Title: PSI 2017/2018 - Machine Learning for Many Body Physics - Lecture 1

Date: Apr 09, 2018 09:00 AM

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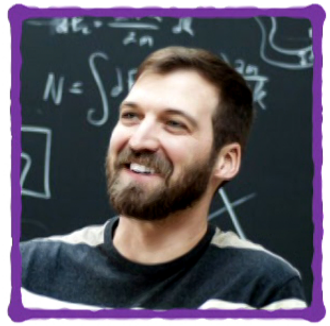
Abstract:

Machine Learning for Many-Body Physics

Lauren Hayward Sierens

Juan Carrasquilla



Roger Melko

Giacomo Torlai

VECTOR INSTITUTE

PERIMETER INSTITUTE

UNIVERSITY OF WATERLOO

PERIMETER SCHOLARS INTERNATIONAL

April 9-27, 2018

Machine learning popularity

PERIMETER SCHOLARS INTERNATIONAL

Image classification

ImageNet Classification with Deep Convolutional Neural Networks

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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.

2012

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Image classification

https://github.com/tensorflow/models

```
toaster (score = 0.99288)
space heater (score = 0.00071)
iPod (score = 0.00034)
printer (score = 0.00024)
pay-phone, pay-station (score = 0.00016)
```


```
mountain bike, all-terrain bike, off-roader (score = 0.80308)
picket fence, paling (score = 0.01216)
bicycle-built-for-two, tandem bicycle, tandem (score = 0.00893)
disk brake, disc brake (score = 0.00346)
sleeping bag (score = 0.00307)
```

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Image classification

https://github.com/tensorflow/models

```
borzoi, Russian wolfhound (score = 0.46677)
quilt, comforter, comfort, puff (score = 0.06664)
whippet (score = 0.06200)
sleeping bag (score = 0.05488)
Cardigan, Cardigan Welsh corgi (score = 0.02153)
```

PERIMETER SCHOLARS INTERNATIONAL

Image classification

https://github.com/tensorflow/models

```
barn (score = 0.19133)
planetarium (score = 0.12688)
dome (score = 0.06614)
church, church building (score = 0.05428)
library (score = 0.03213)
```

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Image classification

https://github.com/tensorflow/models

```
barn (score = 0.19133)
planetarium (score = 0.12688)
dome (score = 0.06614)
church, church building (score = 0.05428)
library (score = 0.03213)
```

```
cinema, movie theater, movie theatre, movie house, picture palace (score = 0.47794)
restaurant, eating house, eating place, eatery (score = 0.10927)
planetarium (score = 0.03705)
library (score = 0.03526)
palace (score = 0.03506)
```

PERIMETER SCHOLARS INTERNATIONAL

AlphaGo

nature
International journal of science

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

Abstract

The game of Go has long been viewed as the most challenging of classic games for artificial intelligence owing to its enormous search space and the difficulty of evaluating board positions and moves. Here we introduce a new approach to computer Go that uses 'value networks' to evaluate board positions and 'policy networks' to select moves. These deep neural networks are trained by a novel combination of supervised learning from human expert games, and reinforcement learning from games of self-play. Without any lookahead search, the neural networks play Go at the level of state-of-the-art Monte Carlo tree search programs that simulate thousands of random games of self-play. We also introduce a new search algorithm that combines Monte Carlo simulation with value and policy networks. Using this search algorithm, our program AlphaGo achieved a 99.8% winning rate against other Go programs, and defeated the human European Go champion by 5 games to 0. This is the first time that a computer program has defeated a human professional player in the full-sized game of Go, a feat previously thought to be at least a decade away.

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 10.12 GMT

https://www.theguardian.com

2016

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Self-driving cars

End to End Learning for Self-Driving Cars

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Lawrence D. Jackel NVIDIA Corporation Holmdel, NJ 07735

Mathew Monfort NVIDIA Corporation Holmdel, NJ 07735

Urs Muller NVIDIA Corporation Holmdel, NJ 07735

Jiakai Zhang NVIDIA Corporation Holmdel, NJ 07735

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Jake Zhao NVIDIA Corporation Holmdel, NJ 07735

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Abstract

We trained a convolutional neural network (CNN) to map raw pixels from a single front-facing camera directly to steering commands. This end-to-end approach proved surprisingly powerful. With minimum training data from humans the system learns to drive in traffic on local roads with or without lane markings and on highways. It also operates in areas with unclear visual guidance such as in parking lots and on unpaved roads.

The system automatically learns internal representations of the necessary processing steps such as detecting useful road features with only the human steering angle as the training signal. We never explicitly trained it to detect, for example, the outline of roads.

Compared to explicit decomposition of the problem, such as lane marking detection, path planning, and control, our end-to-end system optimizes all processing steps simultaneously. We argue that this will eventually lead to better performance and smaller systems. Better performance will result because the internal components self-optimize to maximize overall system performance, instead of optimizing human-selected intermediate criteria, e. g., lane detection. Such criteria understandably are selected for ease of human interpretation which doesn't automatically guarantee maximum system performance. Smaller networks are possible because the system learns to solve the problem with the minimal number of processing steps.

We used an NVIDIA DevBox and Torch 7 for training and an NVIDIA DRIVE™ PX self-driving car computer also running Torch 7 for determining where to drive. The system operates at 30 frames per second (FPS).

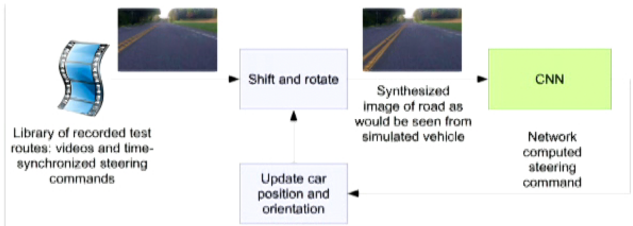

Figure 5: Block-diagram of the drive simulator.

2016

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Language translation

arXiv:1609.08144v2 [cs.CL] 8 Oct 2016

Google's Neural Machine Translation System: Bridging the Gap between Human and Machine Translation

Yonghui Wu, Mike Schuster, Zhifeng Chen, Quoc V. Le, Mohammad Norouzi
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Wolfgang Macherey, Maxim Krikun, Yuan Cao, Qin Gao, Klaus Macherey, Jeff Klingner, Apurva Shah, Melvin Johnson, Xiaobing Liu, Łukasz Kaiser, Stephan Gouws, Yoshikiyo Kato, Taku Kudo, Hideto Kazawa, Keith Stevens, George Kurian, Nishant Patil, Wei Wang, Cliff Young, Jason Smith, Jason Riesa, Alex Rudnick, Oriol Vinyals, Greg Corrado, Macduff Hughes, Jeffrey Dean

Abstract

Neural Machine Translation (NMT) is an end-to-end learning approach for automated translation, with the potential to overcome many of the weaknesses of conventional phrase-based translation systems. Unfortunately, NMT systems are known to be computationally expensive both in training and in translation inference – sometimes prohibitively so in the case of very large data sets and large models. Several authors have also charged that NMT systems lack robustness, particularly when input sentences contain rare words. These issues have hindered NMT's use in practical deployments and services, where both accuracy and speed are essential. In this work, we present GNMT, Google's Neural Machine Translation system, which attempts to address many of these issues. Our model consists of a deep LSTM network with 8 encoder and 8 decoder layers using residual connections as well as attention connections from the decoder network to the encoder. To improve parallelism and therefore decrease training time, our attention mechanism connects the bottom layer of the decoder to the top layer of the encoder. To accelerate the final translation speed, we employ low-precision arithmetic during inference computations. To improve handling of rare words, we divide words into a limited set of common sub-word units ("wordpieces") for both input and output. This method provides a good balance between the flexibility of "character"-delimited models and the efficiency of "word"-delimited models, naturally handles translation of rare words, and ultimately improves the overall accuracy of the system. Our beam search technique employs a length-normalization procedure and uses a coverage penalty, which encourages generation of an output sentence that is most likely to cover all the words in the source sentence. To directly optimize the translation BLEU scores, we consider refining the models by using reinforcement learning, but we found that the improvement in the BLEU scores did not reflect in the human evaluation. On the WMT'14 English-to-French and English-to-German benchmarks, GNMT achieves competitive results to state-of-the-art. Using a human side-by-side evaluation on a set of isolated simple sentences, it reduces translation errors by an average of 60% compared to Google's phrase-based production system.

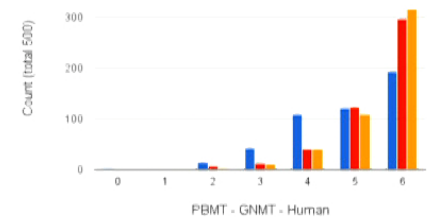

Figure 6: Histogram of side-by-side scores on 500 sampled sentences from Wikipedia and news websites for a typical language pair, here English → Spanish (PBMT blue, GNMT red, Human orange). It can be seen that there is a wide distribution in scores, even for the human translation when rated by other humans, which shows how ambiguous the task is. It is clear that GNMT is much more accurate than PBMT.

2016

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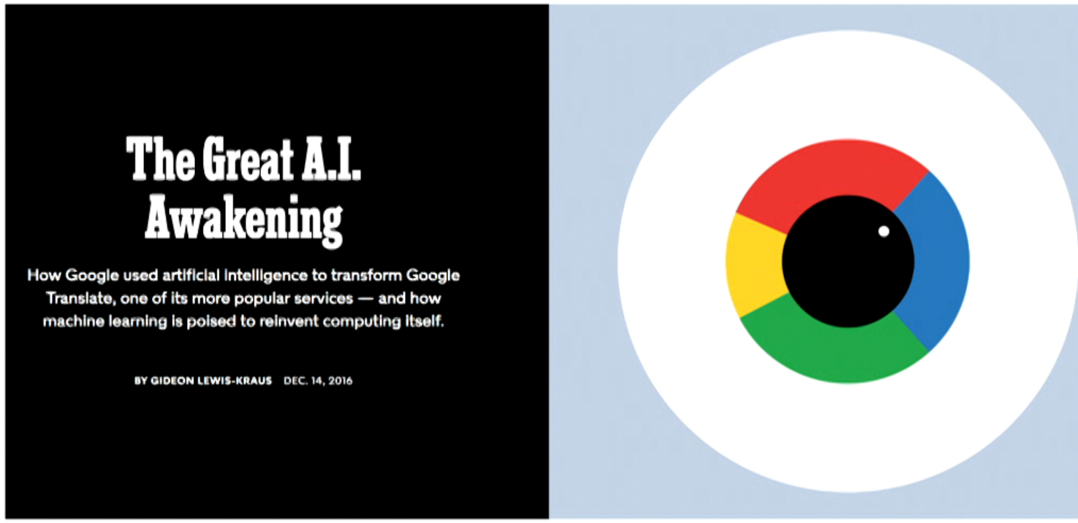
The New York Times



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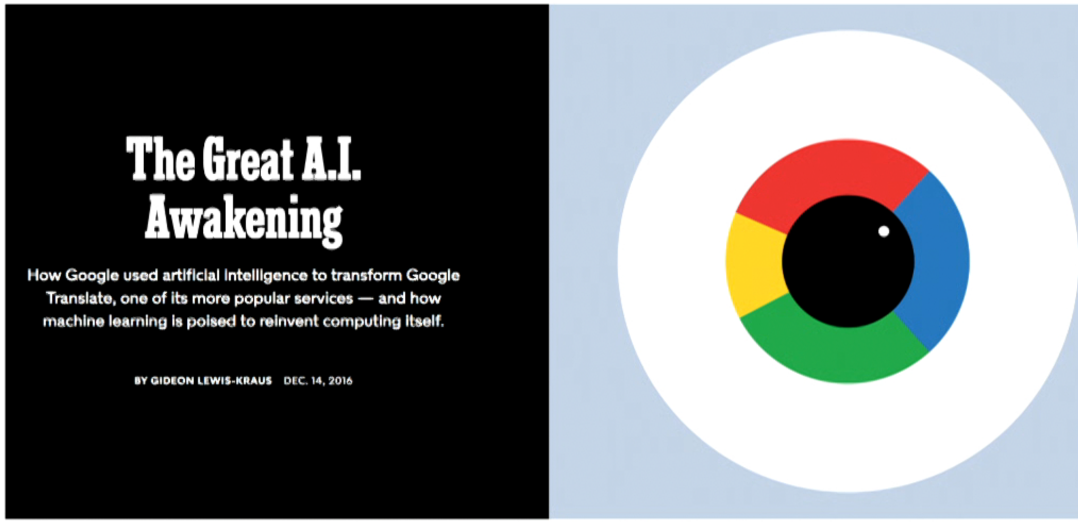
The New York Times



Translation #1:

Kilimanjaro is 19,710 feet of the mountain covered with snow, and it is said that the highest mountain in Africa. Top of the west, “Ngaje Ngai” in the Maasai language, has been referred to as the house of God. The top close to the west, there is a dry, frozen carcass of a leopard. Whether the leopard had what the demand at that altitude, there is no that nobody explained.

Translation #2:

Kilimanjaro is a mountain of 19,710 feet covered with snow and is said to be the highest mountain in Africa. The summit of the west is called “Ngaje Ngai” in Masai, the house of God. Near the top of the west there is a dry and frozen dead body of leopard. No one has ever explained what leopard wanted at that altitude.

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Medical diagnosis

CheXNet: Radiologist-Level Pneumonia Detection on Chest X-Rays with Deep Learning

Pranav Rajpurkar[*1] Jeremy Irvin[*1] Kaylie Zhu[1] Brandon Yang[1] Hershel Mehta[1] Tony Duan[1] Daisy Ding[1] Aarti Bagul[1] Robyn L. Ball[2] Curtis Langlotz[3] Katie Shpanskaya[3] Matthew P. Lungren[3] Andrew Y. Ng[1]

arXiv:1711.05225v3 [cs.CV] 25 Dec 2017

Abstract

We develop an algorithm that can detect pneumonia from chest X-rays at a level exceeding practicing radiologists. Our algorithm, CheXNet, is a 121-layer convolutional neural network trained on ChestX-ray14, currently the largest publicly available chest X-ray dataset, containing over 100,000 frontal-view X-ray images with 14 diseases. Four practicing academic radiologists annotate a test set, on which we compare the performance of CheXNet to that of radiologists. We find that CheXNet exceeds average radiologist performance on the F1 metric. We extend CheXNet to detect all 14 diseases in ChestX-ray14 and achieve state of the art results on all 14 diseases.

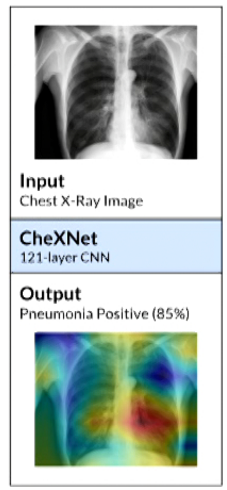

Figure 1. CheXNet is a 121-layer convolutional neural network that takes a chest X-ray image as input, and outputs the probability of a pathology. On this example, CheXnet correctly detects pneumonia and also localizes areas in the image most indicative of the pathology.

2017

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Generating art

https://deepart.io/

Step 1: Upload photo

Step 2: Choose style

PERIMETER SCHOLARS INTERNATIONAL

Generating art

https://deepart.io/

Step 1: Upload photo

Step 2: Choose style

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What is machine learning?

"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

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What is machine learning?

"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

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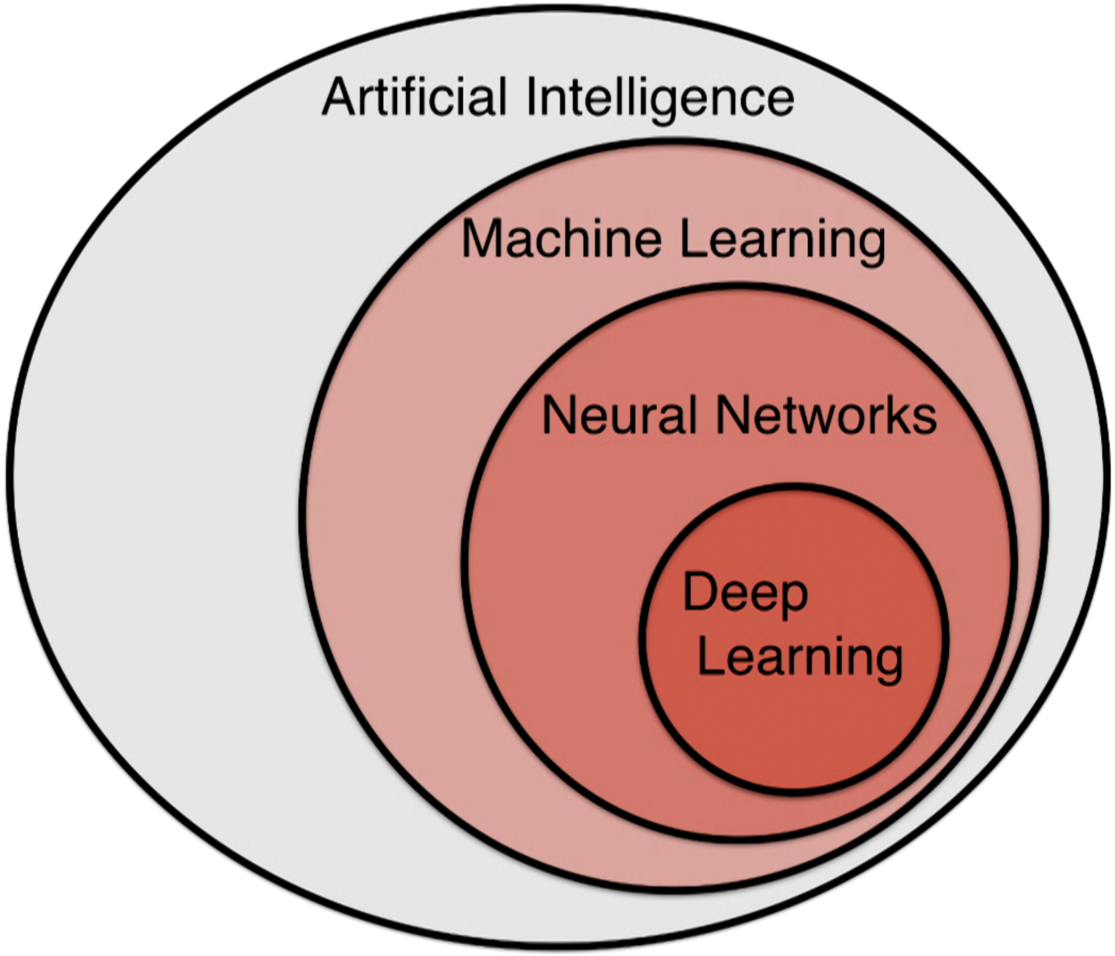

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Machine learning (ML)

↳ training computers to detect and characterize features from data

Compare in many-body physics

↳ predict and explain $\underbrace{\text{macroscopic phenomena}}_{\text{features}}$ from $\underbrace{\text{microscopic quantities}}_{\text{data}}$

Many-body physics:

↳ fundamentally relies on many particles interacting

↳ high-T superconductivity, fractional quantum Hall, many-qubit quantum computers

↳ <u>not</u> needed for solid state problems like e^- conduction, semiconductors

Computational methods

↳ useful because solving the Schrödinger equation is exponentially difficult, quickly becomes intractable as the # of interacting particles increases

Other methods

Monte Carlo
tensor networks
exact diagonalization

Start from microscopic theory, generate data describing the state

ML: fundamentally data driven (take measurements or "data" and learn about macroscopic properties such as phases)

We will study two categories of ML algorithms:

Supervised learning (SL)

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

datapoints $\vec{x} = (x_1, x_2, \ldots, x_{d_x})$

labels $\vec{y} = (y_1, y_2, \ldots, y_{d_y})$

Task: fit some function $f(\vec{x})$ to $\vec{y}$

Unsupervised learning (UL)

Dataset $\mathcal{D} = \{\vec{x}\}$

Unlabelled data

Task: extract meaningful features from the data to represent the data's prob. distribution $p_{data}(\vec{x})$

We will study two categories of ML algorithms:

Supervised learning (SL)

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datapoints $\vec{x} = (x_1, x_2, \ldots, x_{d_x})$

labels $\vec{y} = (y_1, y_2, \ldots, y_{d_y})$

Task: fit some function $f(\vec{x})$ to $\vec{y}$

(first 6–7 lectures)

Unsupervised learning (UL)

Dataset $\mathcal{D} = \{\vec{x}\}$

Unlabelled data

Task: extract meaningful features from the data to represent the data's prob. distribution $p_{data}(\vec{x})$

(remaining lectures)

SL:

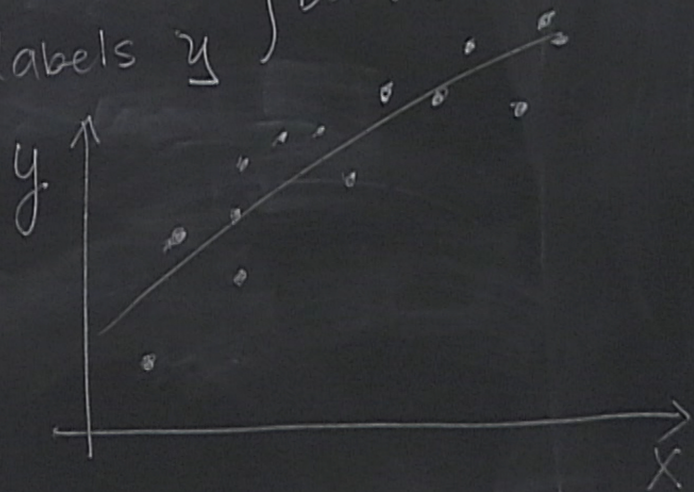
↳ "regression" when the labels are continuous

↳ "classification" when the labels are discrete

Supervised learning examples

#1 Regression

input data x } both 1D real-valued coordinates
labels y



Goal: determine a curve to describe the data

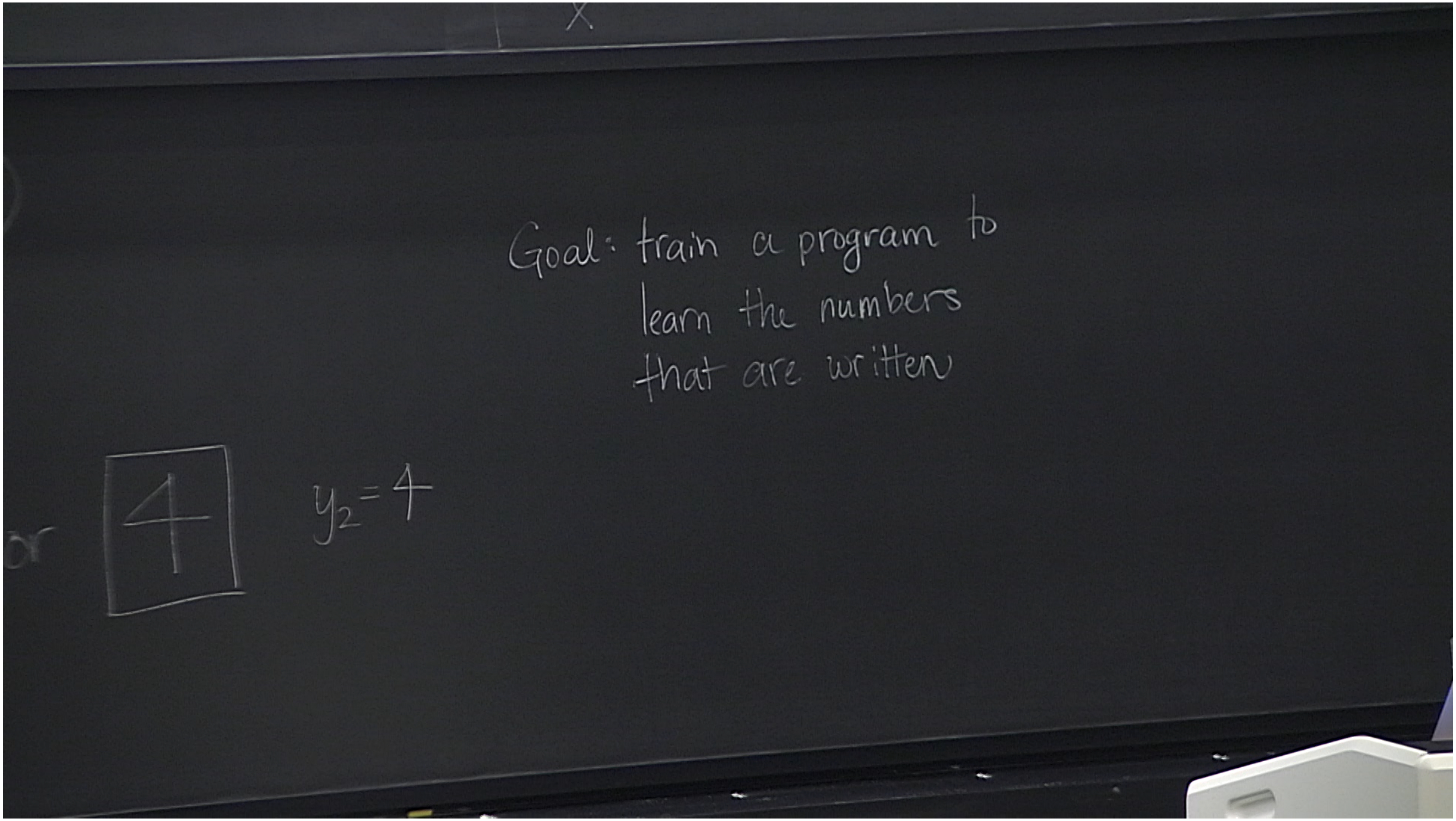
#2 Handwritten digit classification (MNIST)

input data $\vec{x}$: image of a handwritten digit

labels y : the corresponding number

$\vec{x}_1 = \boxed{5}$, $y_1 = 5$

$\vec{x}_2 = \boxed{4}$ or $\boxed{4}$

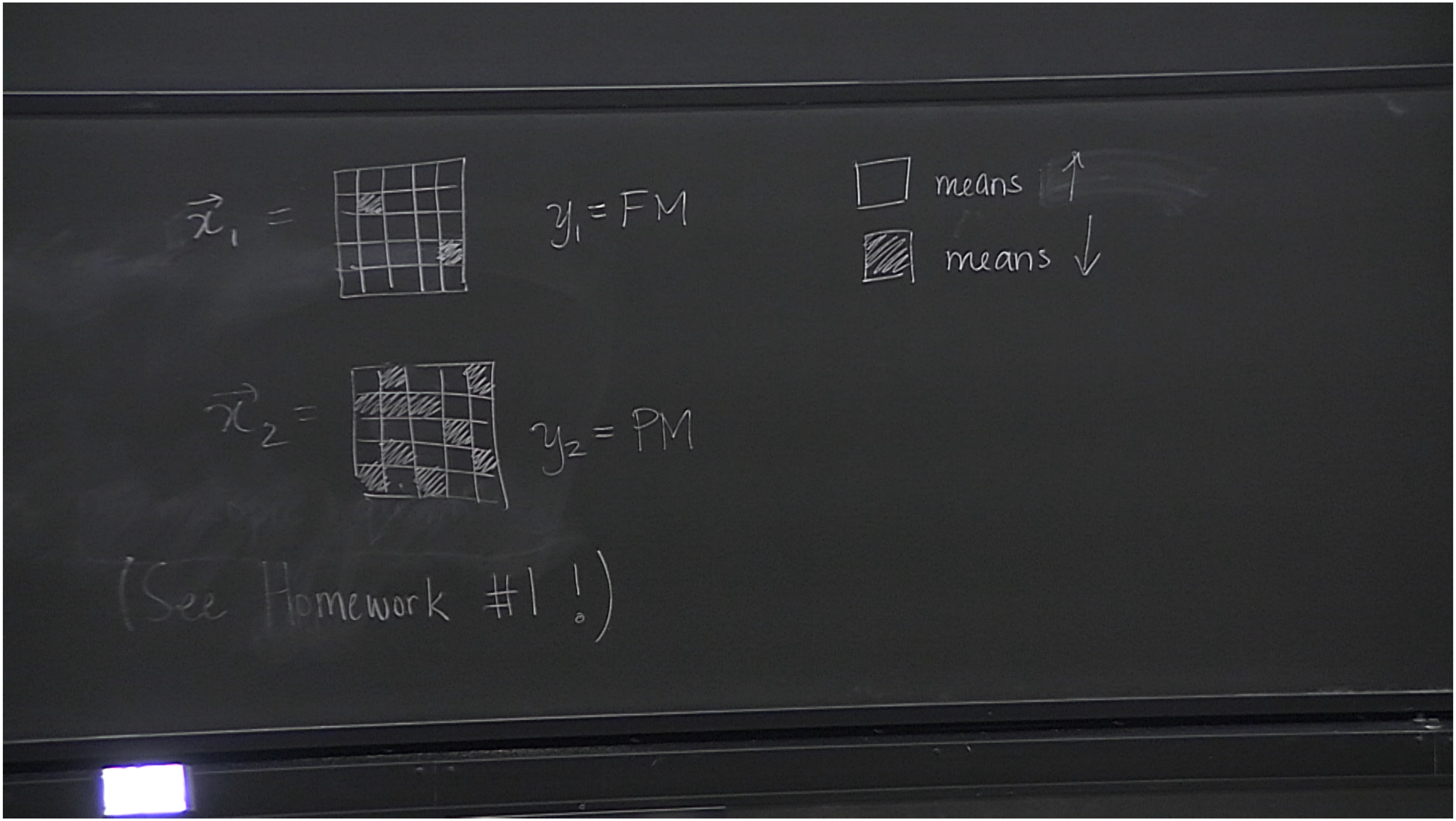

Goal: train a program to
learn the numbers
that are written
4
$y_2 = 4$

semiconductors

#3 Ising model phase classifier

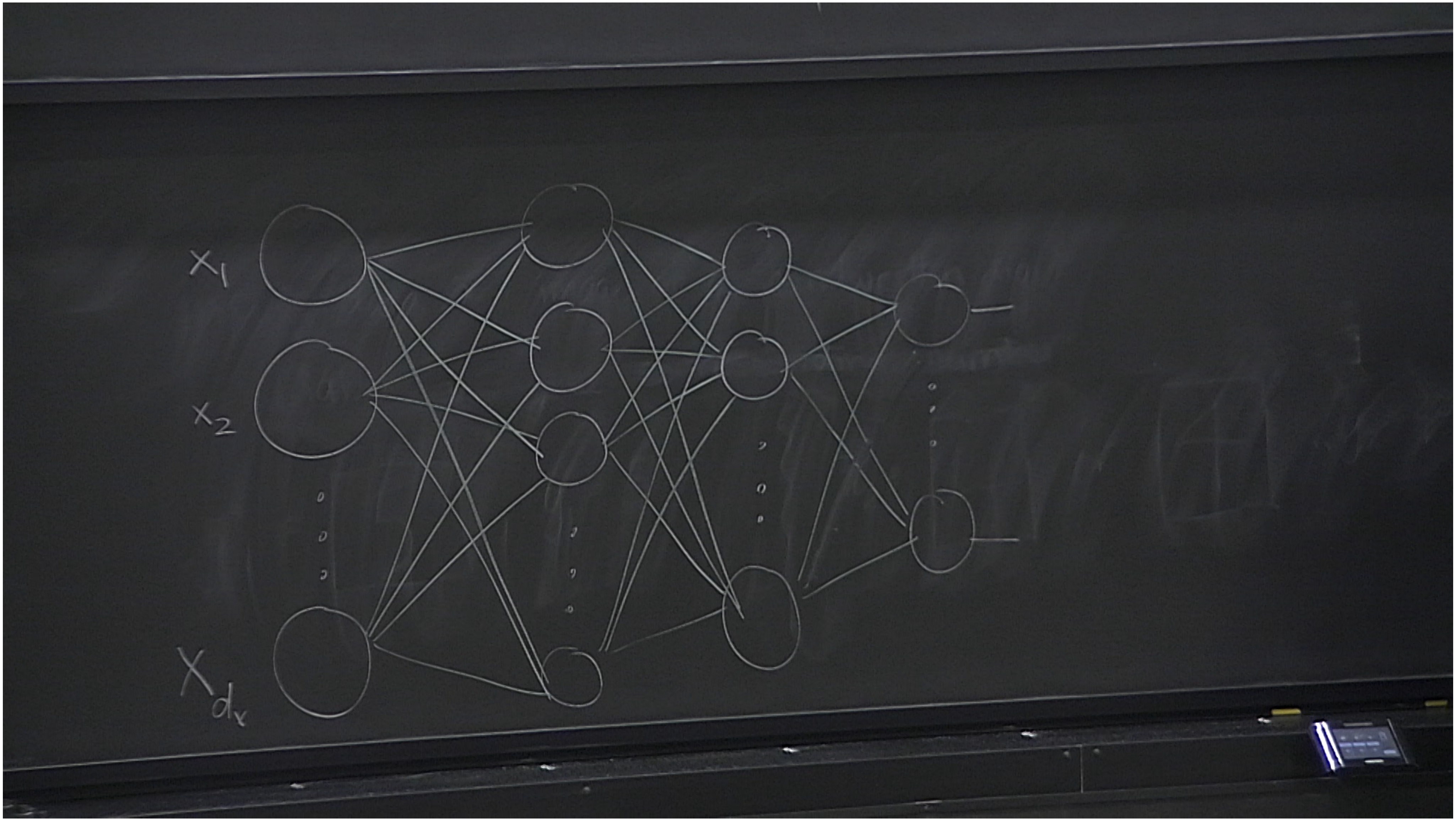
input data $\vec{x}$: spin configuration
(eg. from Monte Carlo simulation)

labels y : ferromagnet (FM)
or paramagnet (PM)

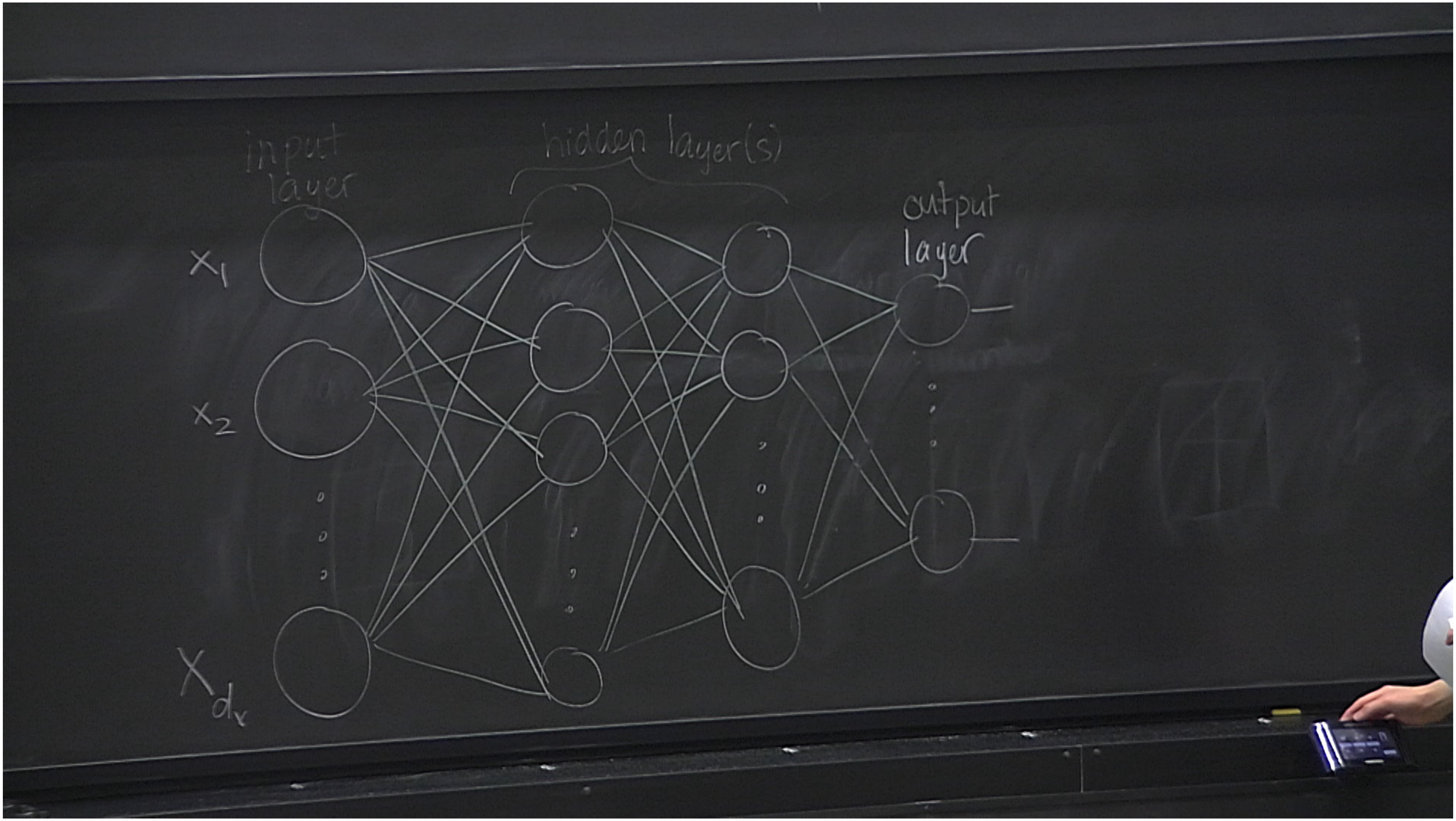

$\vec{x}_1 =$
$y_1 = FM$
means $\uparrow$
means $\downarrow$
$\vec{x}_2 =$
$y_2 = PM$
(See Homework #1 !)

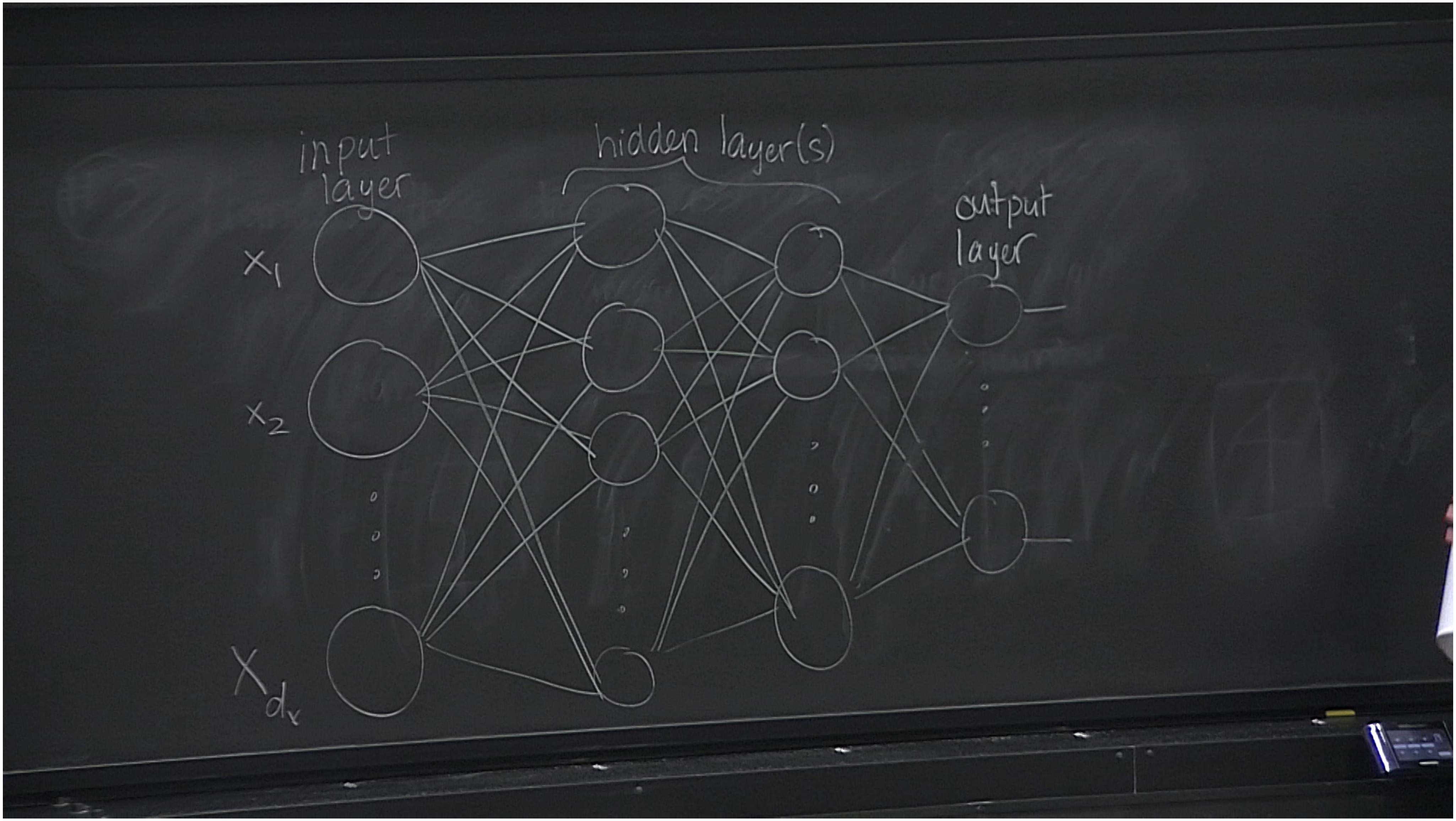
(See Homework #1 !)

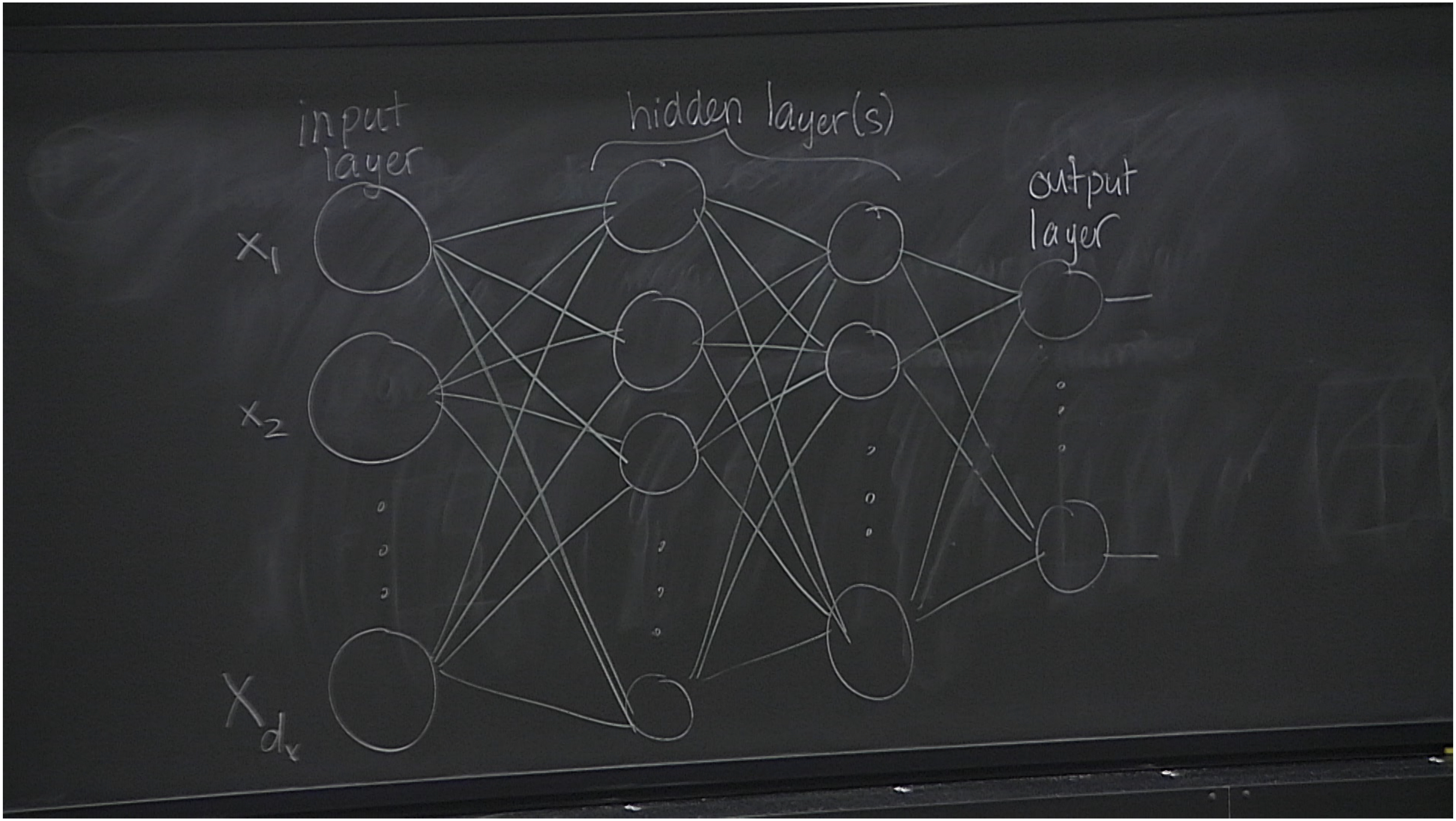
This week: supervised learning with feedforward neural networks (NNs)



x_1
x_2
x_{d_x}


input layer
hidden layer(s)
output layer
x_1
x_2
X_{d_x}


input layer
hidden layer(s)
output layer
x_1
x_2
X_{d_x}


input layer
hidden layer(s)
output layer
x_1
x_2
x_{d_x}

PERIMETER SCHOLARS INTERNATIONAL

Machine Learning for Many-Body Physics
Spring 2018
Lauren Hayward Sierens

Homework 3: Blog post on ⟨ PHYSICS | MACHINE LEARNING ⟩

Due date: Friday, May 4, 2018

Submit online using the link in the PSI wiki

The objective of this homework assignment is to write a blog-style article about current ideas and research within the intersection of physics and machine learning. The best article will be posted online to the blog section of `https://physicsml.github.io`, which is a website currently run by PI graduate student Anna Golubeva.

You can either work alone or form a group of 2–3 students. If you choose to work in a group, then you must also submit a short description of each student's contributions. You can choose to write about work that has already been done by other researchers, or you can write about your own ideas for interdisciplinary research combining physics and machine learning (see below for more information and suggestions). For those students who are writing their PSI essay on topics related to machine learning, you must choose a different topic for this assignment. You must inform Lauren of your group and article topic by **Friday, April 27**, and each group's article must address a different topic.

The target audience for your article should be physicists who are non-experts in both machine learning and the physics subdiscipline of your topic. Your article should be at least 1000 words in length. You are encouraged to incorporate creative visualizations and animations. A PDF copy of the article as well as all documents required to generate it must be submitted in a ZIP file by **Friday, May 4**.

For inspiration, you are highly encouraged to read through posts on blogs such as

- `https://www.ethz.ch/content/specialinterest/phys/theoretical-physics/cmtm/en.html`,
- `https://physicsml.github.io/category/articles.html`,
- `https://deepmind.com/blog` (not physics related),
- `https://distill.pub` (not physics related).

Option 1: Summarize a recent research paper or idea

As a first option, you may choose to write about recent work done by other researchers. During this course, you will have opportunities to attend two journal club meetings and one colloquium that will present current research combining physics and machine learning. You may choose to write about one of the topics from these presentations. Alternatively, you can summarize an idea presented in an article (or articles) of your choice. A list of relevant papers can be found at `https://physicsml.github.io/pages/papers.html`, or you can discuss other options with Lauren.

Option 2: Write about your own ideas

As another option, you can get creative and write about your own ideas or work. Much of the research within the intersection of physics and machine learning can be divided into two categories. The first category uses existing techniques from machine learning to study problems in physics (such as phase transitions in many-body physics). Perhaps you have ideas for some areas of physics research that could benefit from using machine learning as a tool. The second category of research uses ideas from theoretical physics (such as tensor networks and renormalization group theory) to improve machine learning methods and algorithms. You may develop ideas for how to use intuition and theory from physics to explain phenomena in machine learning.