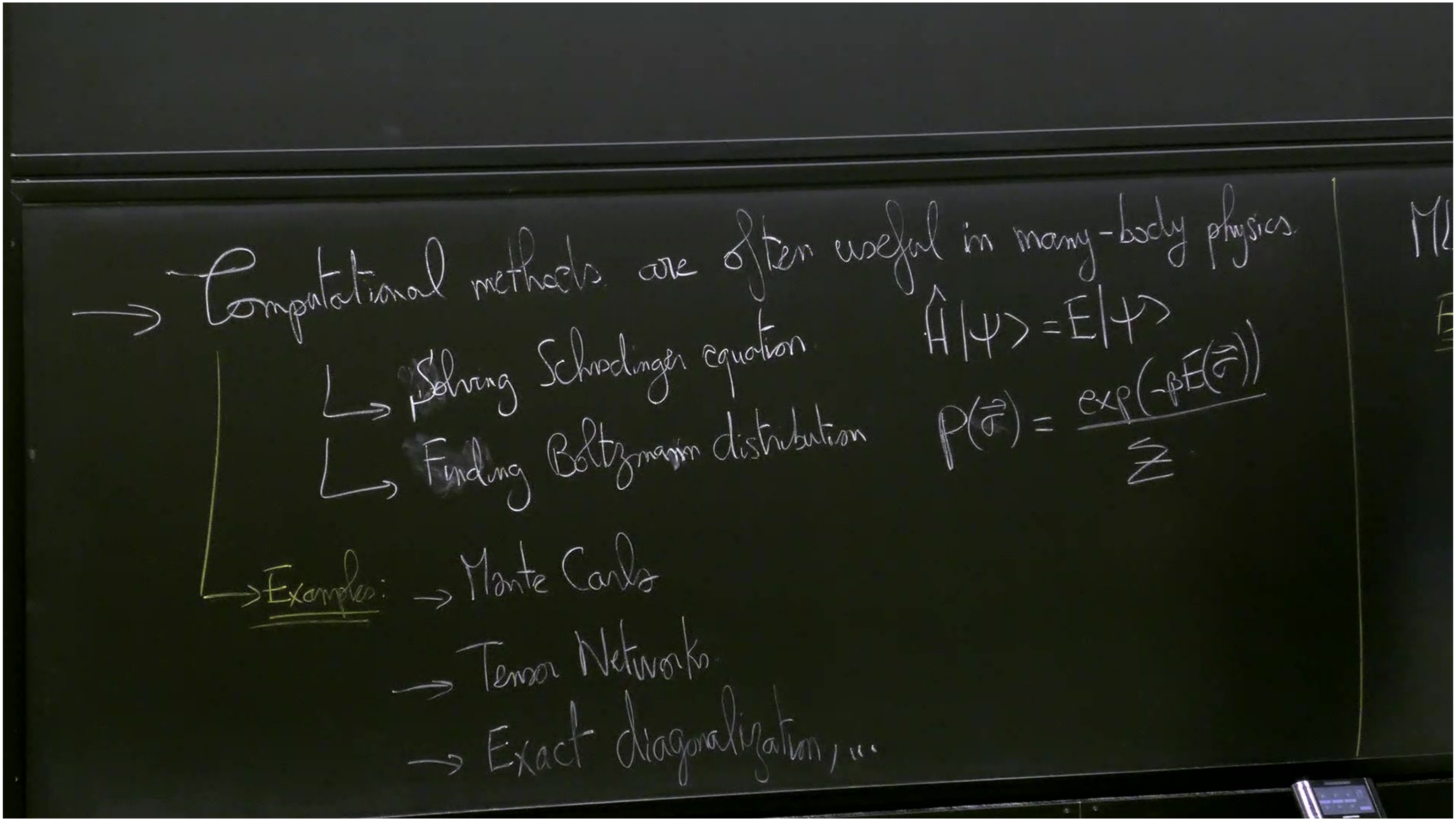
Prize share: 1/2

Ill. Niklas Elmehed © Nobel Prize Outreach

Geoffrey Hinton

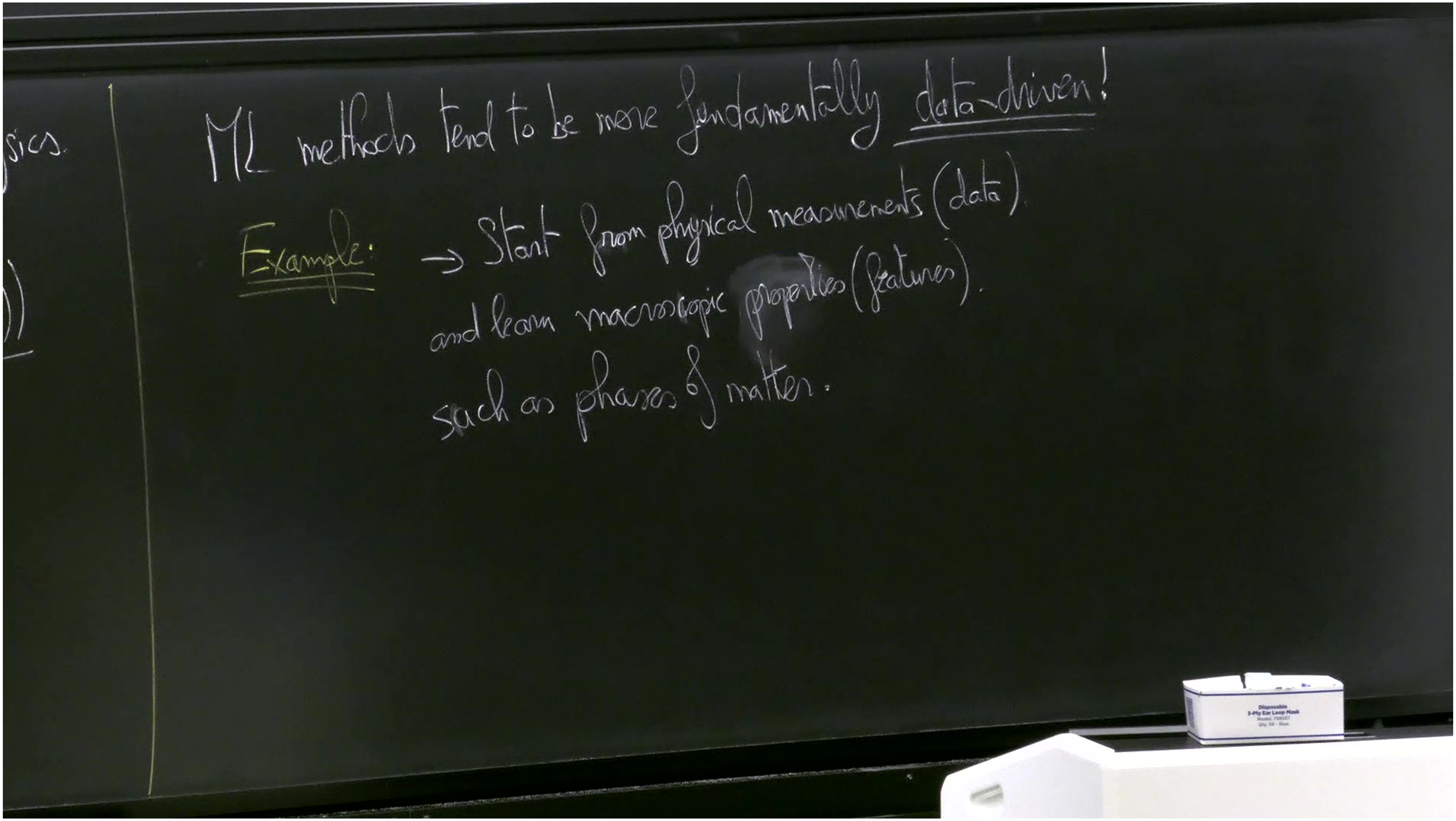
Prize share: 1/2

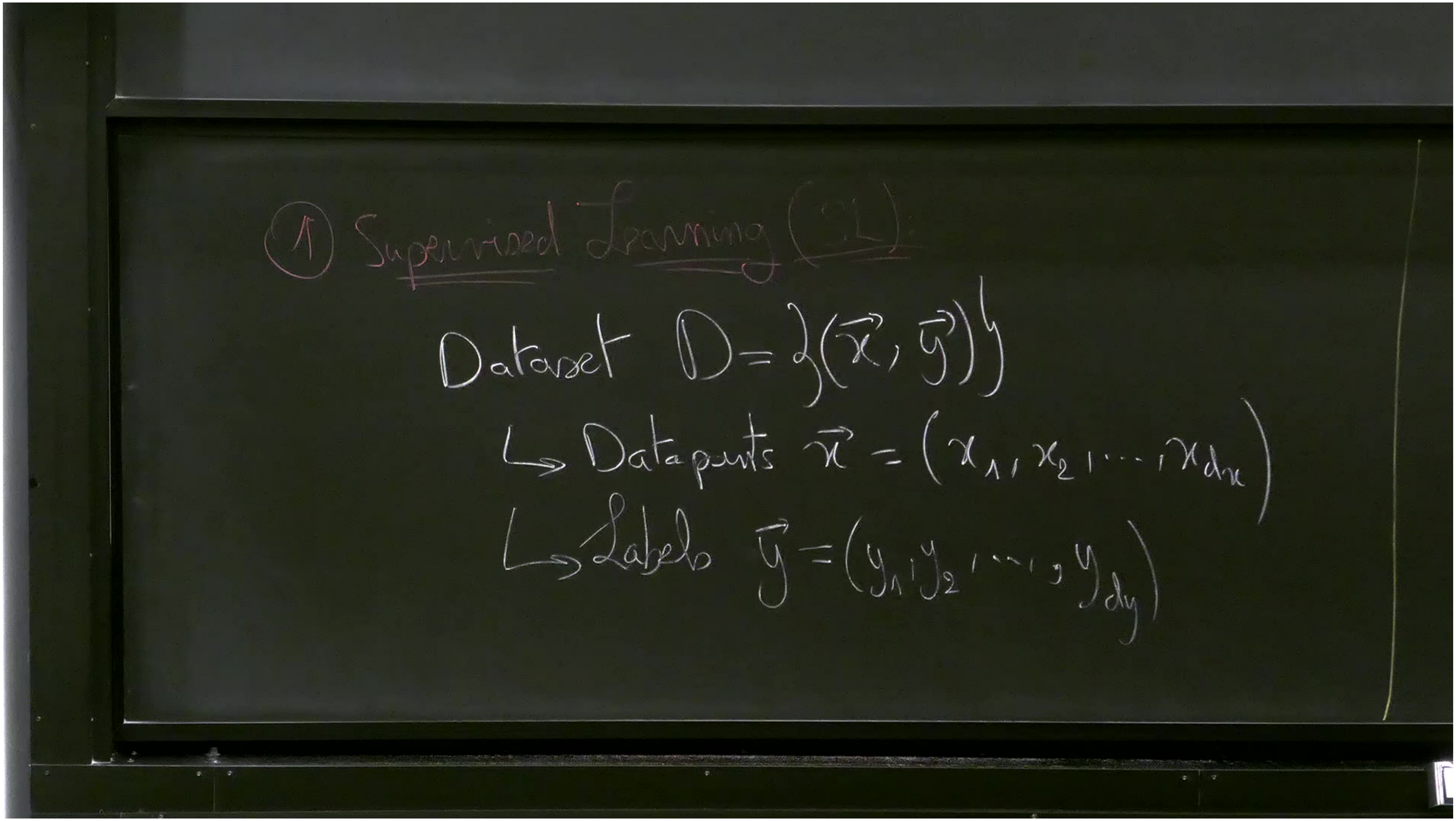

Lecture 1. Machine Learning
for many-body physics

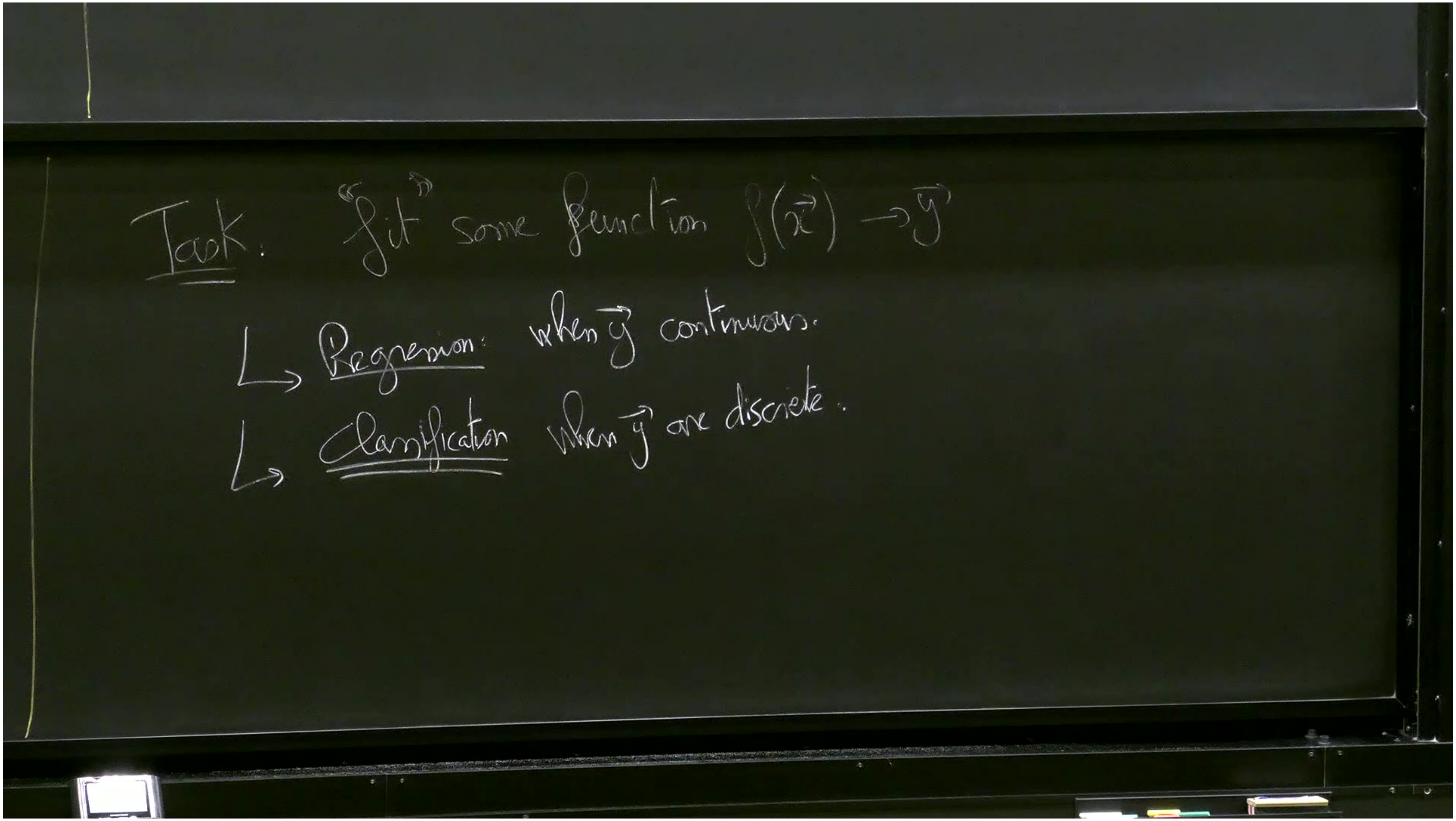

→ Computational methods are often useful in many-body physics
Solving Schrodinger equation
Ĥ|ψ> = E|ψ>
Finding Boltzmann distribution
p(σ⃗) = exp(-βE(σ⃗)) / Z
Examples:
→ Monte Carlo
→ Tensor Networks
→ Exact diagonalization, ...

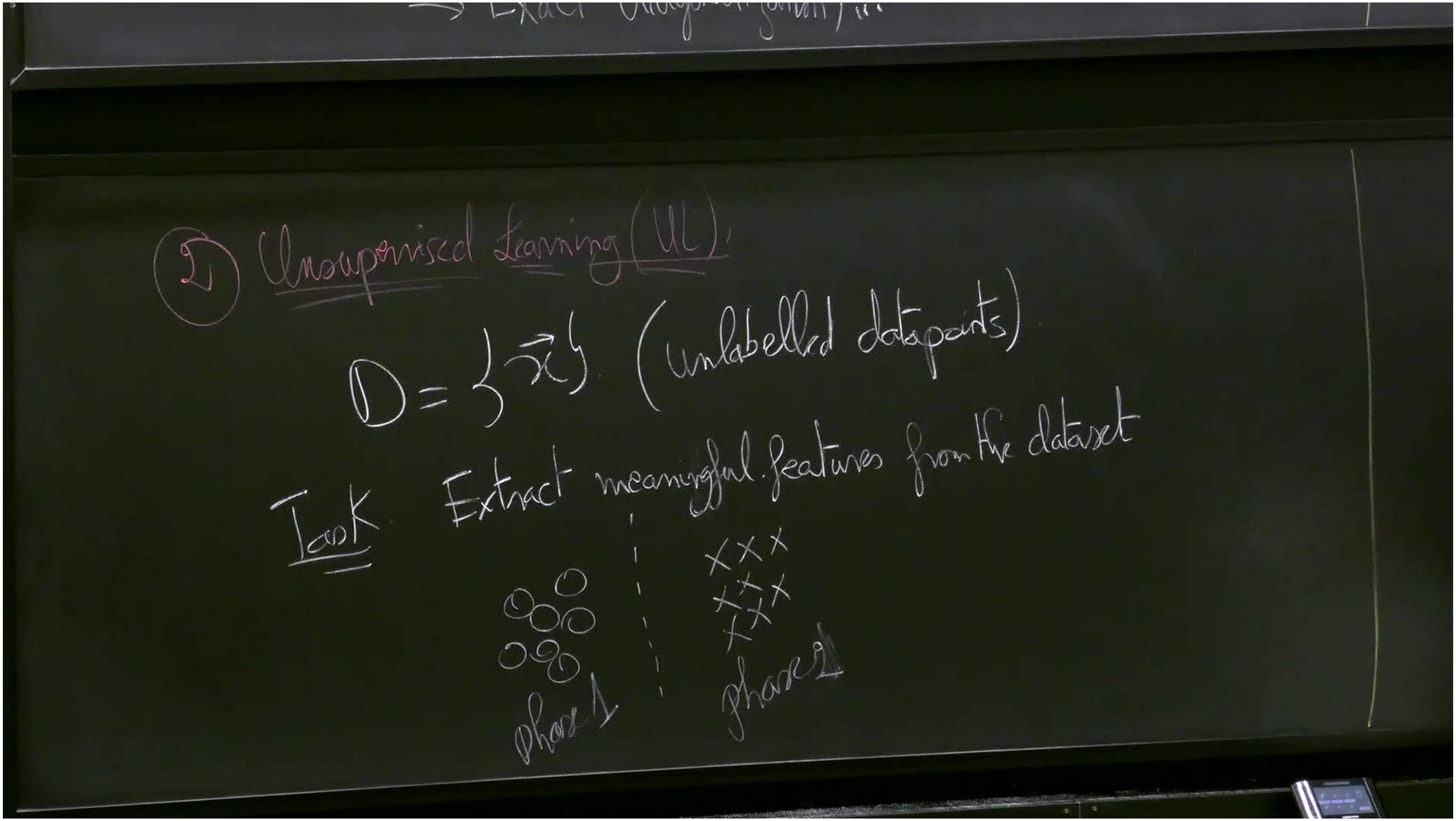
Important points about many-body physics:

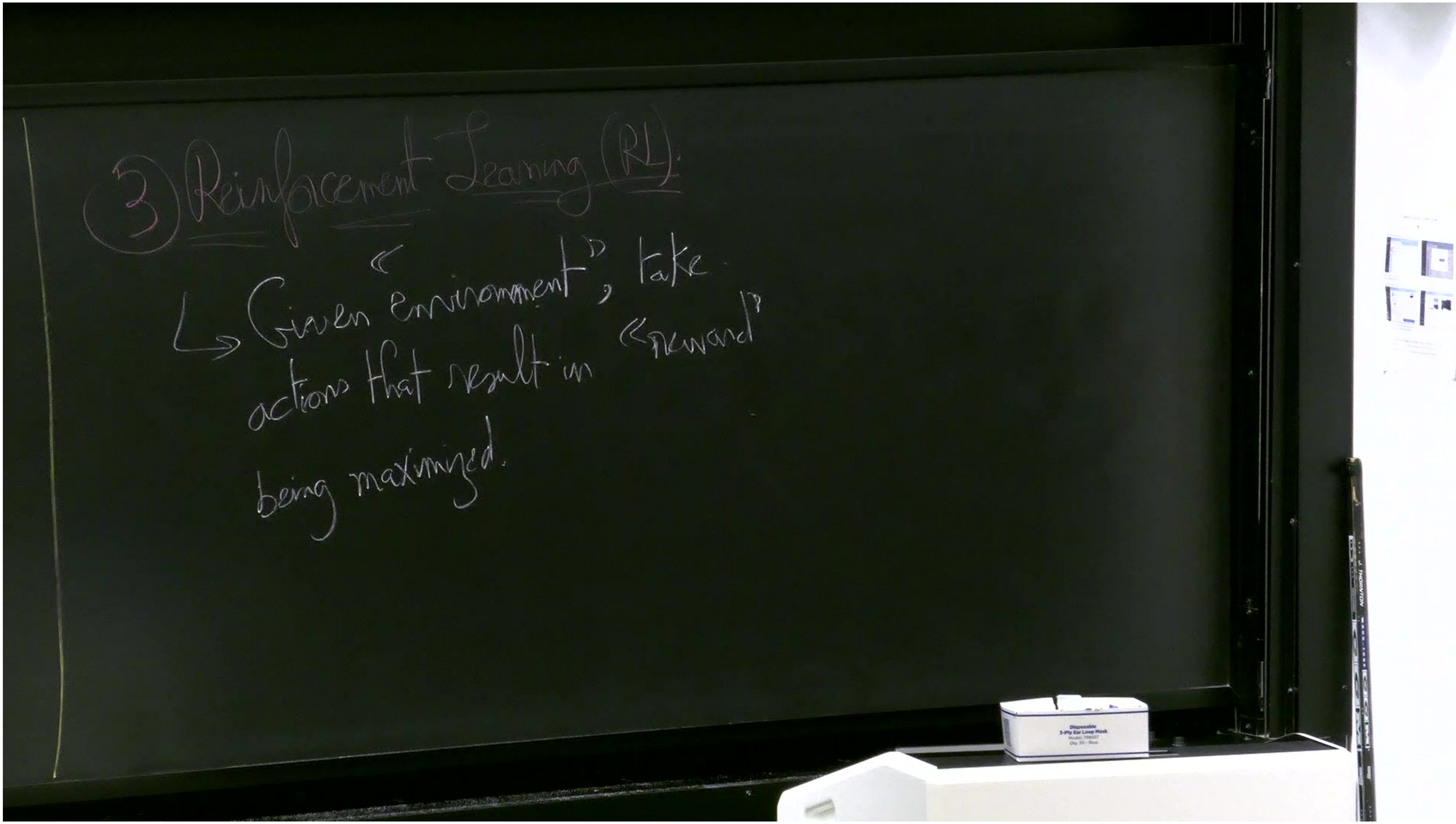
- ↳ Relies on many-particles interacting.
- ↳ Needed to describe phases of matter (excluding single quasi-particle theories).

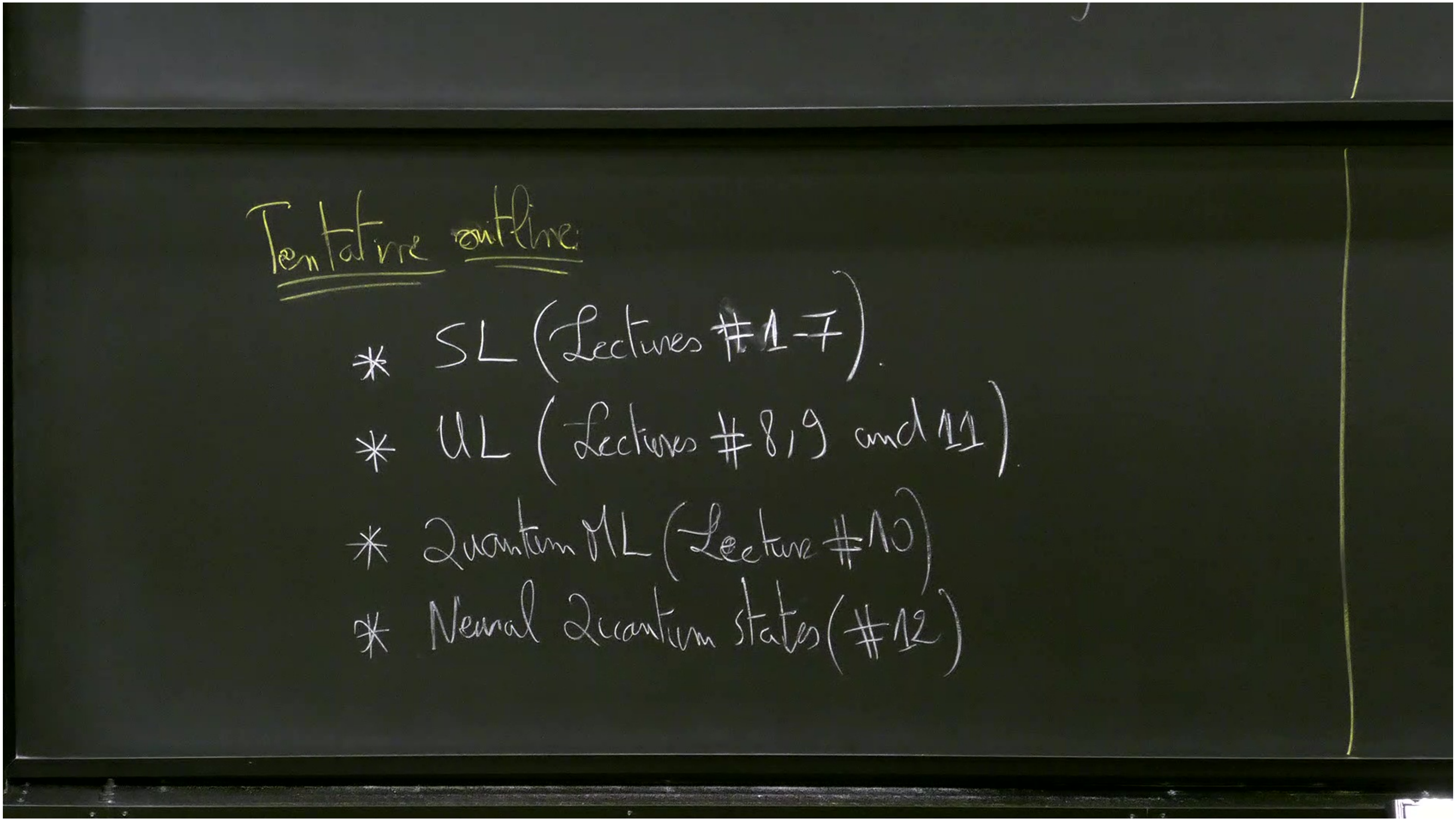

sics.
ML methods tend to be more fundamentally data-driven!
Example:
→ Start from physical measurements (data).
and learn macroscopic properties (features).
such as phases of matter.
Disposable
3-Ply Ear Loop Mask


① Supervised Learning (SL):
Dataset D = {(x⃗, y⃗)}
↳ Datapoints x⃗ = (x1, x2, ..., xdx)
↳ Labels y⃗ = (y1, y2, ..., ydy)


Task: "fit" some function f(x⃗) → y⃗
↳ Regression: when y⃗ continuous.
↳ Classification when y⃗ are discrete.


2) Unsupervised Learning (UL)
D = {x} (unlabelled datapoints)
Task Extract meaningful features from the dataset
phase 1
phase 2

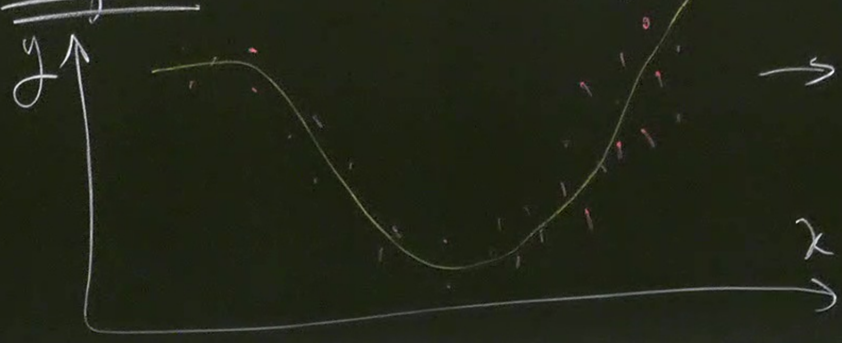

③ Reinforcement Learning (RL).
↳ Given «environment», take
actions that result in «reward»
being maximized.


Tentative outline:
* SL (Lectures #1-7)
* UL (Lectures #8,9 and 11)
* Quantum ML (Lecture #10)
* Neural Quantum states (#12)

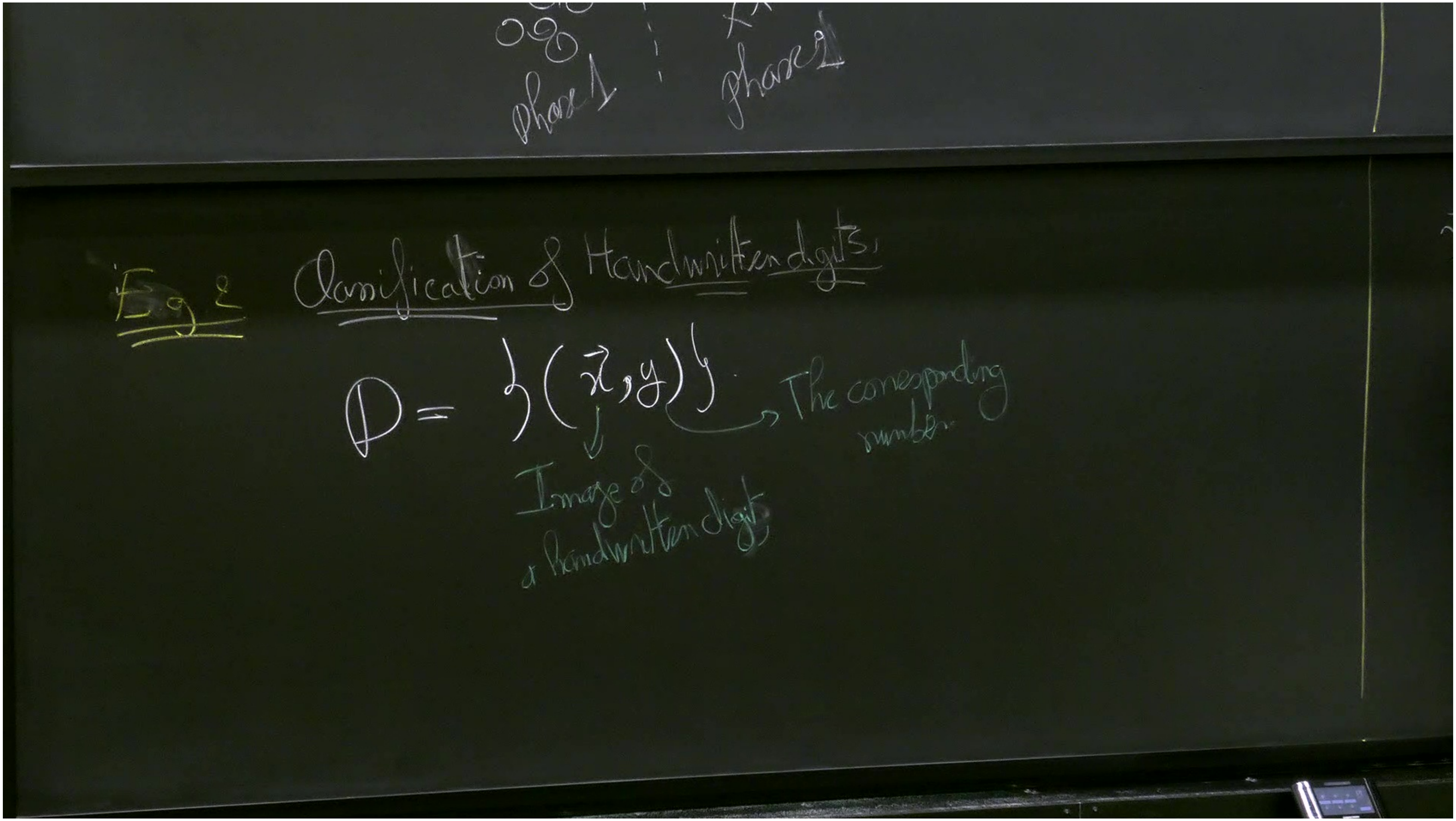
* Recent advances in ⟨ML | many-body phys⟩ + ML ethics

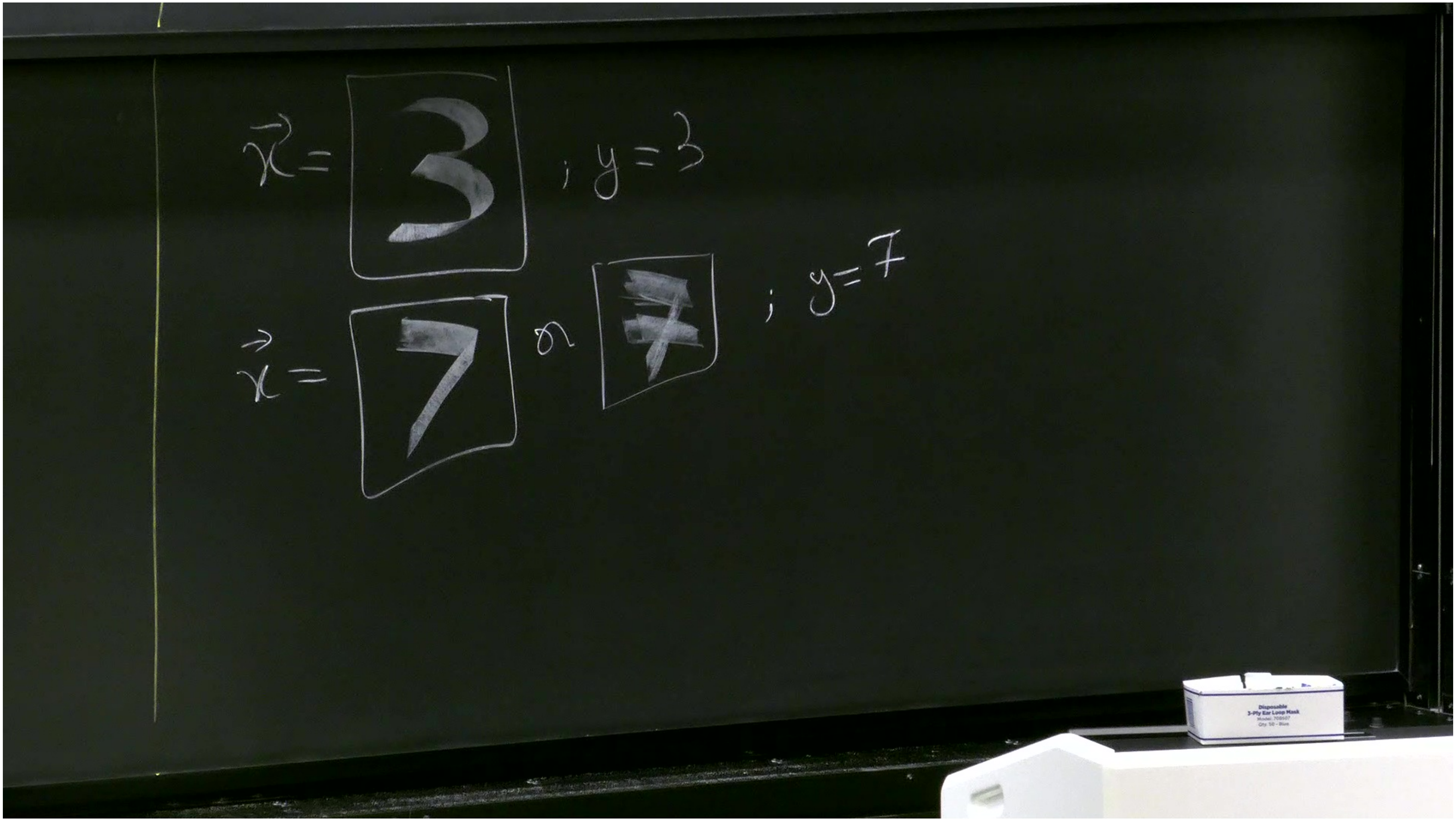
SL examples:

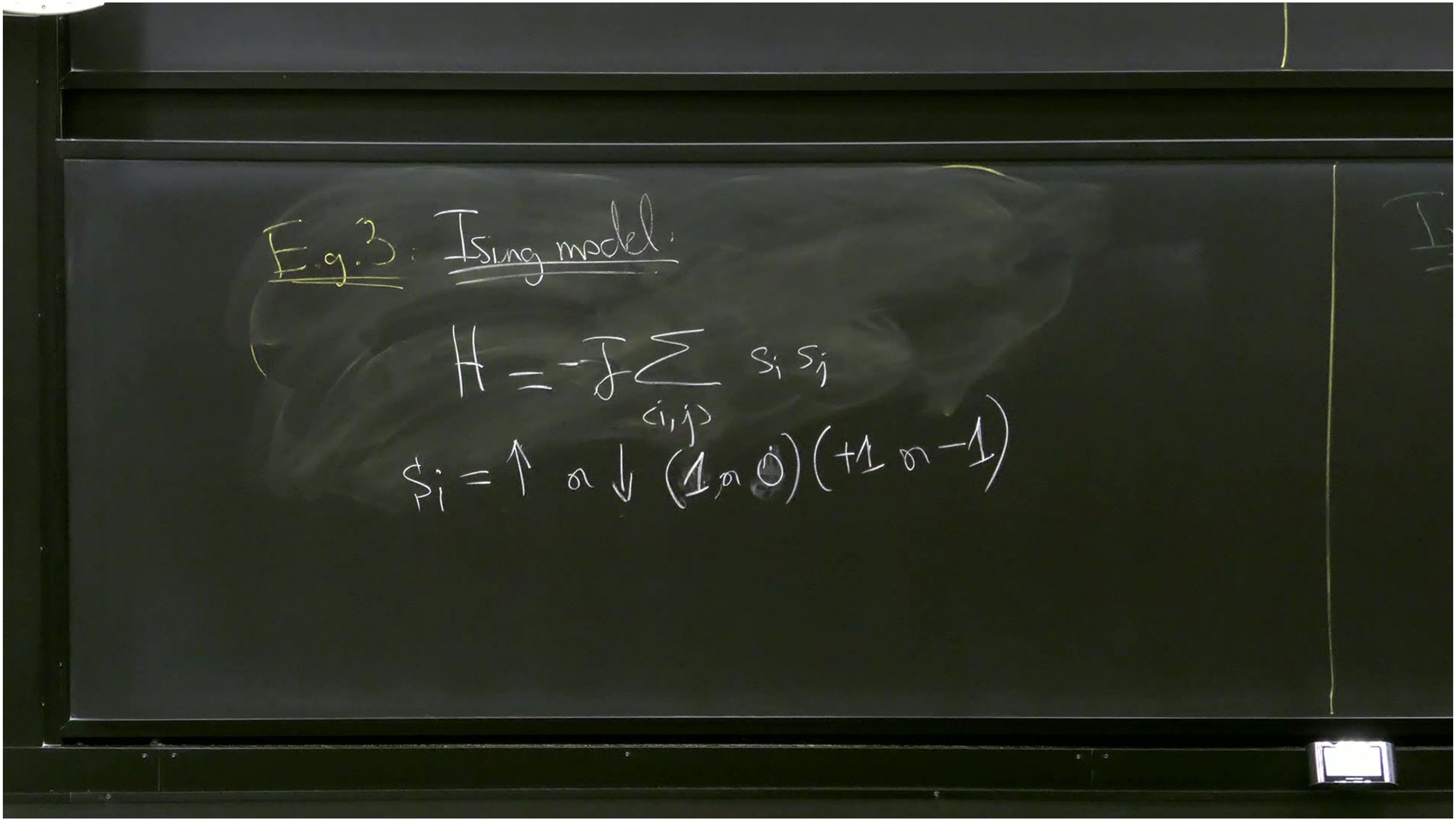
↳ Regression: $D = \{(x, y)\}$ $(d_x = 1 = d_y)$.

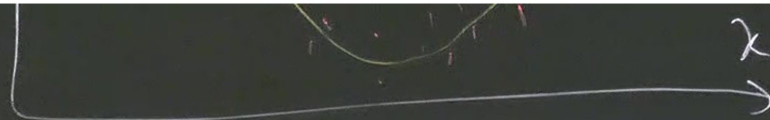


→ Goal: determine a curve to describe the data.


phase 1
phase 2
E.g 2
Classification of Handwritten digits.
D = {(x, y)}
Image of a handwritten digits
The corresponding number


x⃗ = 3 ; y = 3
x⃗ = 7 or 7 ; y = 7
Disposable
3-Ply Ear Loop Mask

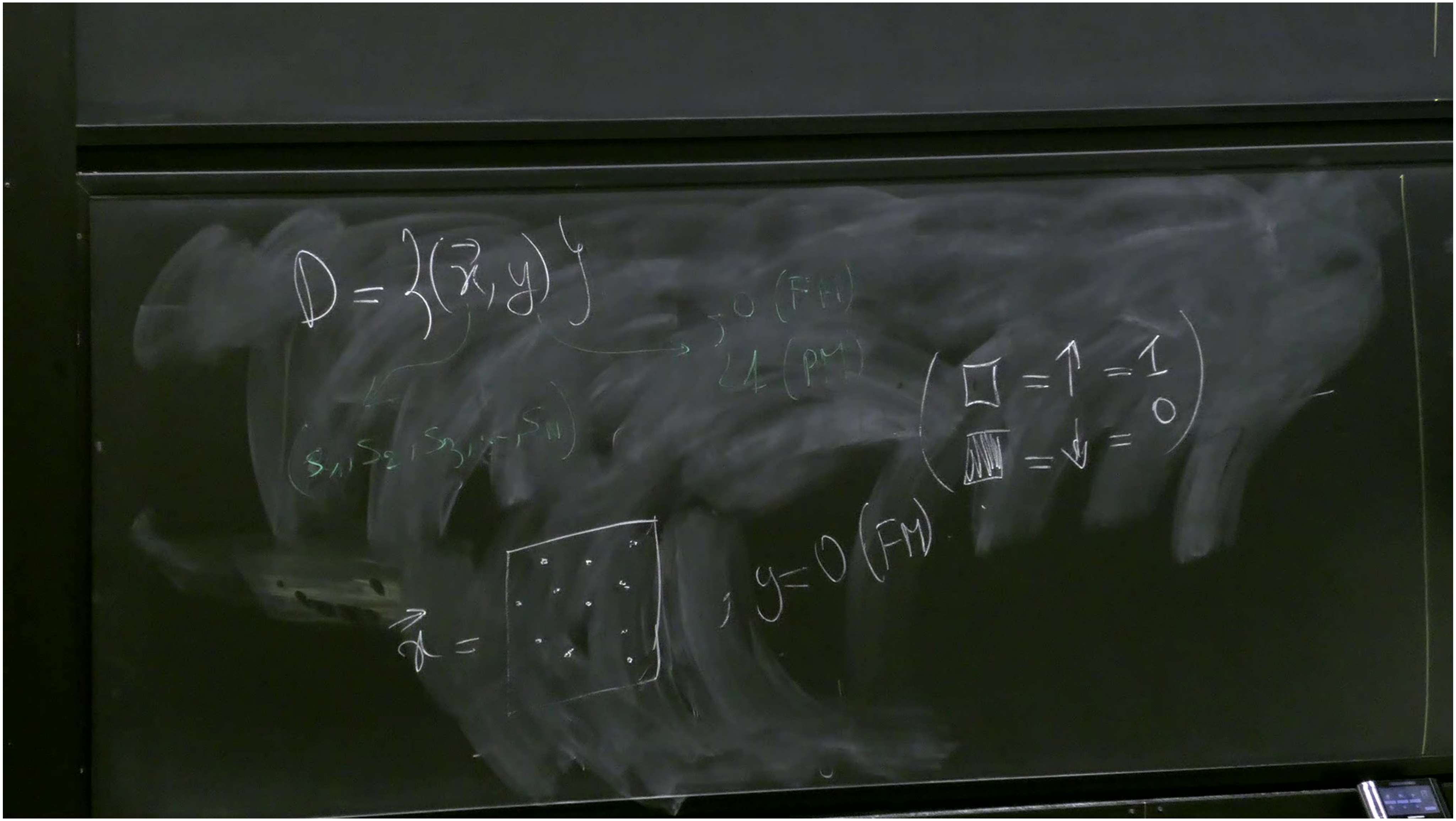

E.g. 3: Ising model.
H = -J Σ s_i s_j
<i,j>
s_i = ↑ or ↓ (1 or 0) (+1 or -1)

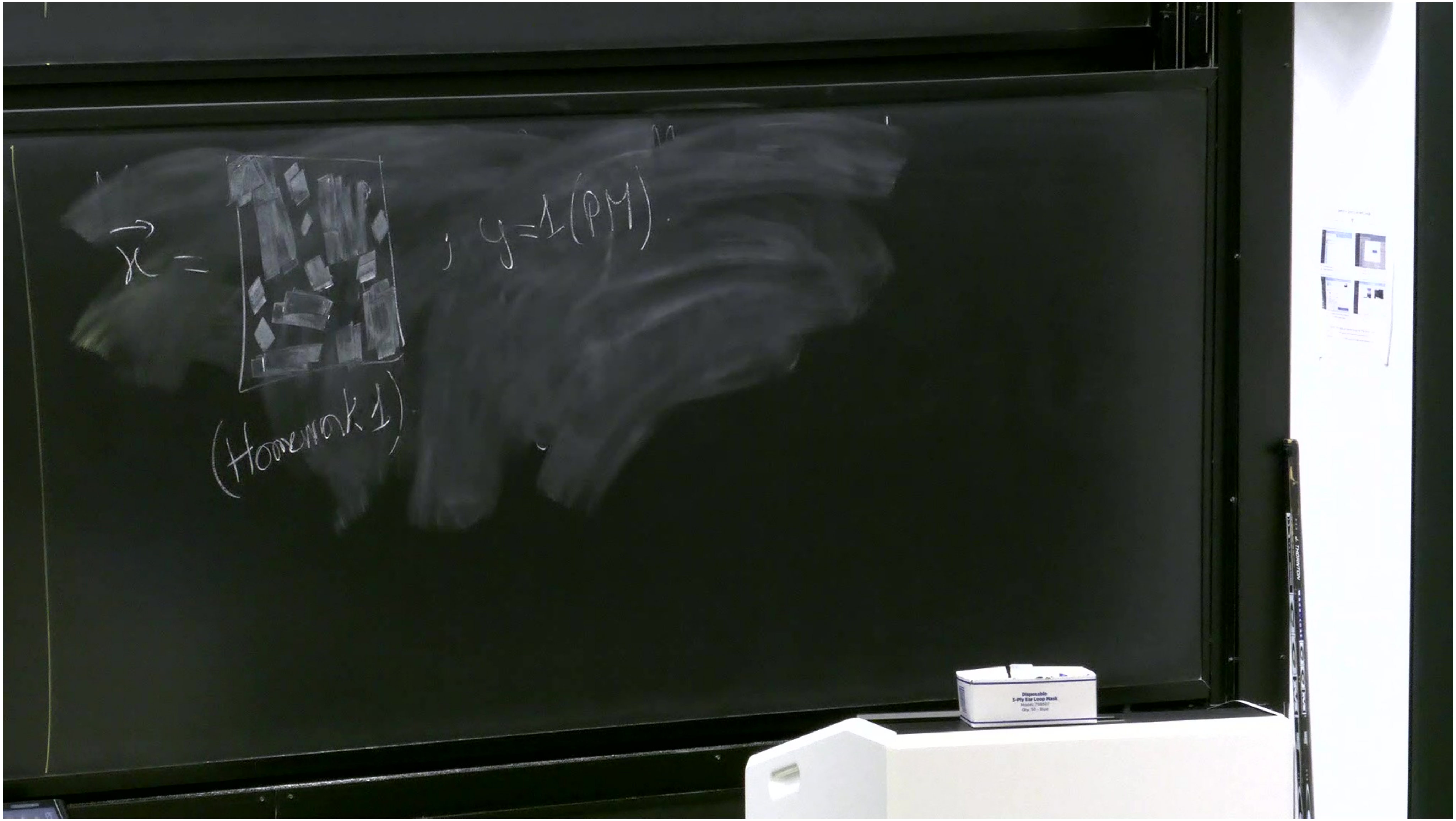


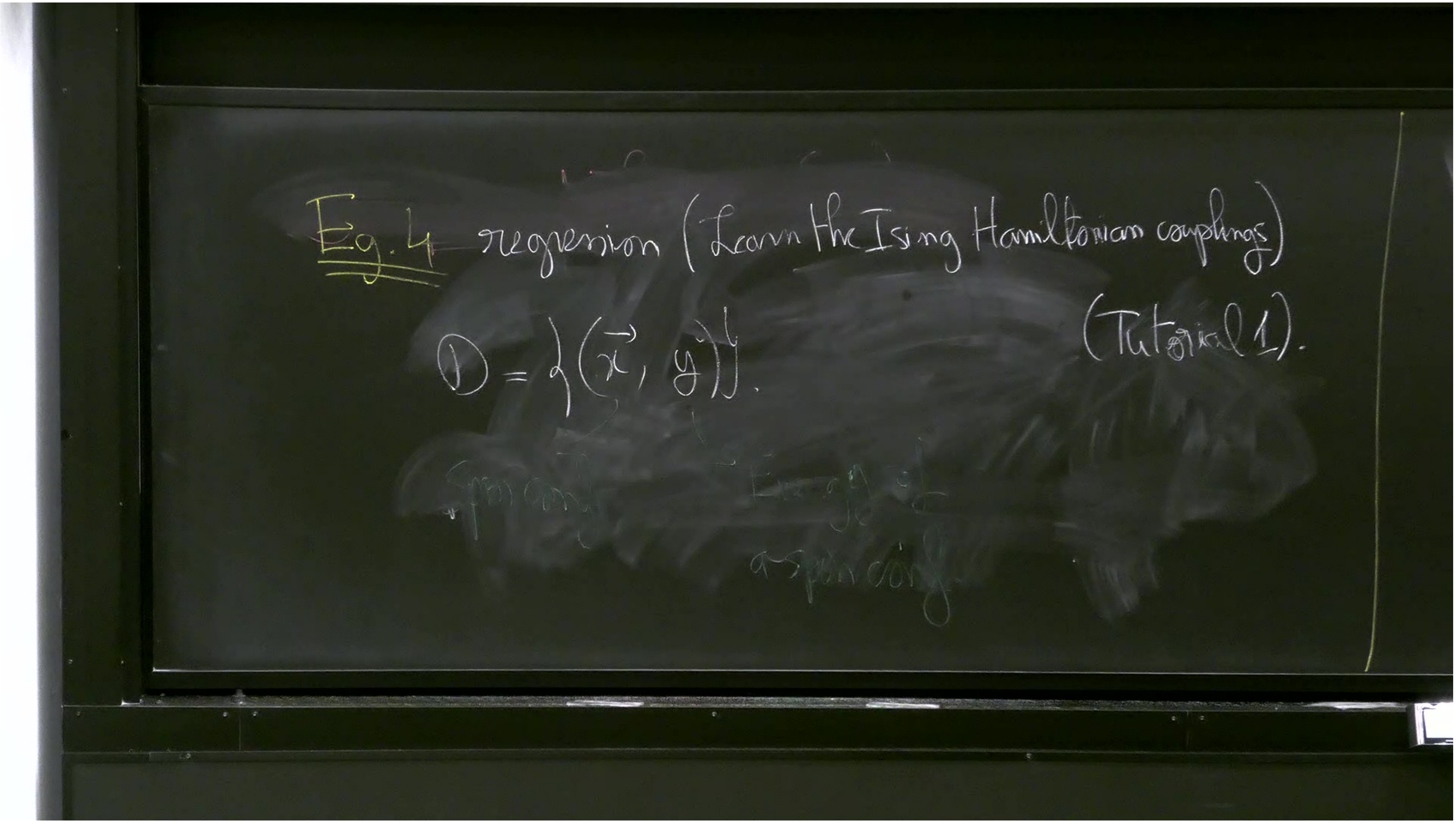
Recall in 2D, the ising model has a phase transition at $T_c/J \simeq 2.269$

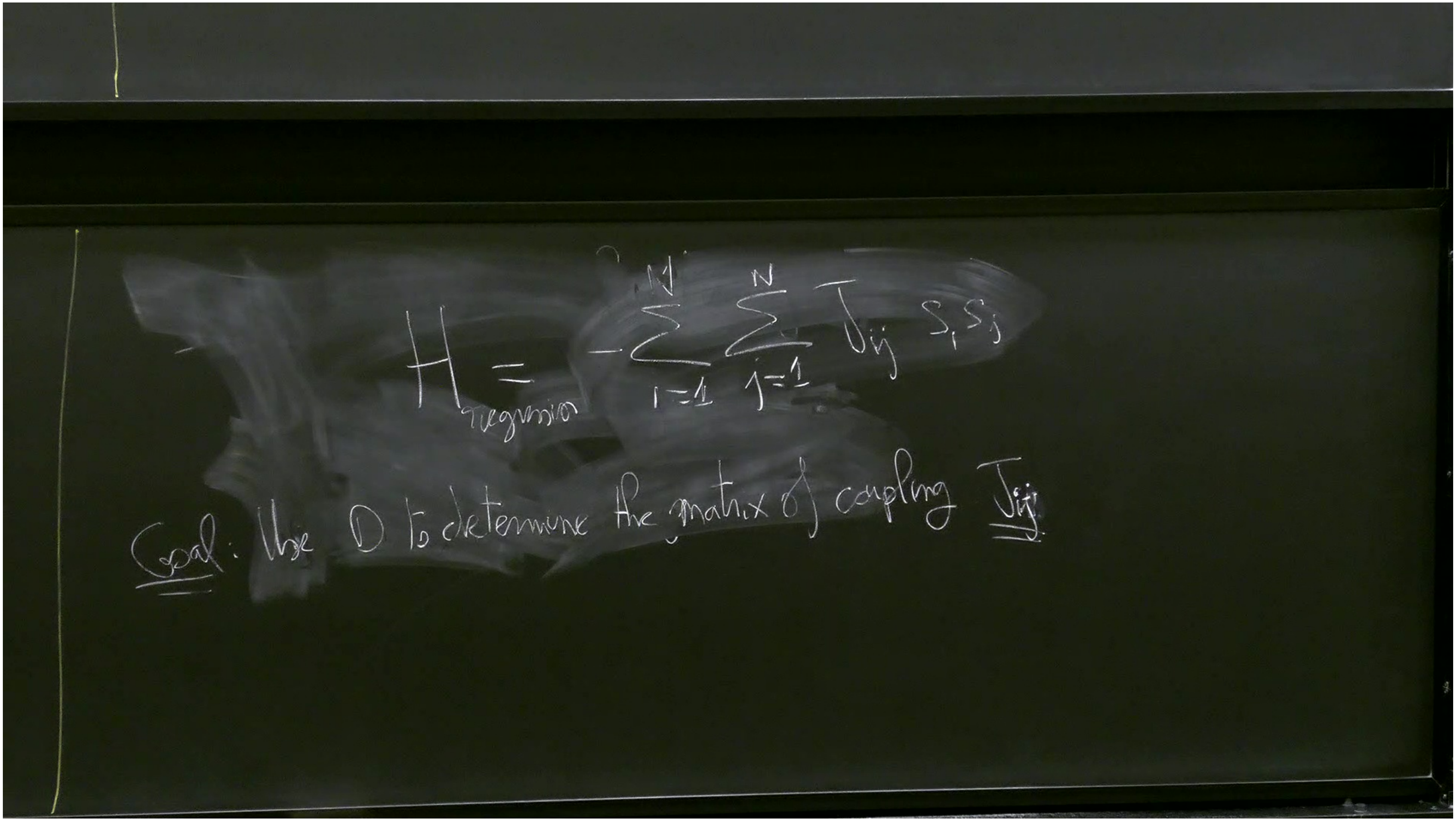
→ For $T < T_c$: Ferromagnetic phase (FM)

→ For $T > T_c$: Paramagnetic phase (PM).


D = {(x, y)}
0 (FM)
1 (PM)
(s1, s2, s3, ..., sN)
= ↑ = 1
= ↓ = 0
x =
y = 0 (FM)


x⃗ =
; y=1 (PM)
(Homework 1)


Eg. 4 regression (Learn the Ising Hamiltonian couplings)
(Tutorial 1).
D = {(x⃗, y)}.


H_regression = - Σ_{i=1}^{N} Σ_{j=1}^{N} J_ij S_i S_j
Goal: Use D to determine the matrix of coupling J_ij

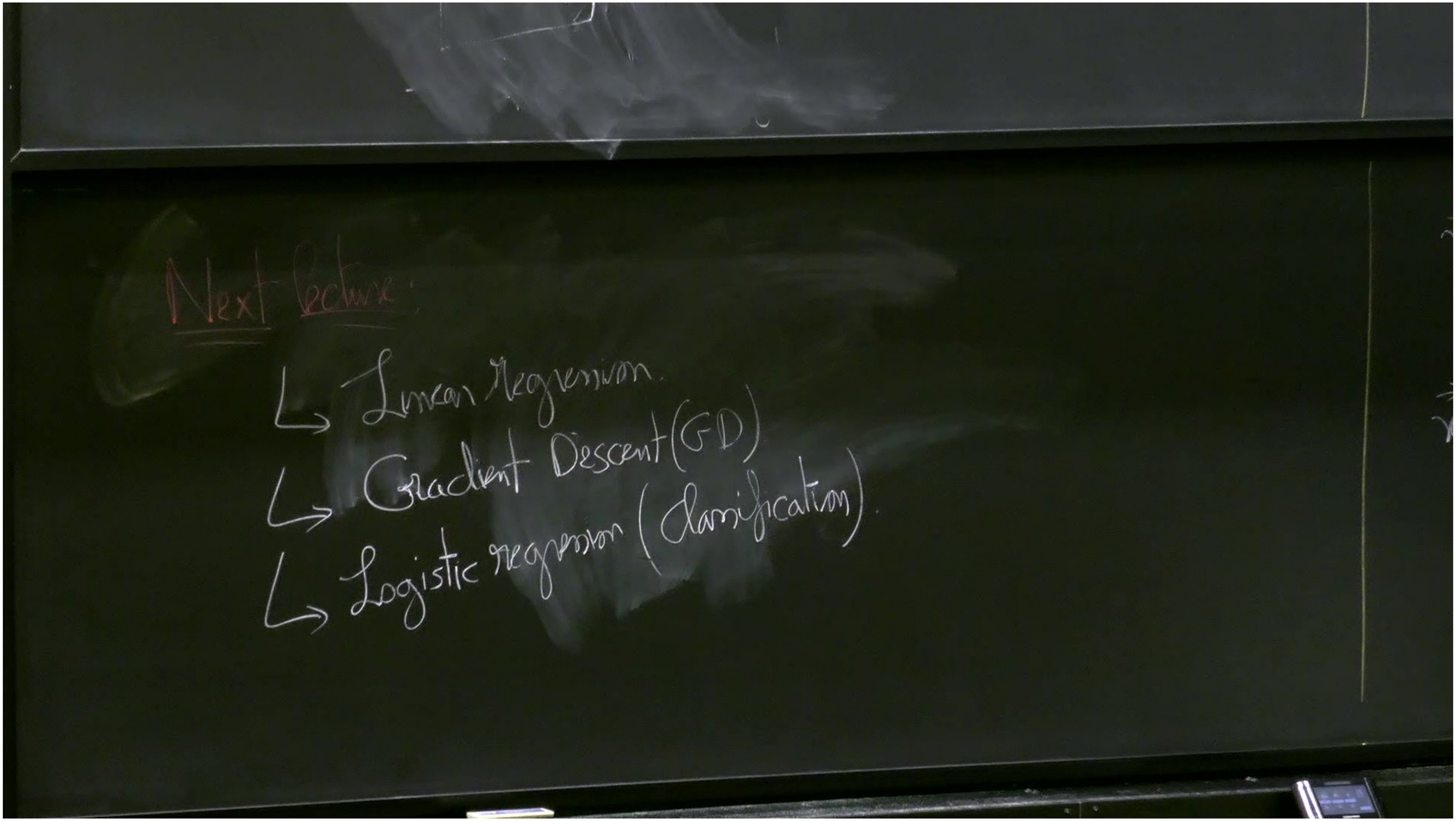
Eg. 4 regression (Learn the Ising Hamiltonian couplings)

(Tutorial 1).

$\mathcal{D} = \{(\vec{x}, y)\}$.

$\vec{x} = (s_1, s_2, \dots, s_N)$

Goal:

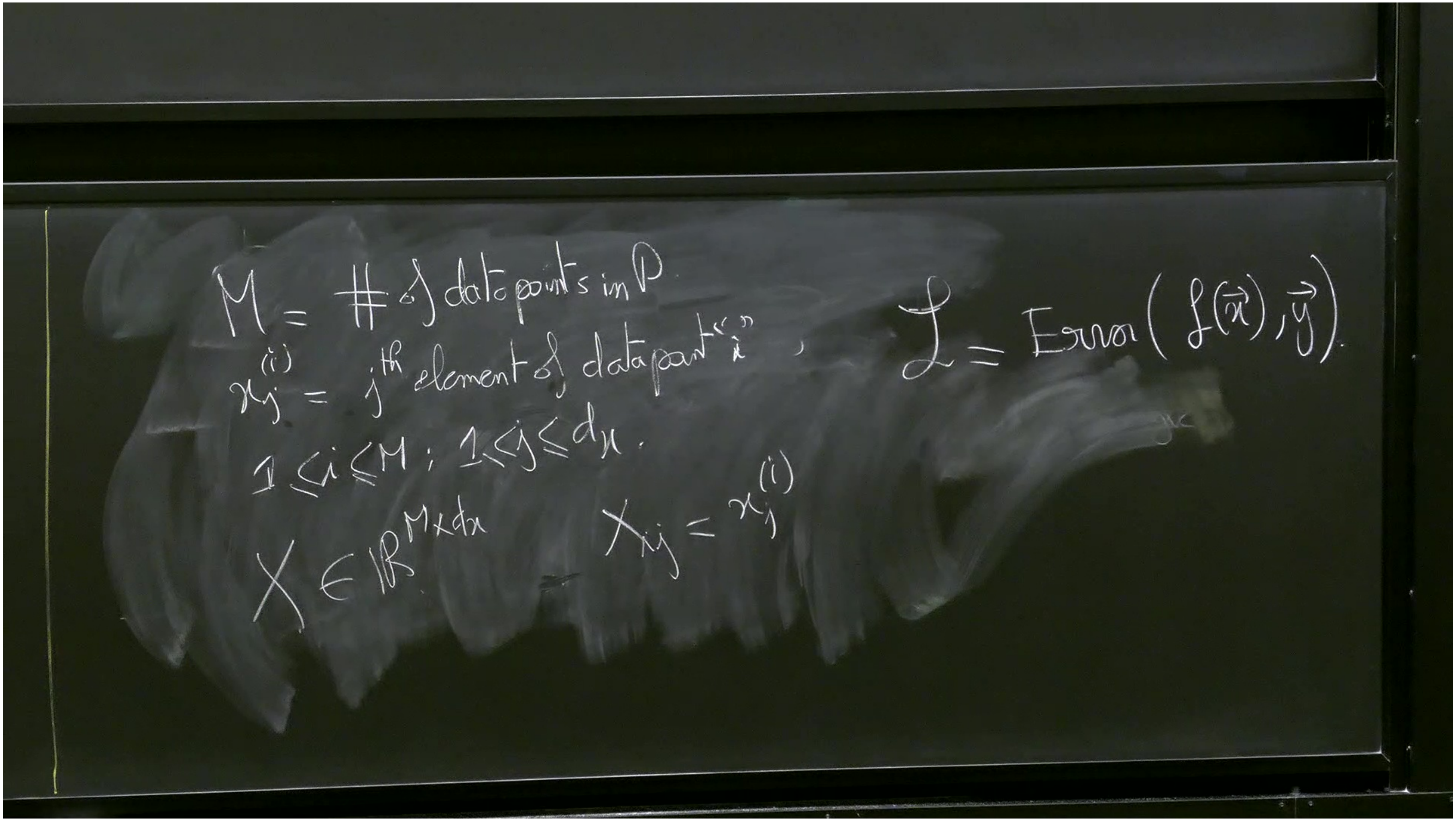

Next Lecture:
↳ Linear Regression.
↳ Gradient Descent (GD)
↳ Logistic regression (Classification).

Linear regression (LR):

$\mathcal{D} = \{(\vec{x}, y)\}$: $f(\vec{x})$ to $y(\vec{x})$ $\quad d_y = 1$

$$f(\vec{x}) = \sum_{j=1}^{d_x} w_j x_j = \vec{w}^T \cdot \vec{x}$$

$$\vec{w}^T = (w_1, \dots, w_{d_x})$$


M = # of datapoints in D
$x_j^{(i)}$ = j^{th} element of datapoint "i"
$1 \leq i \leq M$; $1 \leq j \leq d_x$.
$X \in \mathbb{R}^{M \times d_x}$
$X_{ij} = x_j^{(i)}$
$\mathcal{L}$ = Error($f(\vec{x})$, $\vec{y}$).