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

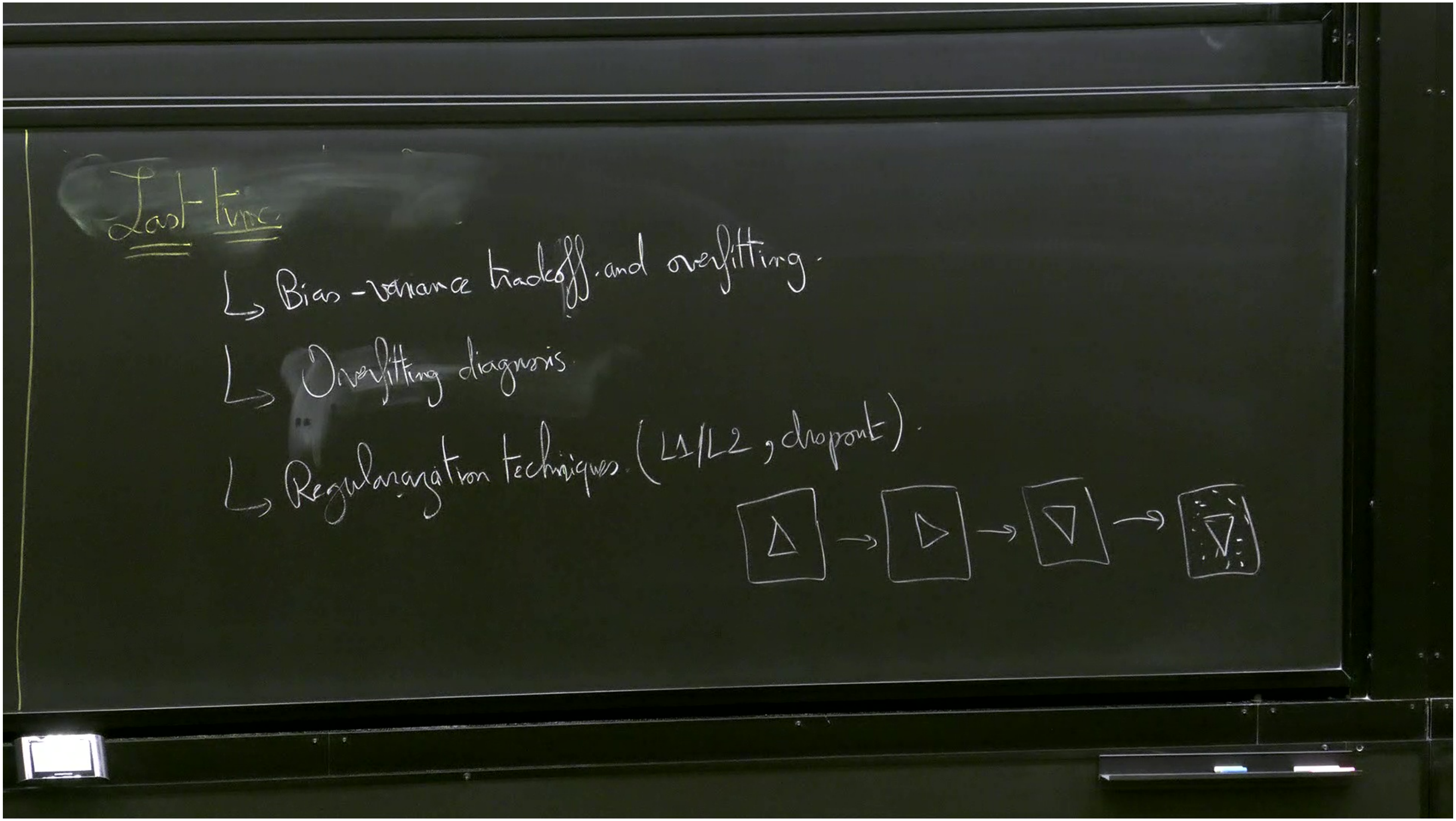
Date: March 07, 2025 - 9:00 AM

URL: https://pirsa.org/25030037

Lecture 6

Outline for today:

1. Recap of hyperparameters in NNs.
2. Monte Carlo Sampling (Data for Homework 1).
3. Using Supervised Learning to learn the phases of the Ising $\mathbb{Z}_2$ gauge theory.


Last time
↳ Bias-variance tradeoff and overfitting.
↳ Overfitting diagnosis.
↳ Regularization techniques (L1/L2, dropout).

① Hyperparams for feed neural networks:

→ # of layers (how deep the NN).

→ # of neurons in each hidden layer.

→ Training alg (GD, mini-batch GD, Momentum, Adam, ...)

→ Hyperparam of each training alg. (learning rate η, "β" momentum param, mini-batch size $|B|$, ...)

→ Activations choise

Regularization (λ param, dropout prob, ...)

...)

tum param, mini-batch size $|B|$, ...)

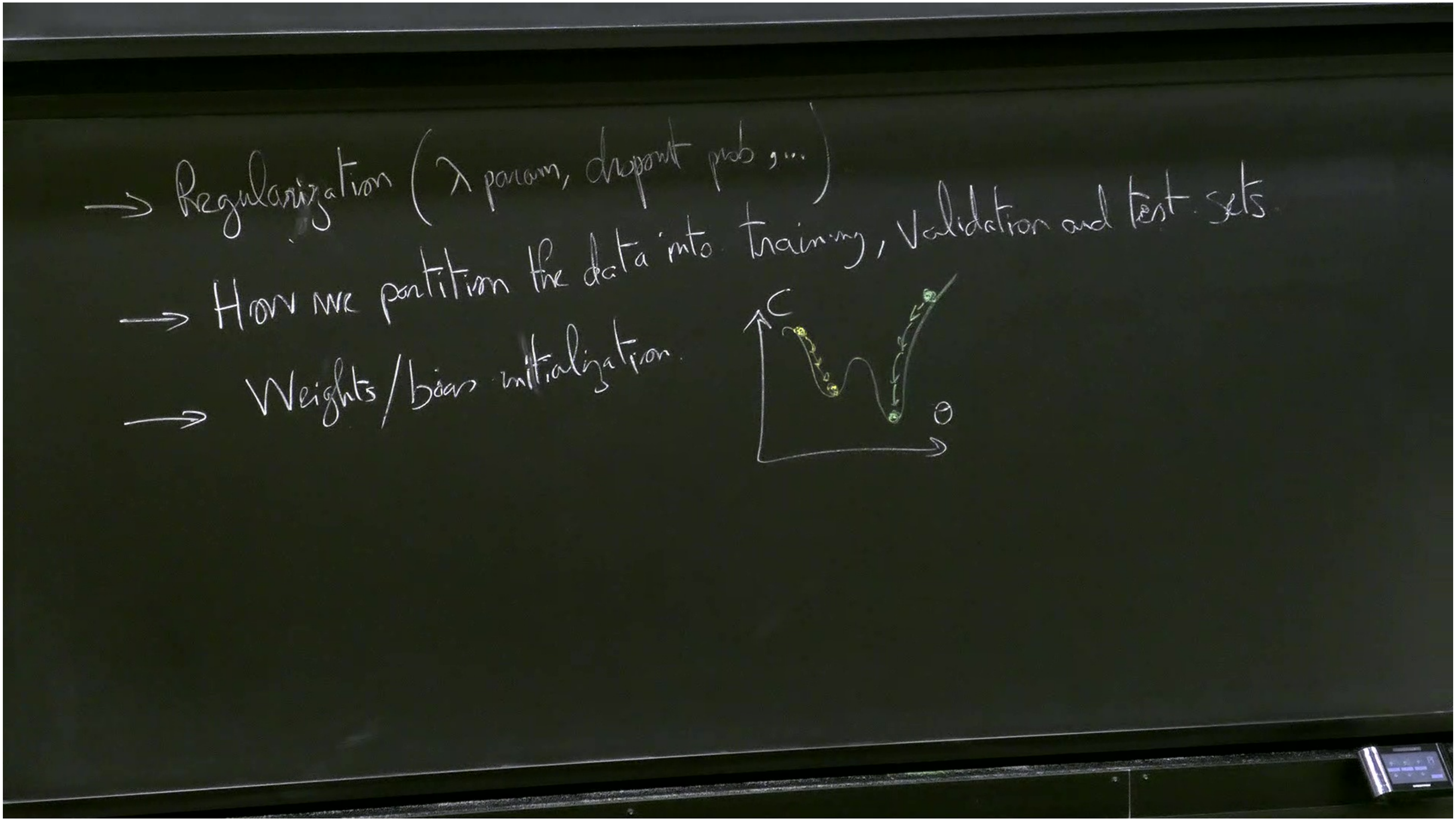
→ Learning rate decay

e.g. $\eta(t) = \frac{\eta_0}{t}$

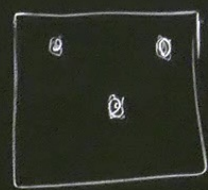
→ Cost function (MSE, CE, ...)

"Works well" with ReLU or Id

"Works well" with Softmax or Sigmoid


→ Regularization (λ param, dropout prob, ...)
→ How we partition the data into training, validation and test sets.
→ Weights / bias initialization.
C
θ

Monte Carlo (MC) sampling:

$\vec{x} =$  , $y = 0$ (FM) $(T < T_c)$

$\vec{x} =$  , $y = 1$ (PM) $(T > T_c)$

→ Consider a classical many-body system at temperature $T = \frac{1}{\beta}$

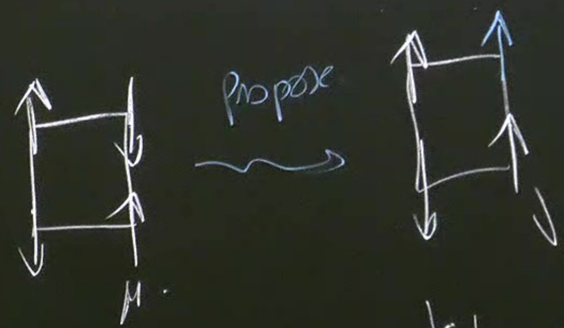
$$p_{\mu} = \frac{\exp(-\beta E_{\mu})}{Z} \; ; \quad Z = \sum_{\mu} \exp(-\beta E_{\mu}).$$

Intractable.

$\#$ of possible "μ" $= 2^N$.

To implement the sampling of "P_μ" $\rightarrow$ we can use Markov Chain Monte Carlo (MCMC).

e.g.)



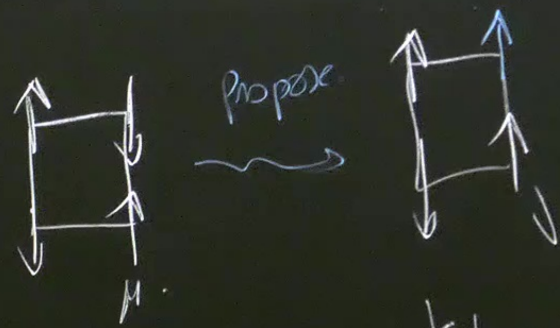
$\rightarrow$ Once a proposal is generated, we choose to accept or reject.

(Simplified) Metropolis algorithm

$$A(\mu \longrightarrow \nu) = \min\left[1,\ \exp\left(-\beta(E_\nu - E_\mu)\right)\right]$$

To implement the sampling of "P_μ" → we can use Markov Chain Monte Carlo (MCMC).

e.g.)



→ Once a proposal is generated, we choose to <u>accept or reject</u>.

(Reference: Newman & Barkema).

Pseudocode for Monte Carlo sampling:

"generates M samples $\mu_1, \mu_2, \dots, \mu_M$ from the dist. $p_\mu = \frac{1}{Z} \exp(-\beta E_\mu)$"

→ choose μ_1 at random. "$g(\mu_i \to \nu)$"

→ For $i = 2, \dots, M$.

→ propose ν from μ_{i-1} with prob. "$\frac{1}{N}$"

→ $r \sim U[0,1)$

(Simplified) Metropolis algorithm

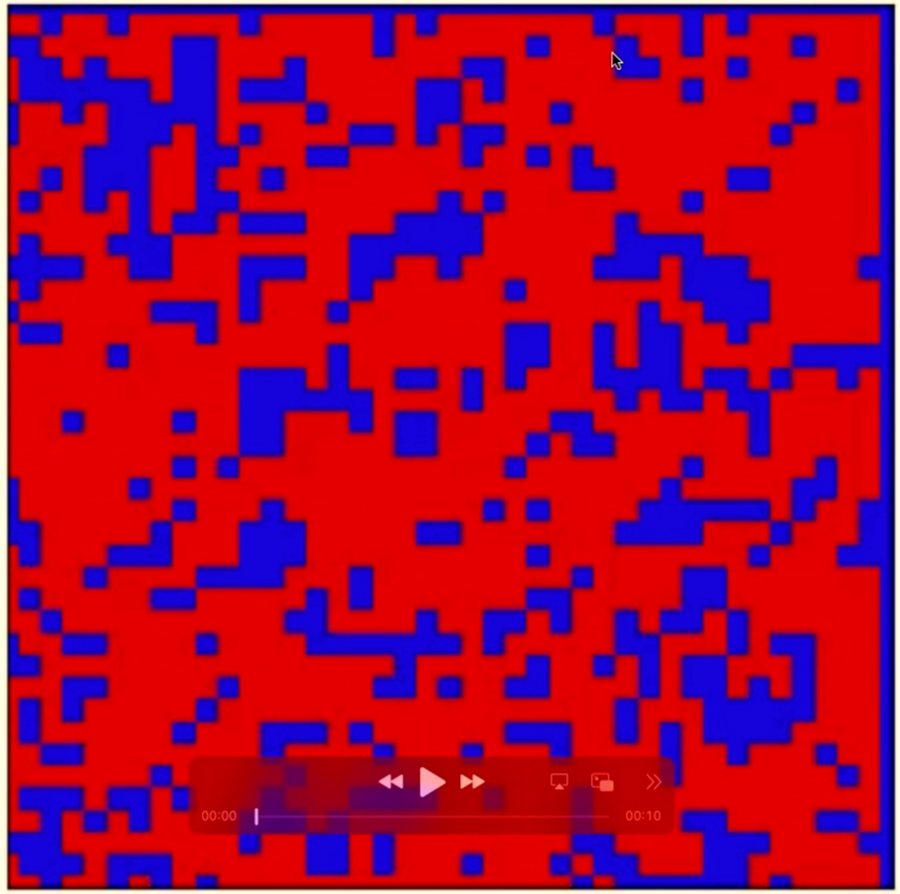
$$A(\mu \to \nu) = \min\left[1,\ \underbrace{\exp\left(-\beta(E_\nu - E_\mu)\right)}_{\frac{p_\nu}{p_\mu}}\right]$$

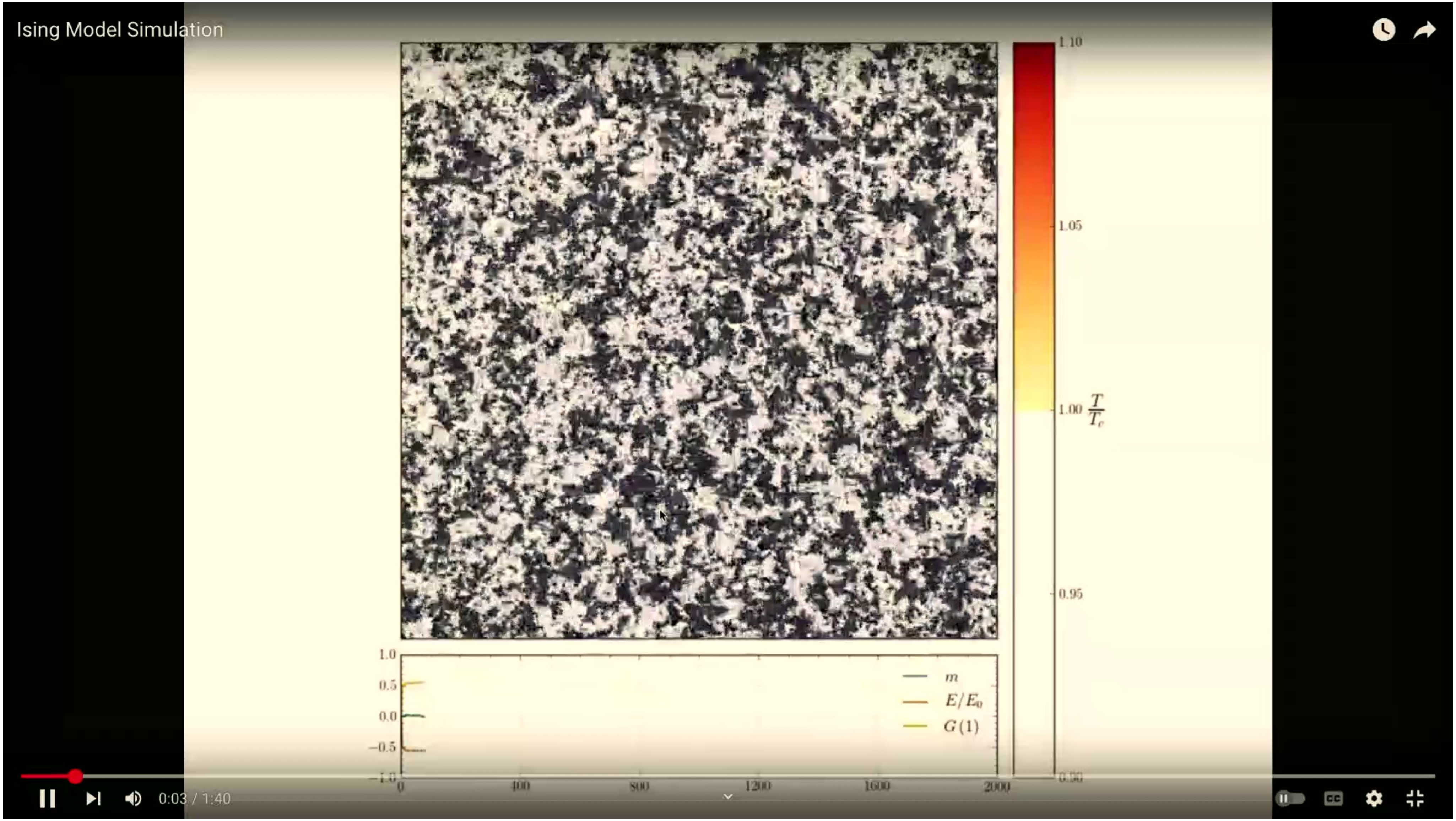
$\to$ If $r < A(\mu_{i-1} \to \nu)$: # Accept

$\mu_i = \nu$

$\to$ Else: $\mu_i = \mu_{i-1}$ # Reject

40 x 40 Ising model, T = 0.010





Ising Model Simulation
1.10
1.05
1.00 $\frac{T}{T_c}$
0.95
1.0
0.5
0.0
−0.5
m
E/E_0
$G(1)$
0
400
800
1200
1600
2000
0:03 / 1:40

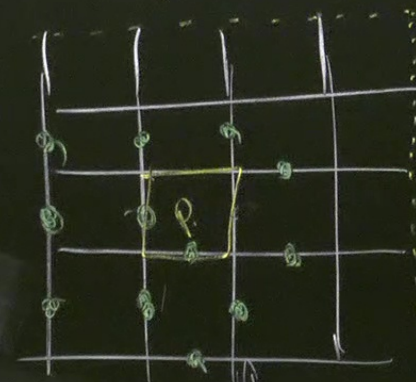
* The classical Ising $\mathbb{Z}_2$ gauge theory.

$$H = -J \sum_{p} \left(\prod_{i \in p} s_i \right)$$

plaquette

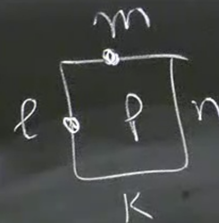
$\rightarrow s_i = +1$

$| \rightarrow s_i = -1$



with periodic boundary conditions.

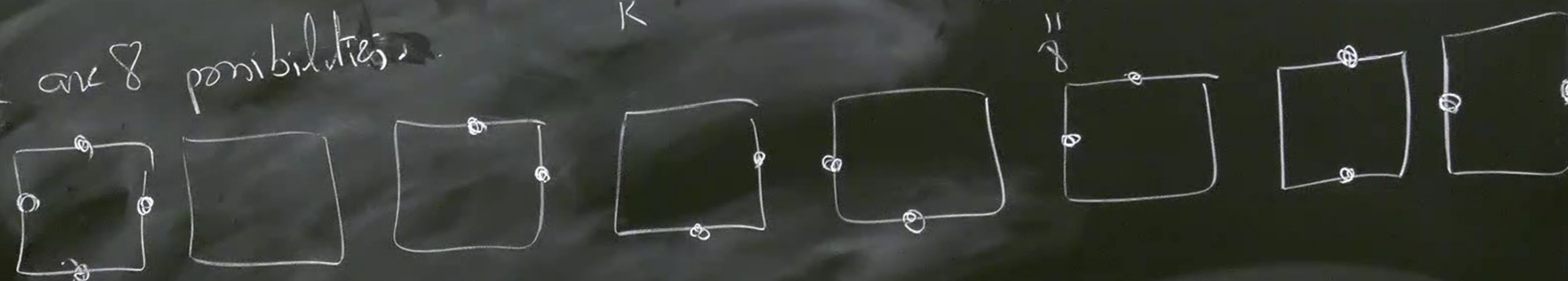
At $T=0$ (Ground State)



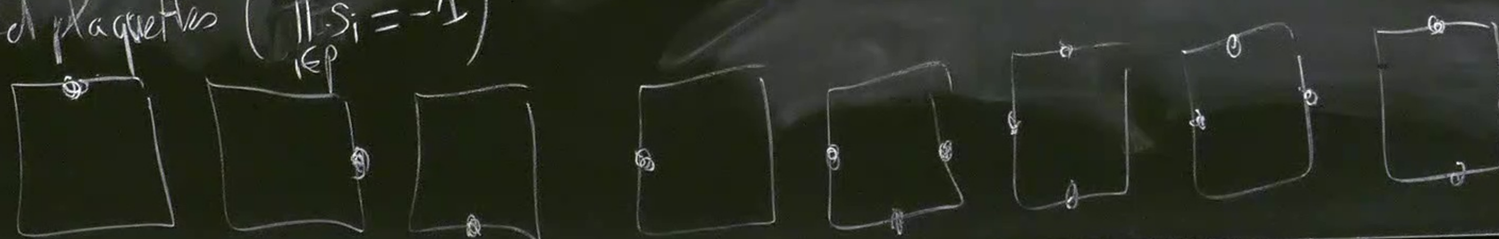
$\prod_{i\in p} s_i = s_k s_l s_m s_n = 1$

$2\times 2\times 2 = 8$

→ There are 8 possibilities.



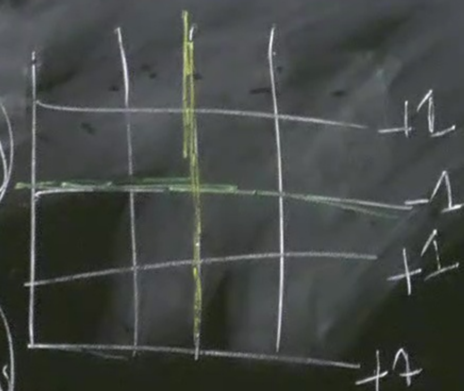
→ 8 "excited plaquettes" $\left(\prod_{i\in p} s_i = -1\right)$



→ At $T = 0$, there is a topologically-ordered phase.

→ At $T > 0$, no order.

$$W_{C_x} = \prod_{i \in C_x} s_i \quad \text{(constant along rows)}$$



$$W_{C_y} = \prod_{i \in C_y} s_i \quad \text{(constant along columns)}$$