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 25, 2025 - 9:00 AM

URL: https://pirsa.org/25030042

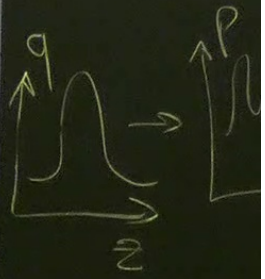
Lecture 11

Today:

↳ Generative modeling: Variational auto-encoders (VAE) and Generative Adversarial Networks (GANs)

↳ Work at the intersection of "Quantum" and ML.

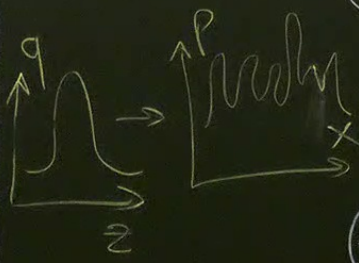
Last



Last time: Generative models

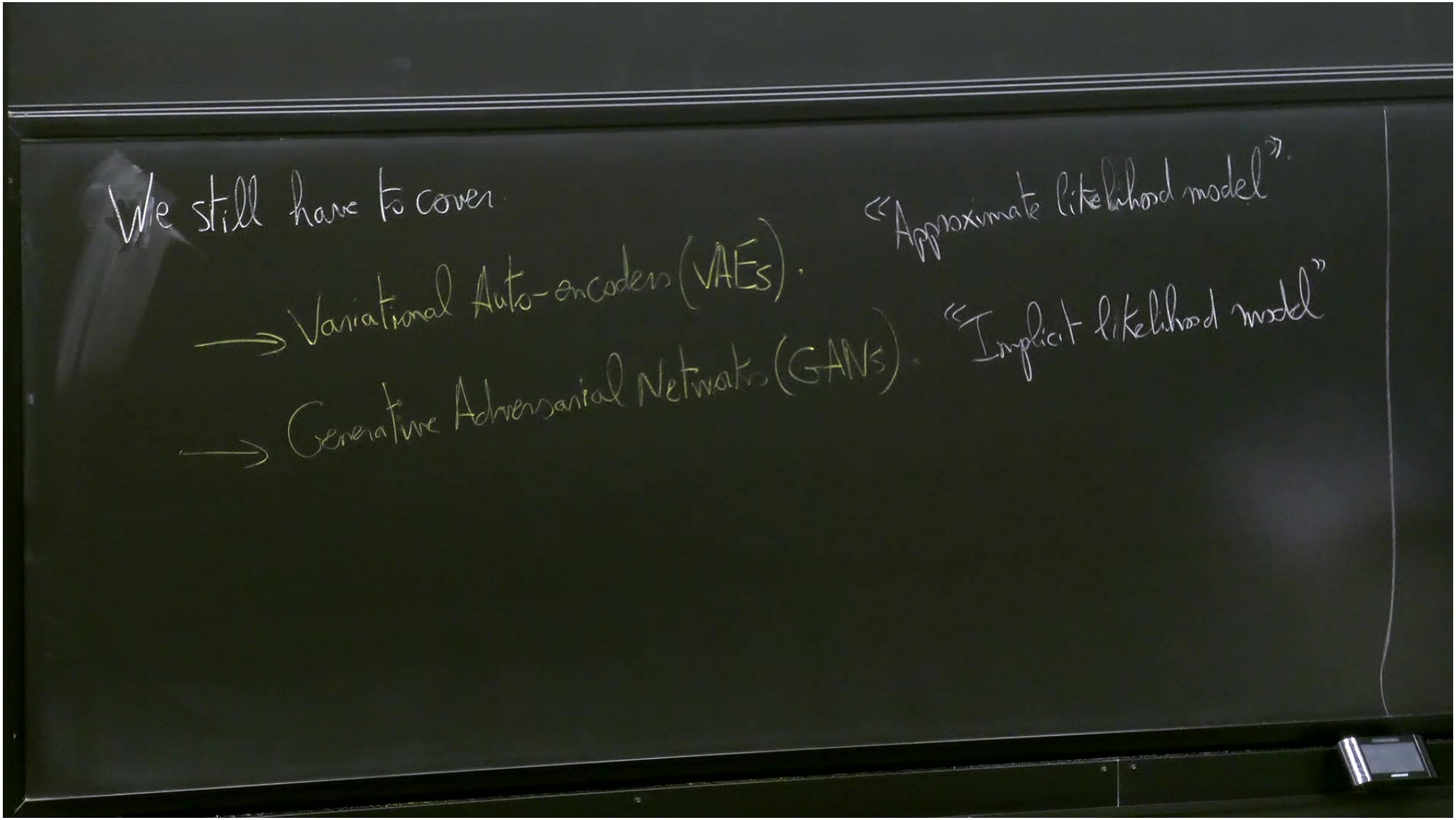
$$P(\vec{x}) = P(x_1)\,P(x_2|x_1)\cdots P(x_N|x_{N-1},\ldots,x_1)$$

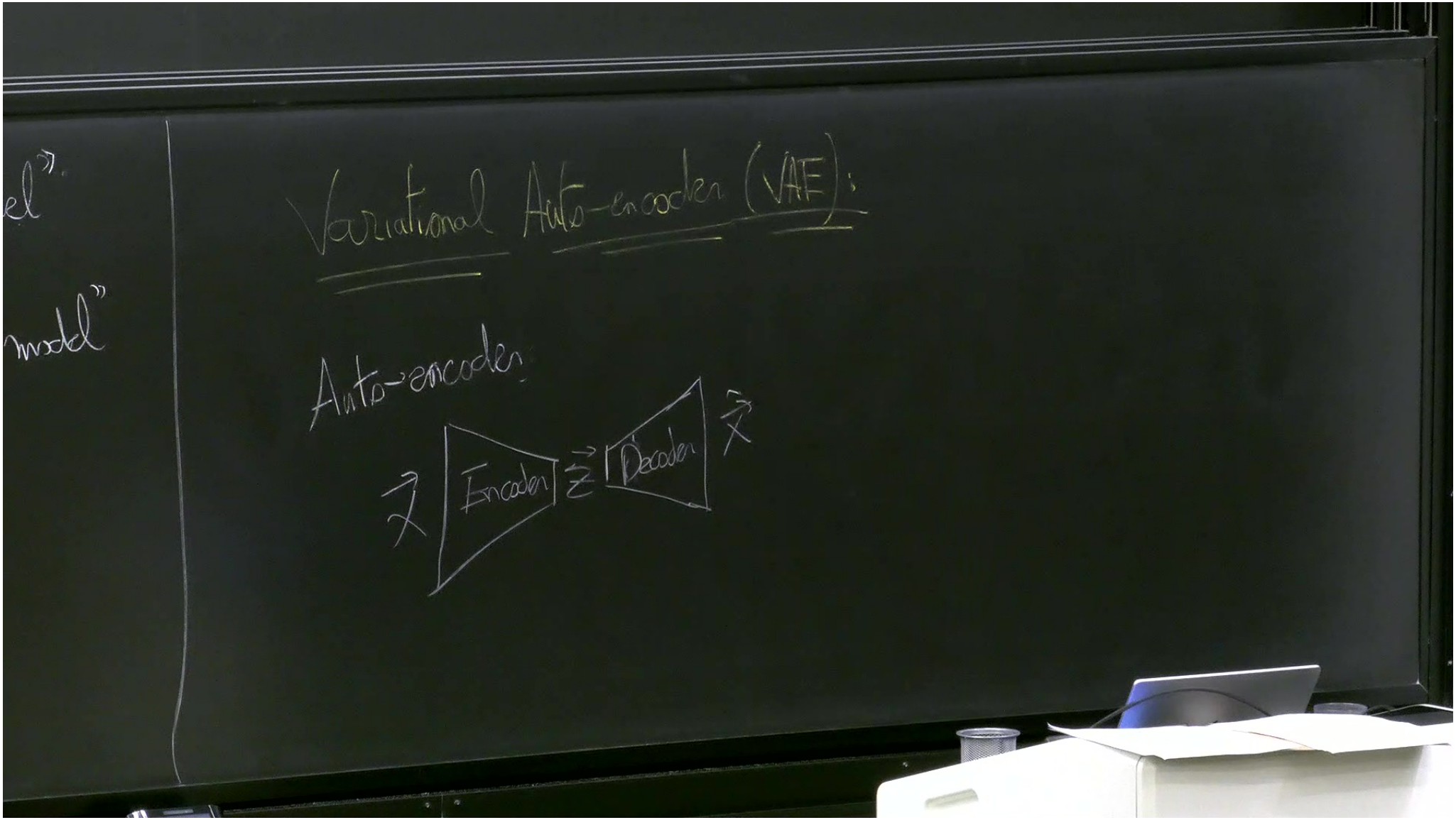
(1) Exact likelihood models
→ Autoregressive models (Discrete data)
→ Normalizing flows (Continuous data)

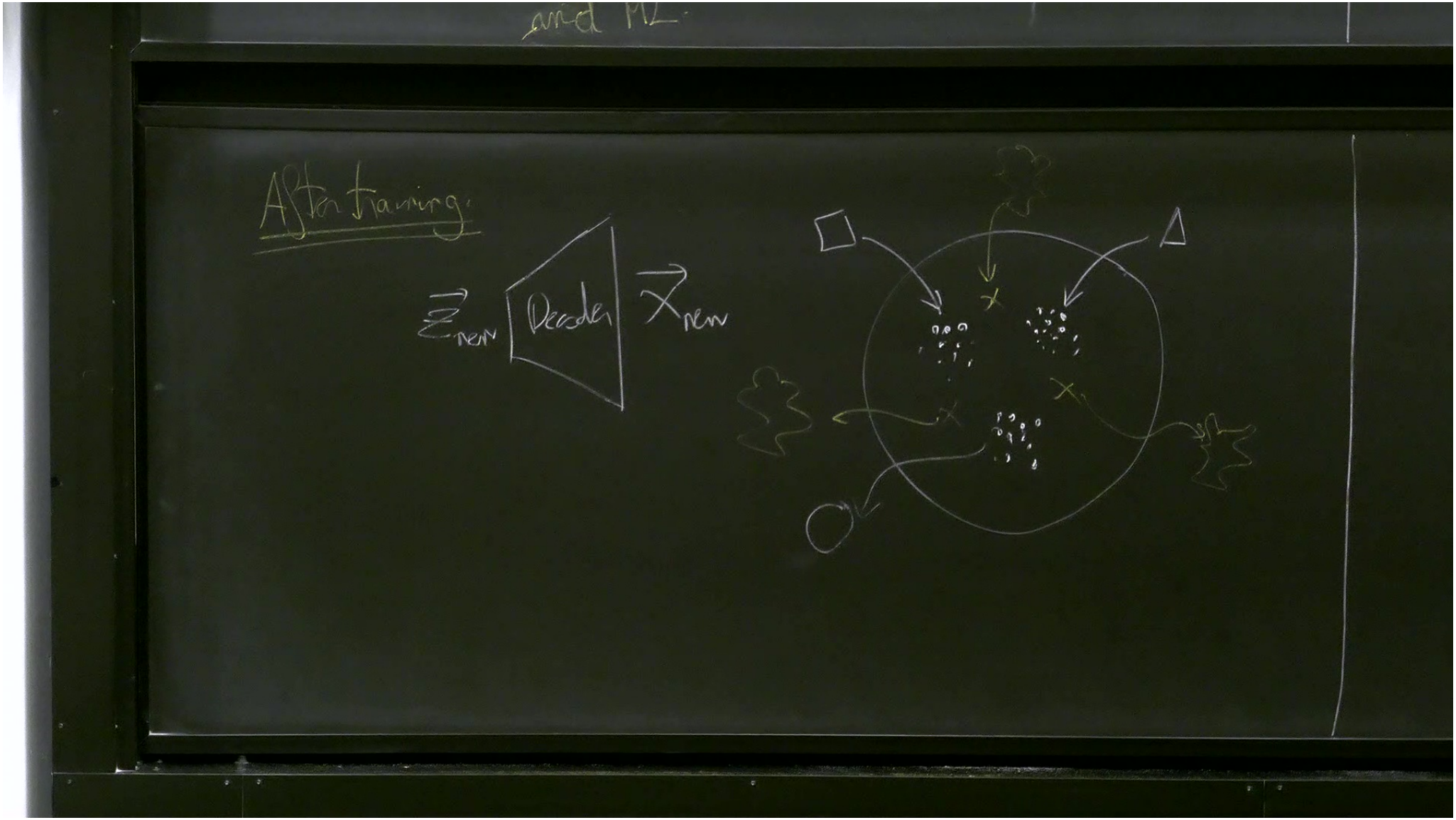


(2) Approximate likelihood models
→ Energy-based models

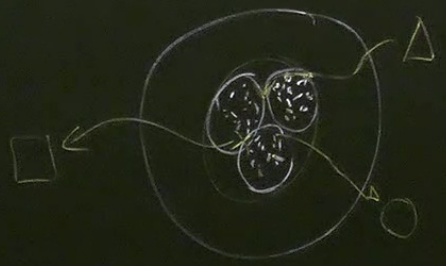
$$P_\theta(\vec{x}) = \frac{\exp(-E_\theta(\vec{x}))}{Z}$$


We still have to cover.
→ Variational Auto-encoders (VAEs). "Approximate likelihood model"
→ Generative Adversarial Networks (GANs). "Implicit likelihood model"


Variational Auto-encoder (VAE):
Auto-encoder:
Encoder
Decoder


and ML.
After training:
$\vec{z}_{new}$
Decoder
$\vec{x}_{new}$

In a VAE.



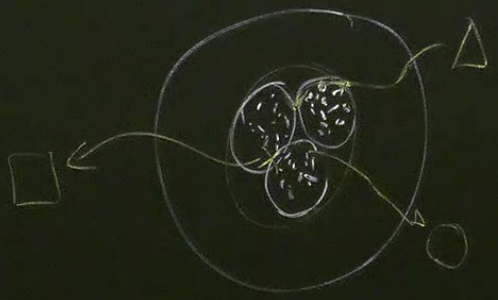
x → Encoder → $\vec{\mu}$, $\vec{\sigma}$ → $\vec{z}$ → Decoder

$\vec{z} \sim N(\vec{\mu}, \vec{\sigma}^2)$

$\vec{z} = \vec{\mu}_\theta + \vec{\sigma}_\theta \odot \vec{\varepsilon}$

$\vec{\varepsilon} \sim N(0, I)$.

In a VAE.

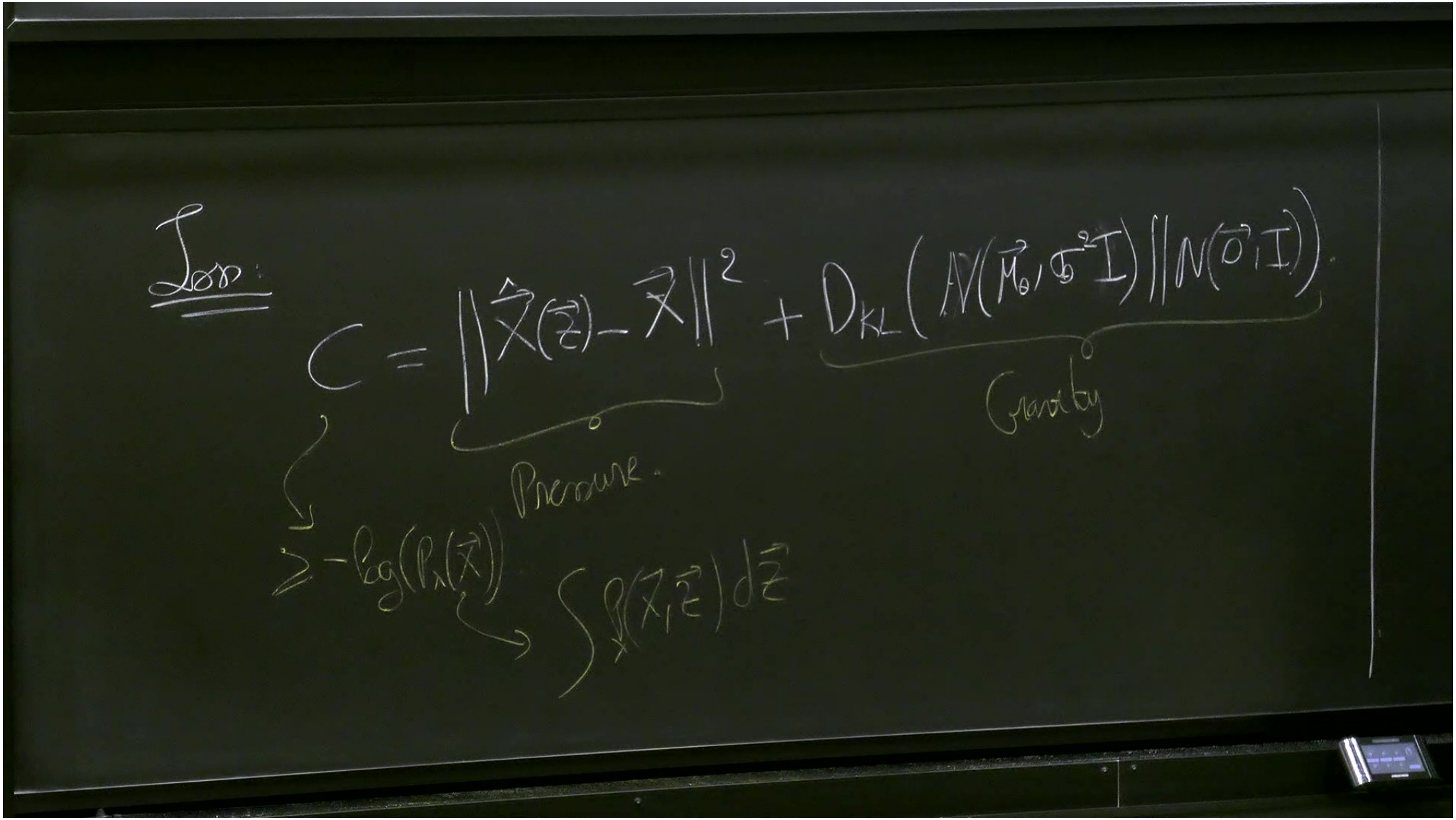


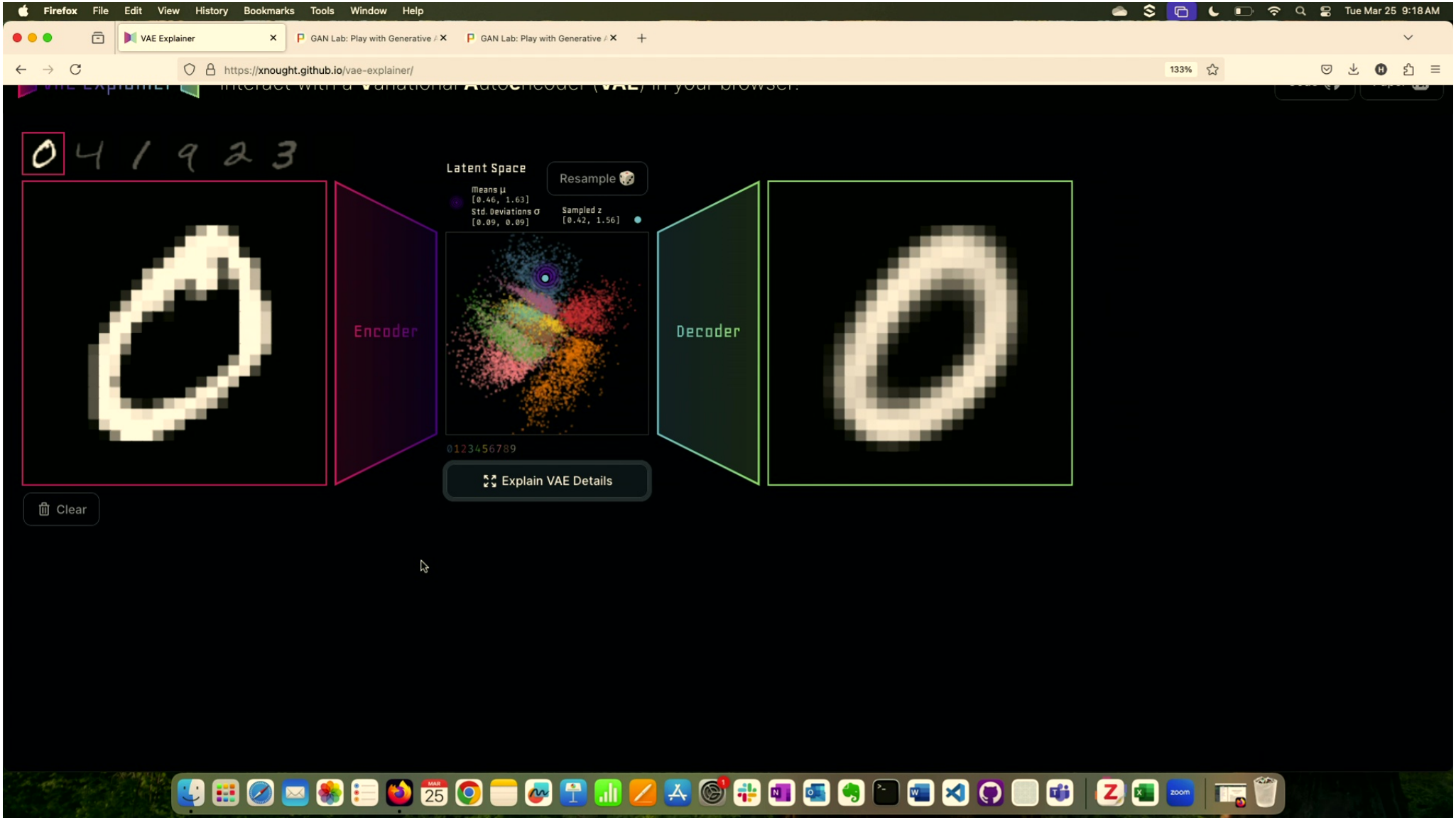
x → Encoder → $\vec{\mu}$, $\vec{\sigma}$ → $\vec{z}$ → Decoder → $\hat{x}$

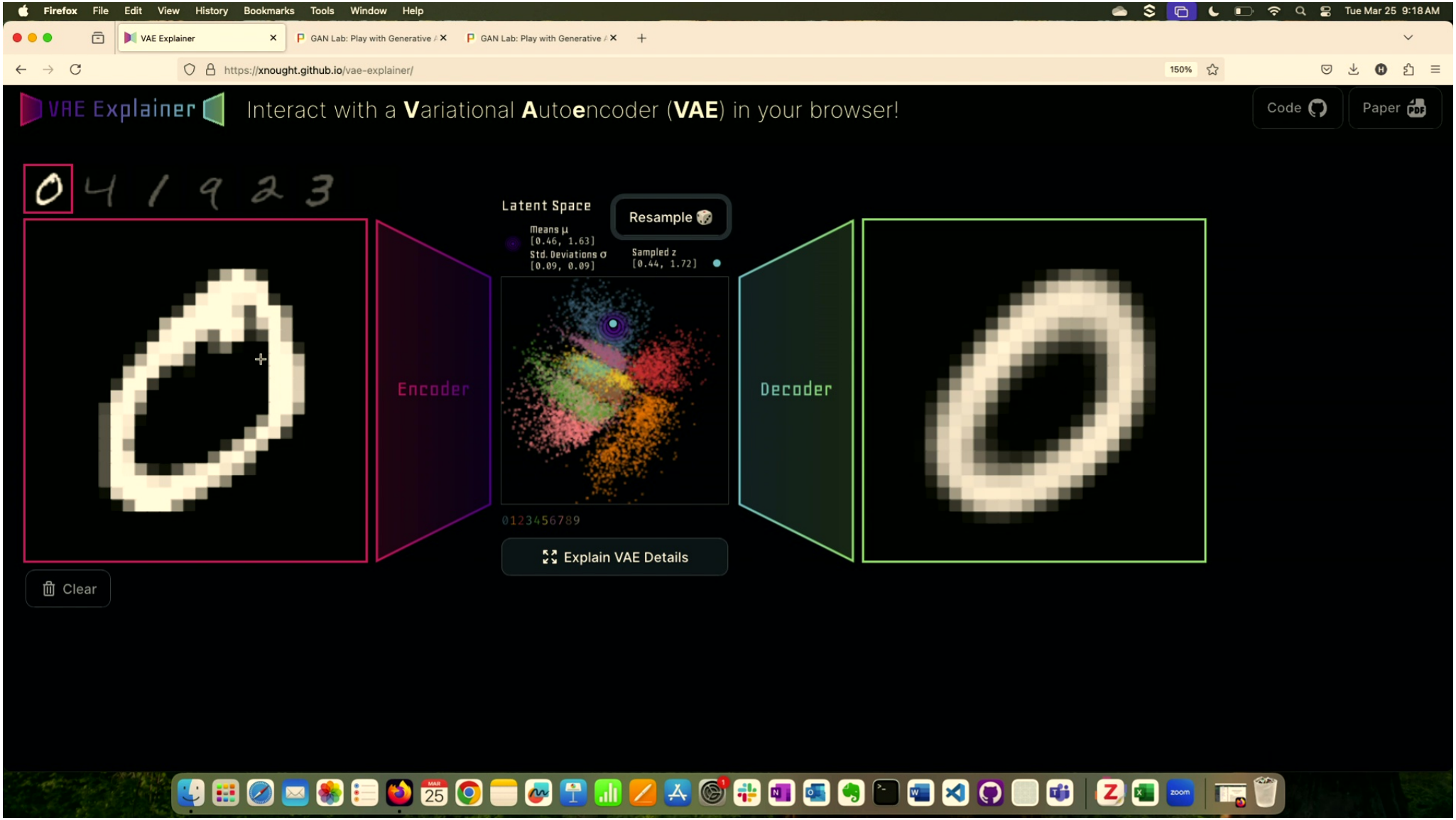
$\vec{z} \sim N(\vec{\mu}, \vec{\sigma}^2) \longrightarrow N(\vec{0}, I)$

$\vec{z} = \vec{\mu}_\theta + \vec{\sigma}_\theta \odot \vec{\varepsilon}$

$\vec{\varepsilon} \sim N(\vec{0}, I)$.


Loss:
$C = \|\hat{\vec{x}}(\vec{z}) - \vec{x}\|^2 + D_{KL}\left(N(\vec{\mu}_\theta, \sigma^2 I) \,\|\, N(\vec{0}, I)\right)$
Pressure
Gravity
$\geq -\log(P_x(\vec{x}))$
$\int P(\vec{x}, \vec{z})\, d\vec{z}$


Firefox File Edit View History Bookmarks Tools Window Help
Tue Mar 25 9:18 AM
VAE Explainer
GAN Lab: Play with Generative
GAN Lab: Play with Generative
https://xnought.github.io/vae-explainer/
133%
0 4 1 9 2 3
Latent Space
Resample
Means μ
[0.46, 1.63]
Std. Deviations σ
[0.09, 0.09]
Sampled z
[0.42, 1.56]
Encoder
Decoder
0123456789
Explain VAE Details
Clear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VAE Explainer
GAN Lab: Play with Generative
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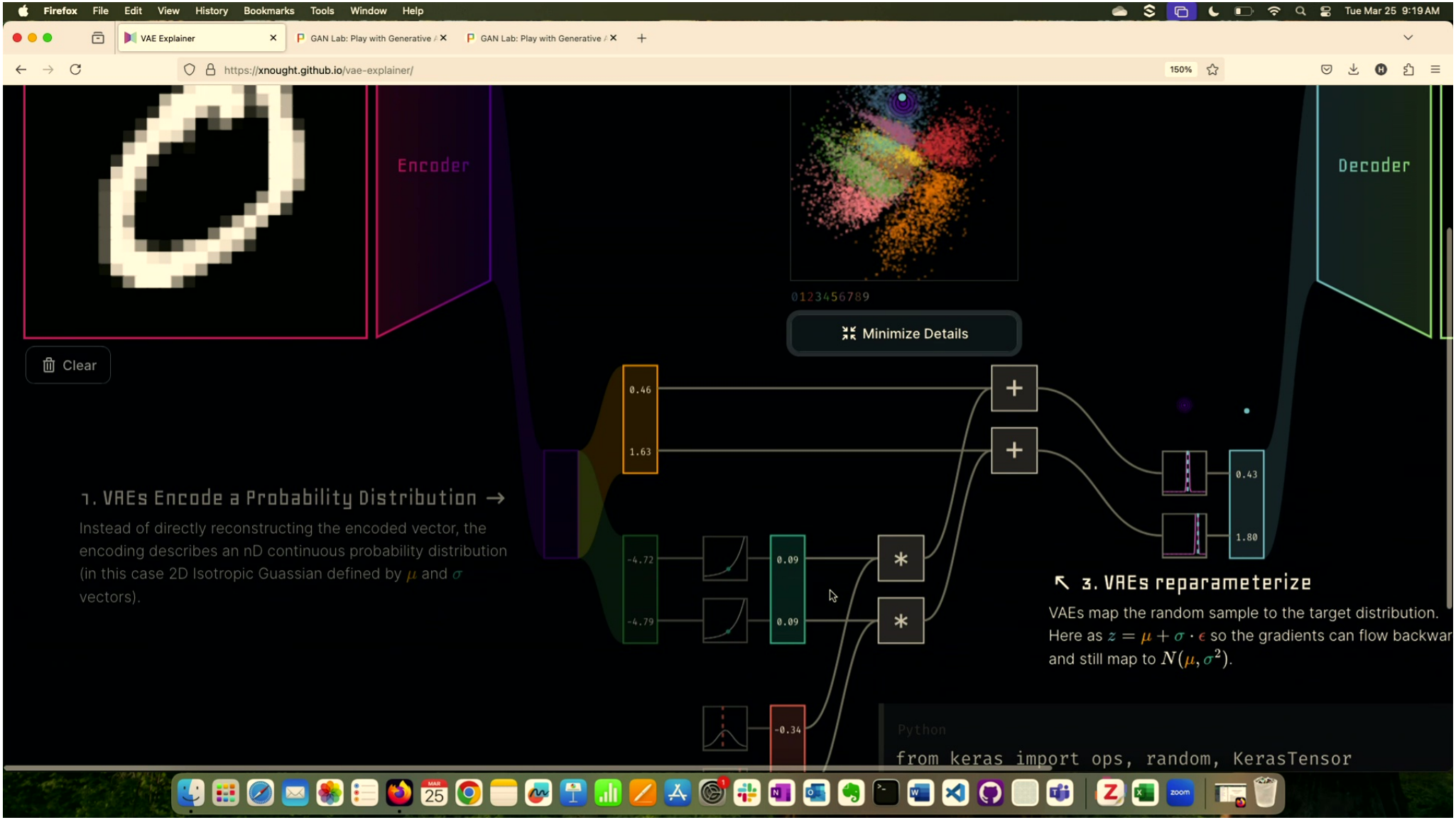
https://xnought.github.io/vae-explainer/
150%
VAE Explainer
Interact with a Variational Autoencoder (VAE) in your browser!
Code
Paper
Latent Space
Resample
Means μ
[0.46, 1.63]
Std. Deviations σ
[0.09, 0.09]
Sampled z
[0.44, 1.72]
Encoder
Decoder
0123456789
Explain VAE Details
Clear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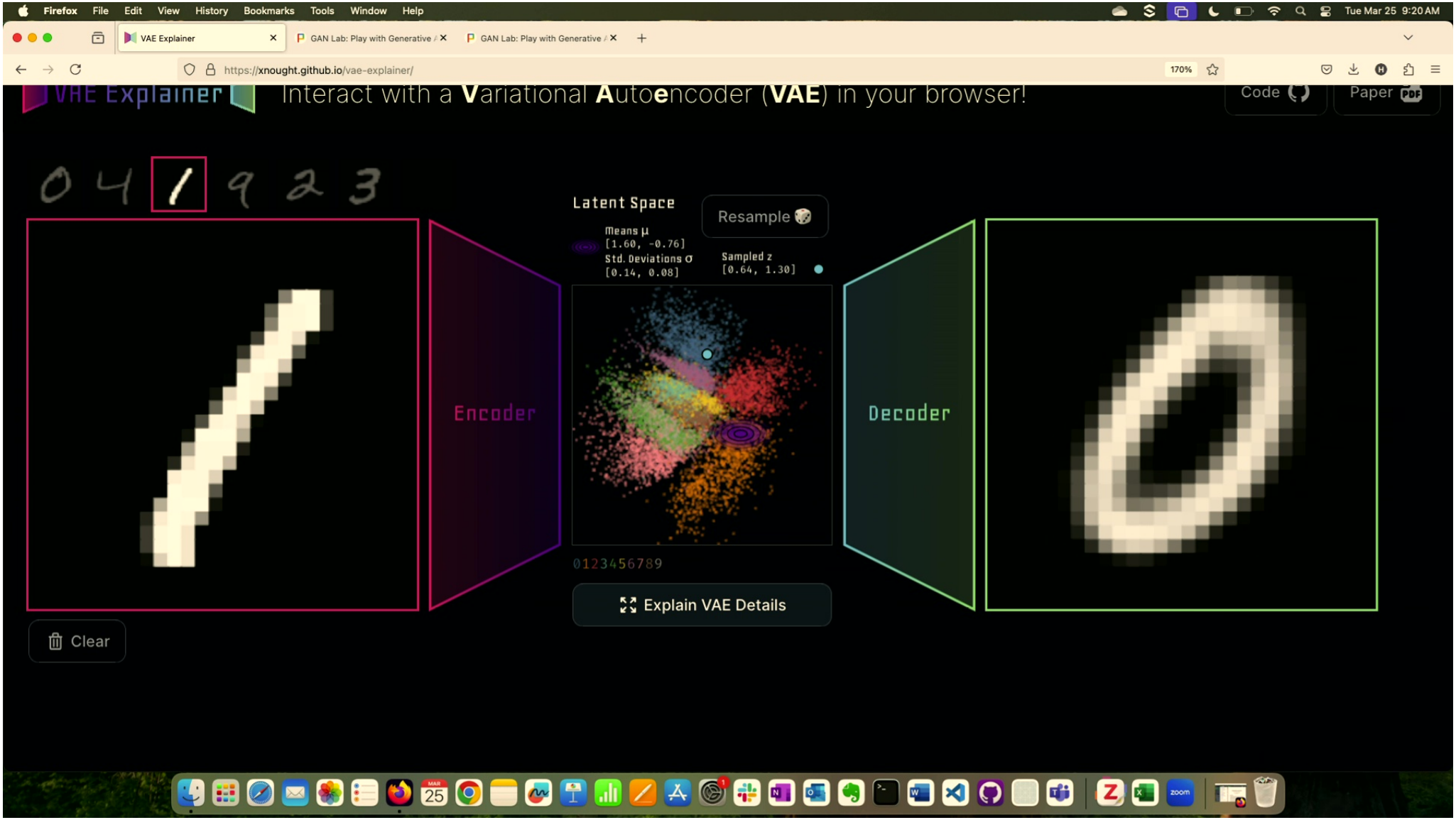
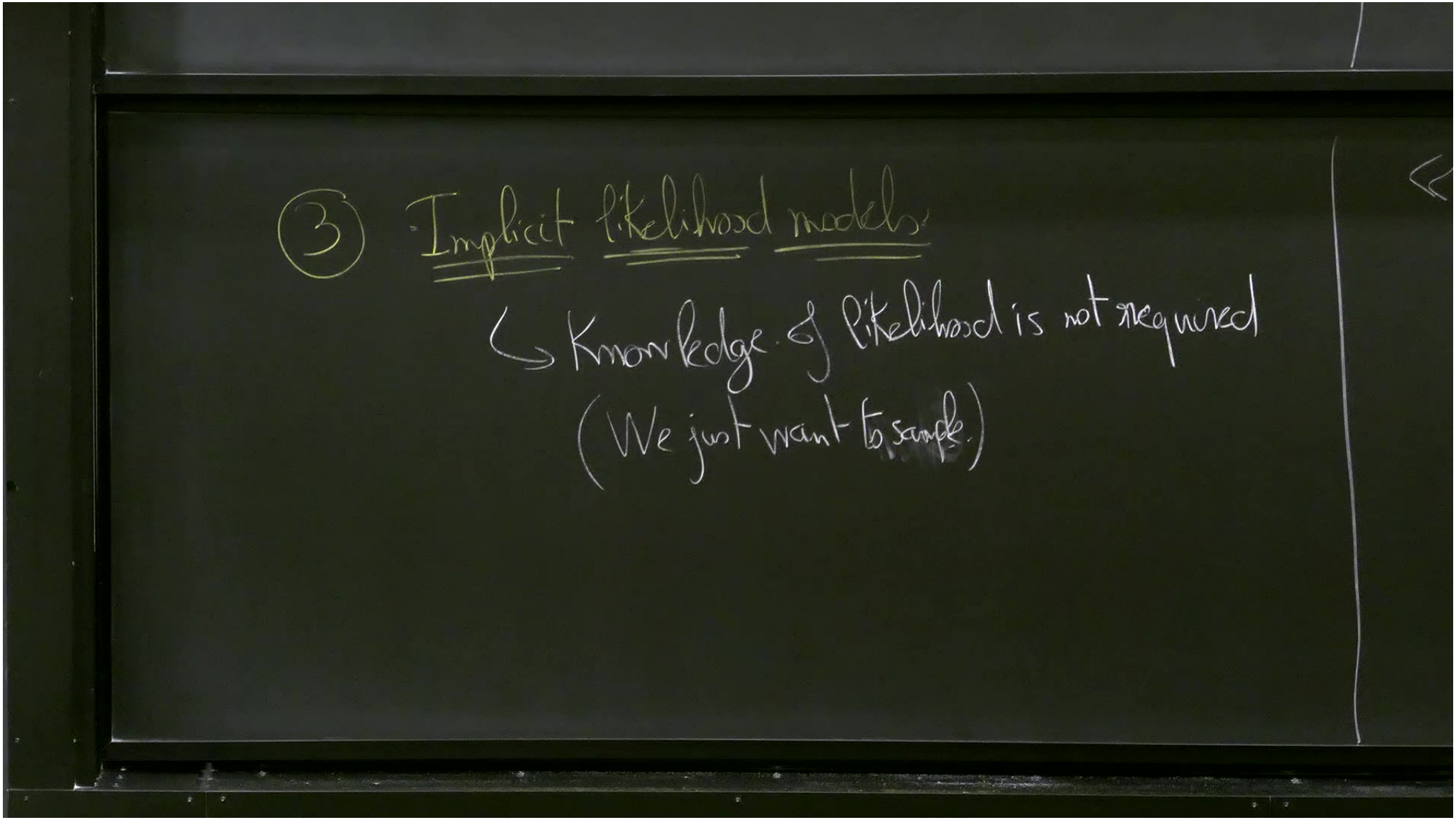
Tue Mar 25 9:19 AM
VAE Explainer
GAN Lab: Play with Generative
GAN Lab: Play with Generative
https://xnought.github.io/vae-explainer/
150%
Encoder
Decoder
0123456789
Minimize Details
Clear
0.46
1.63
-4.72
-4.79
0.09
0.09
-0.34
0.43
1.80
1. VAEs Encode a Probability Distribution →
Instead of directly reconstructing the encoded vector, the encoding describes an nD continuous probability distribution (in this case 2D Isotropic Guassian defined by μ and σ vectors).
↖ 3. VAEs reparameterize
VAEs map the random sample to the target distribution. Here as $z = \mu + \sigma \cdot \epsilon$ so the gradients can flow backwar
and still map to $N(\mu, \sigma^2)$.
Python
from keras import ops, random, KerasTensor

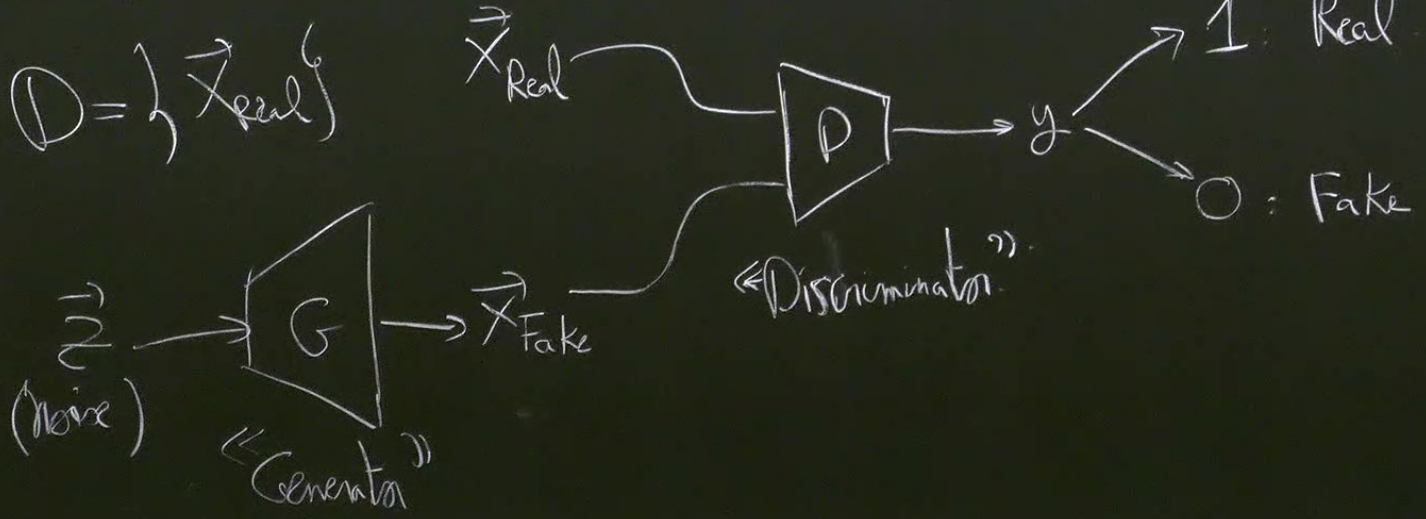

Firefox File Edit View History Bookmarks Tools Window Help
Tue Mar 25 9:20 AM
VAE Explainer
GAN Lab: Play with Generative
GAN Lab: Play with Generative
https://xnought.github.io/vae-explainer/
170%
VAE Explainer
Interact with a Variational Autoencoder (VAE) in your browser!
Code
Paper
Latent Space
Resample
Means μ
[1.60, -0.76]
Std. Deviations σ
[0.14, 0.08]
Sampled z
[0.64, 1.30]
Encoder
Decoder
0123456789
Explain VAE Details
Clear

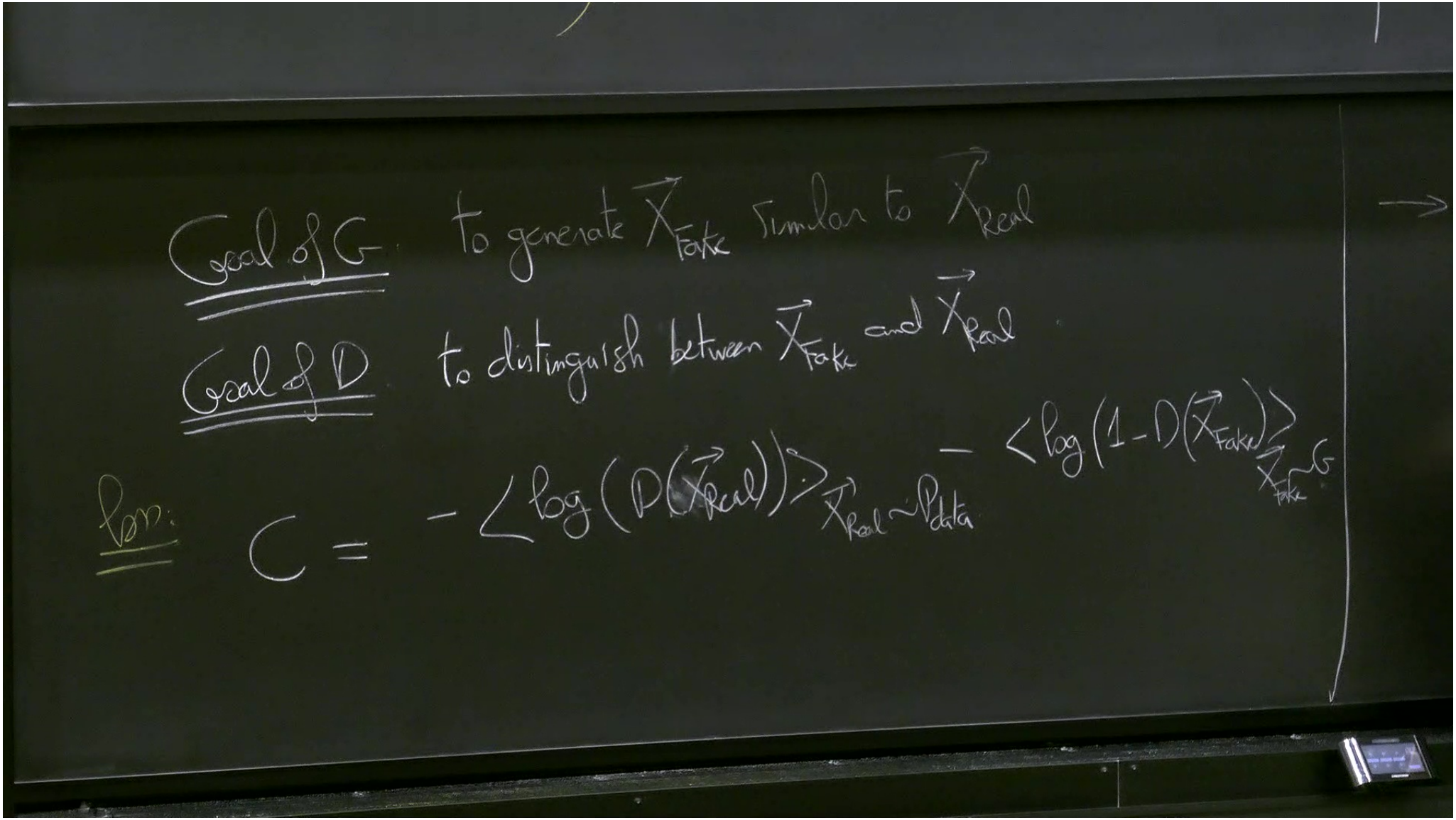

③ Implicit likelihood models
↳ Knowledge of likelihood is not required
(We just want to sample.)

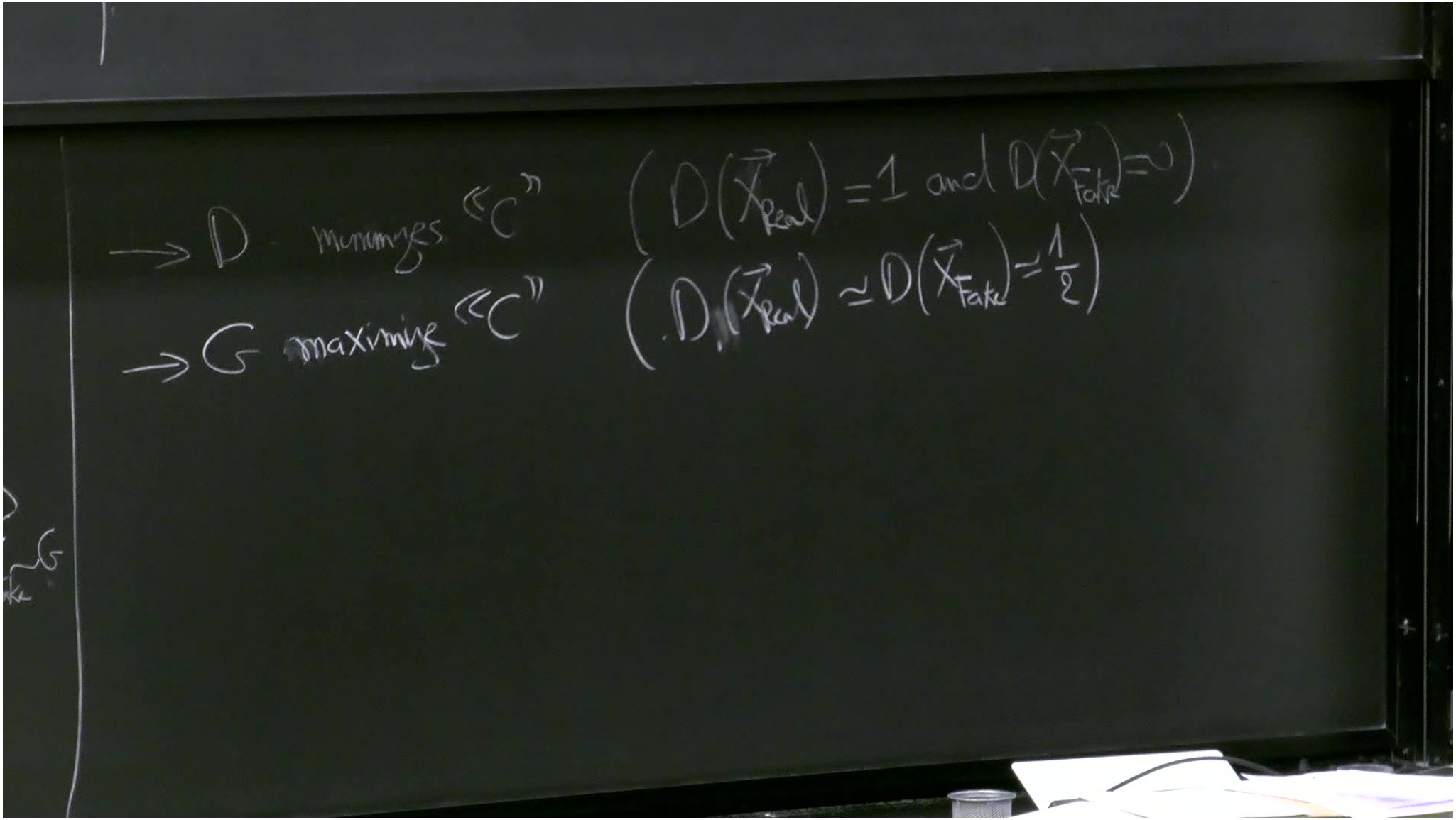
$\varepsilon \sim N(0, I)$.

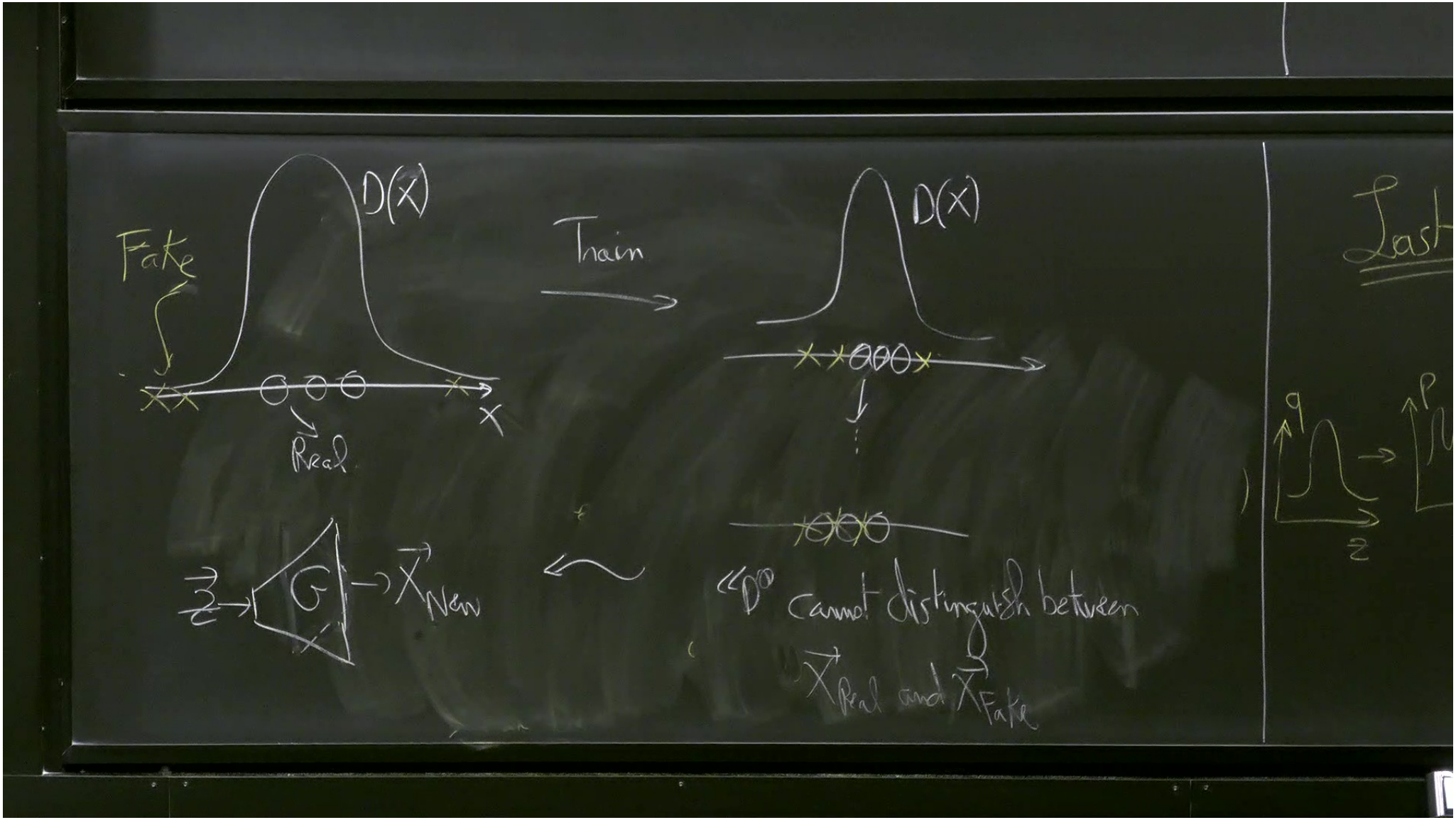
"Generative Adversarial Networks" (GAN).

$D = \{\vec{x}_{real}\}$




Goal of G: to generate $\vec{X}_{Fake}$ similar to $\vec{X}_{Real}$
Goal of D: to distinguish between $\vec{X}_{Fake}$ and $\vec{X}_{Real}$
Loss: $C = -\langle \log(D(\vec{X}_{Real})) \rangle_{\vec{X}_{Real} \sim P_{data}} - \langle \log(1 - D(\vec{X}_{Fake})) \rangle_{\vec{X}_{Fake} \sim G}$


→ D minimizes « C »
(D(X_Real) = 1 and D(X_Fake) = 0)
→ G maximizing « C »
(D(X_Real) ≃ D(X_Fake) ≃ 1/2)


Fake
D(x)
Real
x
Train
D(x)
Last
q
p
z
G
$\vec{x}_{New}$
"D" cannot distinguish between
$\vec{x}_{Real}$ and $\vec{x}_{Fake}$

Play with Generative Adversarial Networks (GANs) in your browser!

Fork us on GitHub

GAN Lab

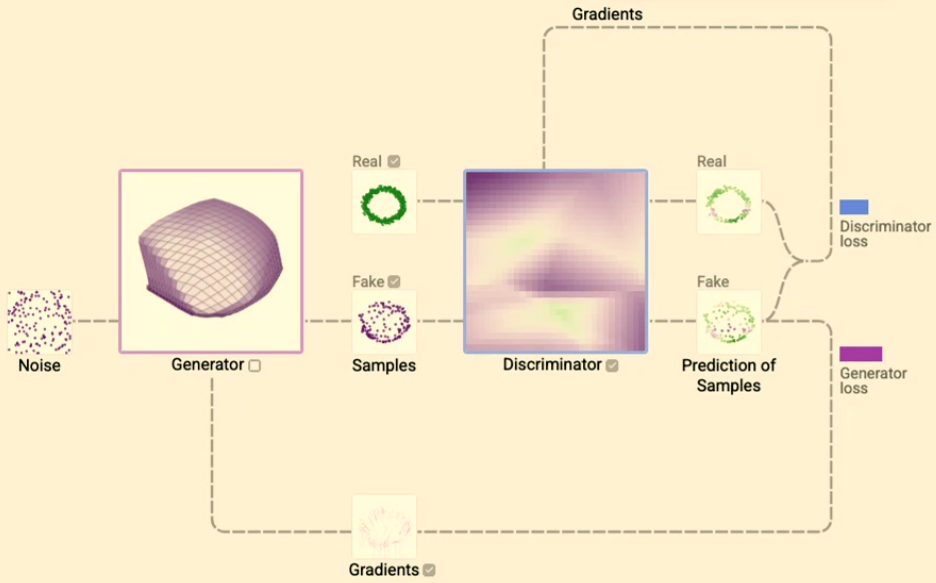
Data Distribution

Use pre-trained model

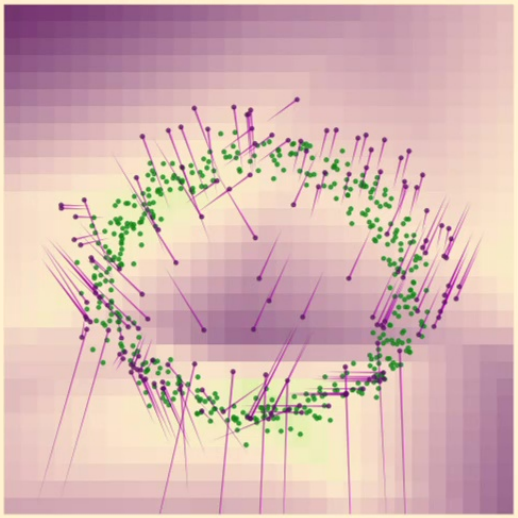
Epoch
001,048

MODEL OVERVIEW GRAPH

Shows the architecture of a model and data flow



LAYERED DISTRIBUTIONS



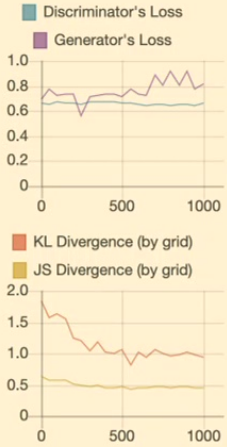
Each dot is a 2D data sample: real samples; fake samples.

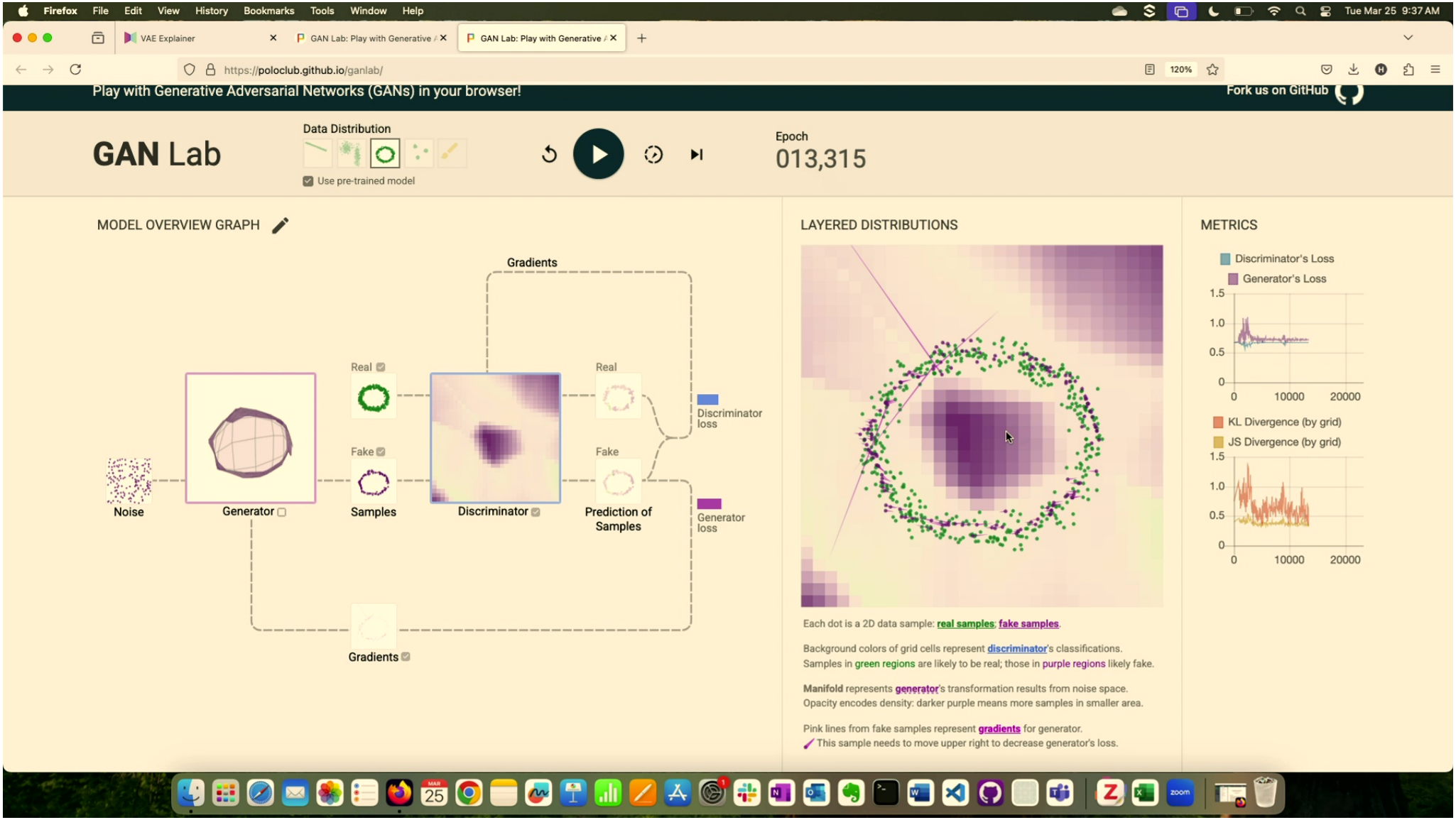
Background colors of grid cells represent discriminator's classifications.
Samples in green regions are likely to be real; those in purple regions likely fake.

Manifold represents generator's transformation results from noise space.
Opacity encodes density: darker purple means more samples in smaller area.

Pink lines from fake samples represent gradients for generator.
This sample needs to move upper right to decrease generator's loss.

METRICS

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Tue Mar 25 9:37 AM
VAE Explainer
GAN Lab: Play with Generative
GAN Lab: Play with Generative
https://poloclub.github.io/ganlab/
120%
Play with Generative Adversarial Networks (GANs) in your browser!
Fork us on GitHub
GAN Lab
Data Distribution
Use pre-trained model
Epoch
013,315
MODEL OVERVIEW GRAPH
Gradients
Real
Fake
Noise
Generator
Samples
Discriminator
Real
Fake
Prediction of Samples
Discriminator loss
Generator loss
Gradients
LAYERED DISTRIBUTIONS
Each dot is a 2D data sample: real samples; fake samples.
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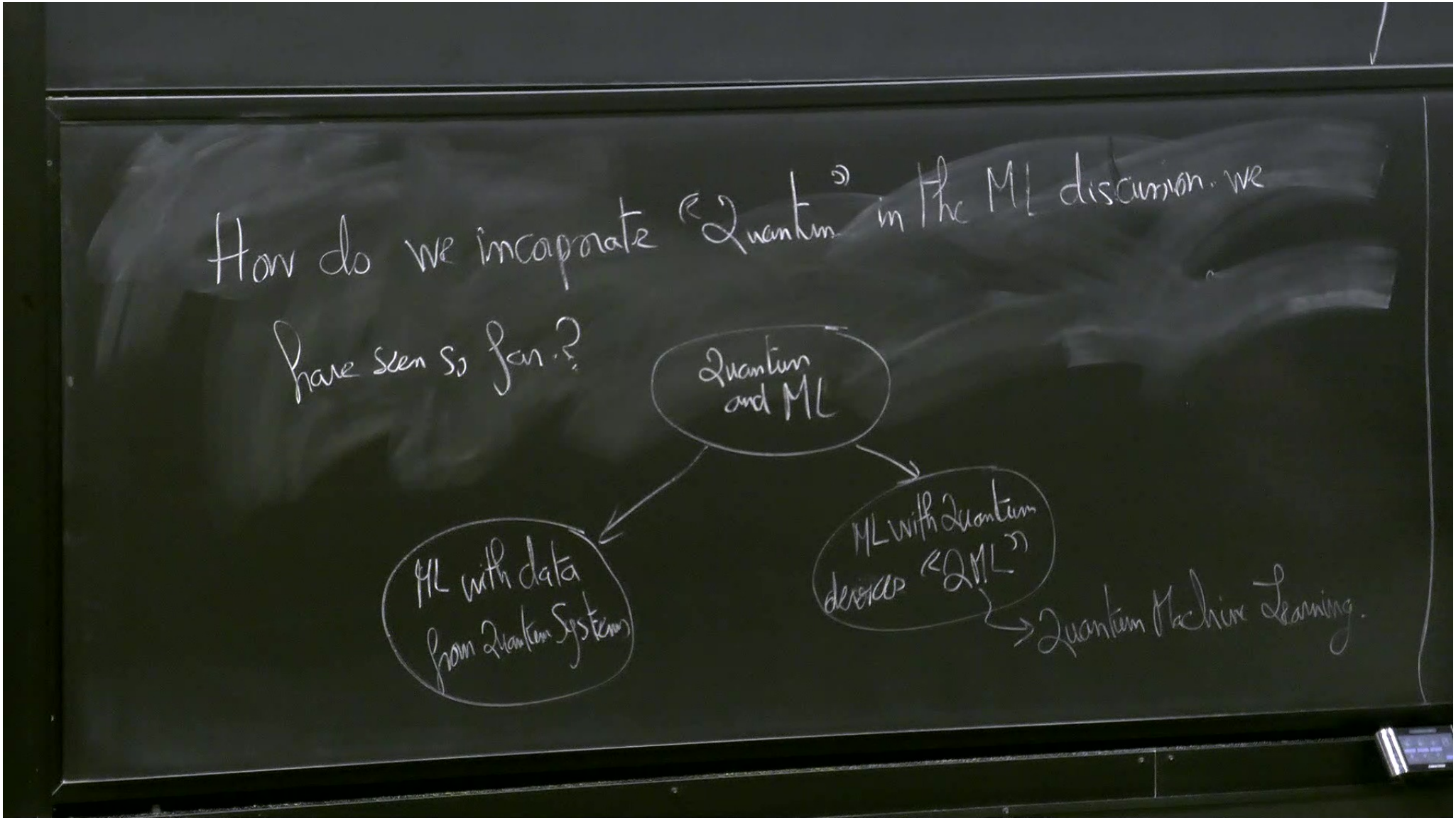
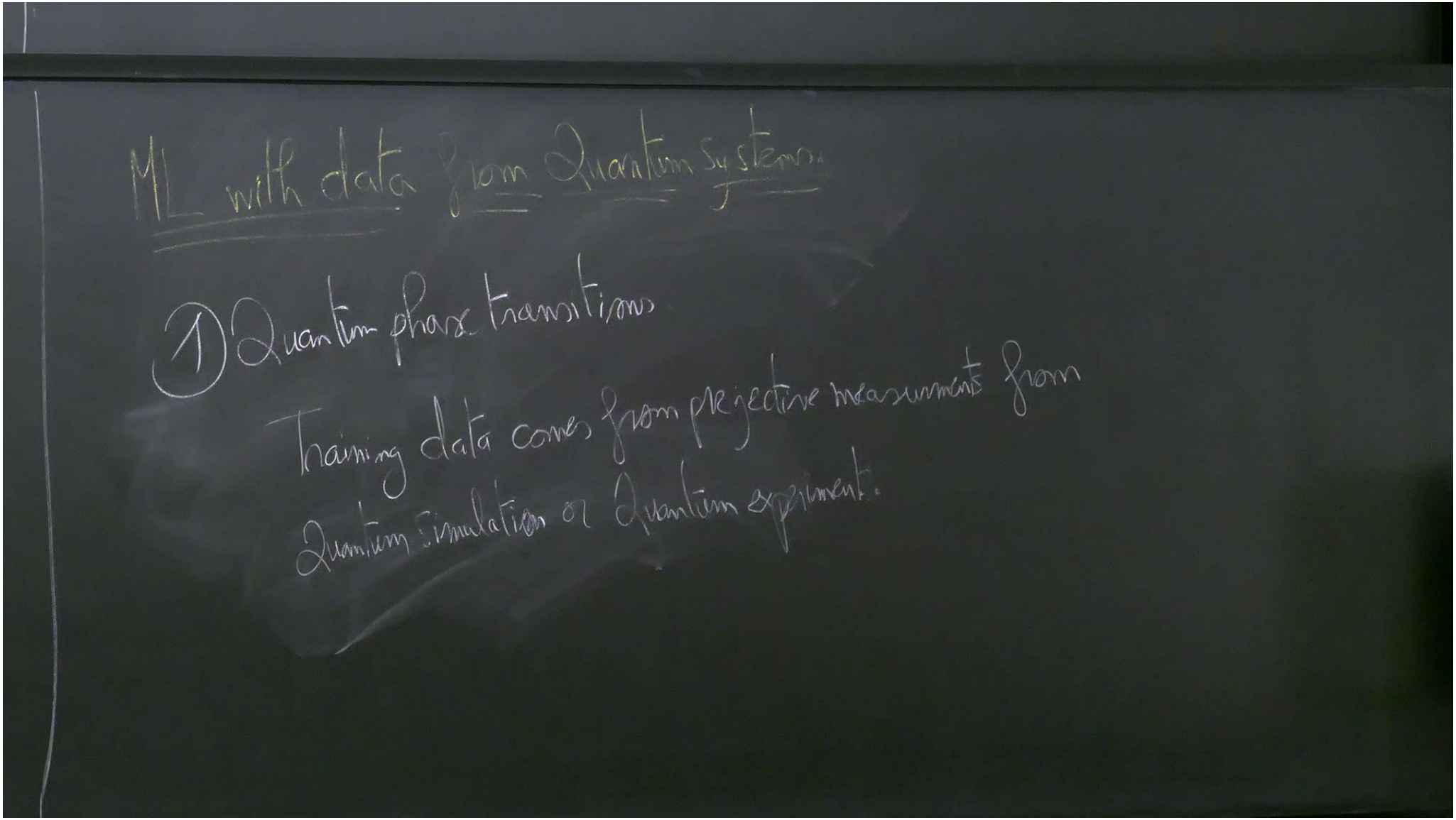
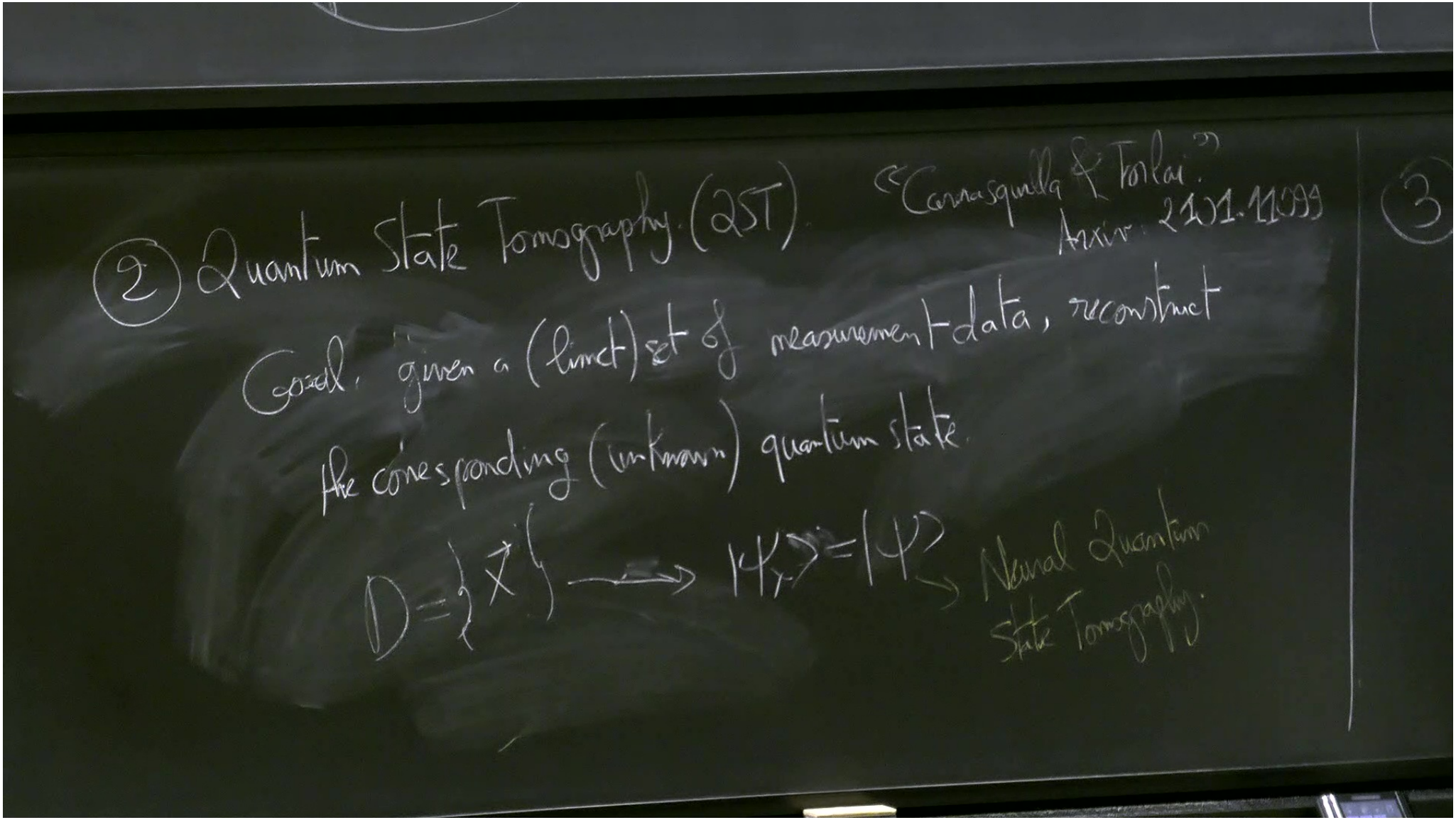
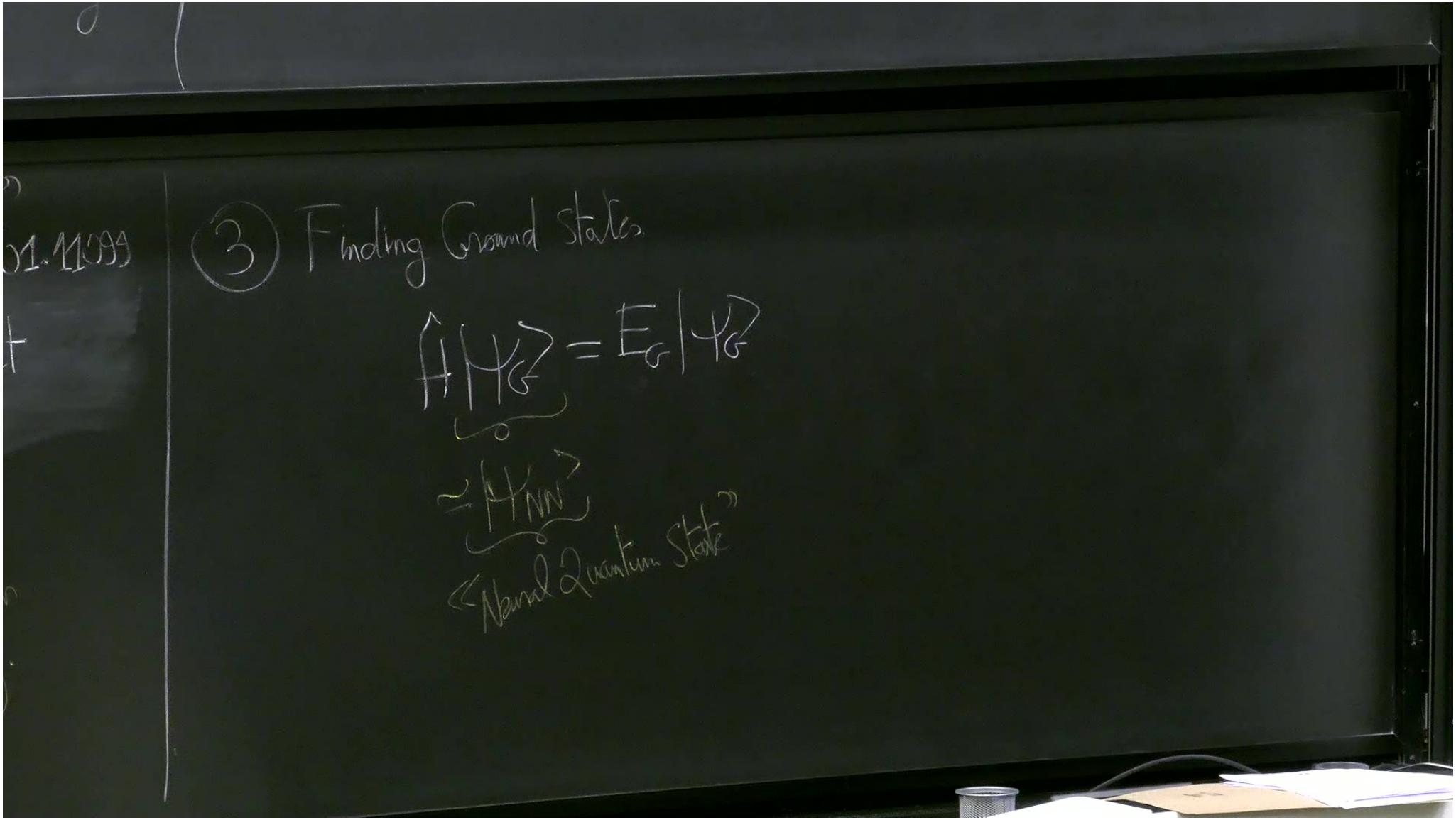
Pink lines from fake samples represent gradients for generator.
This sample needs to move upper right to decrease generator's loss.
METRICS
Discriminator's Loss
Generator's Loss
1.5
1.0
0.5
0
0
10000
20000
KL Divergence (by grid)
JS Divergence (by grid)
1.5
1.0
0.5
0
0
10000
20000


How do we incorporate "Quantum" in the ML discussion. We have seen so far.?
Quantum and ML
ML with data from Quantum Systems
ML with Quantum devices "QML"
→ Quantum Machine Learning.


ML with data from Quantum Systems
1) Quantum phase transitions
Training data comes from projective measurements from
Quantum simulation or Quantum experiment.


② Quantum State Tomography (QST)
"Carrasquilla & Torlai"
Anxiv: 2101.11099
Goal: given a (finite) set of measurement data, reconstruct
the corresponding (unknown) quantum state.
$D = \{\vec{x}_i\} \longrightarrow |\psi_\lambda\rangle = |\psi\rangle$
Neural Quantum
State Tomography.
③


01.11099
3 Finding Ground states
$\hat{H}|\Psi_G\rangle = E_G|\Psi_G\rangle$
$\simeq |\Psi_{NN}\rangle$
"Neural Quantum State"

→ Quantum Machine Learning (QML)

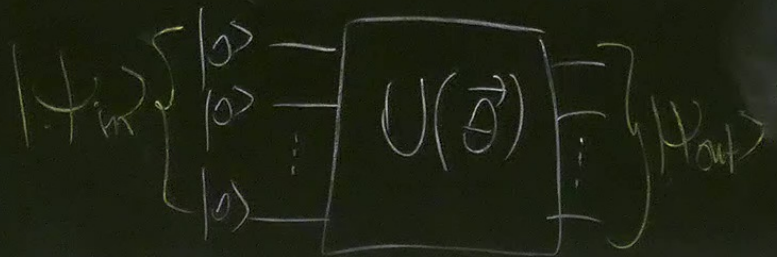
Goal: Use quantum computers/Devices to help with (speed or innovate) ML tasks

Generator

Variational Circuits → Depend on parameters $\theta = \{\theta_1, \theta_2, \dots\}$

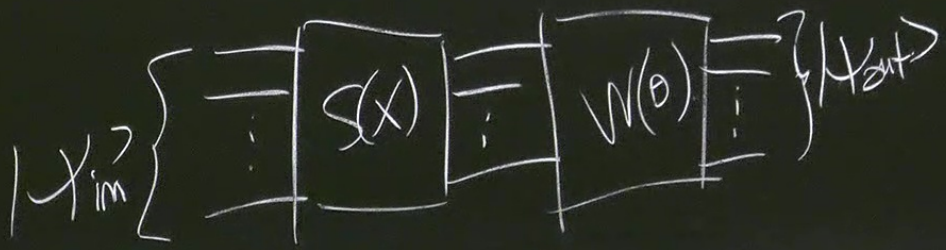
$$|\psi_{in}\rangle = |00\dots0\rangle$$

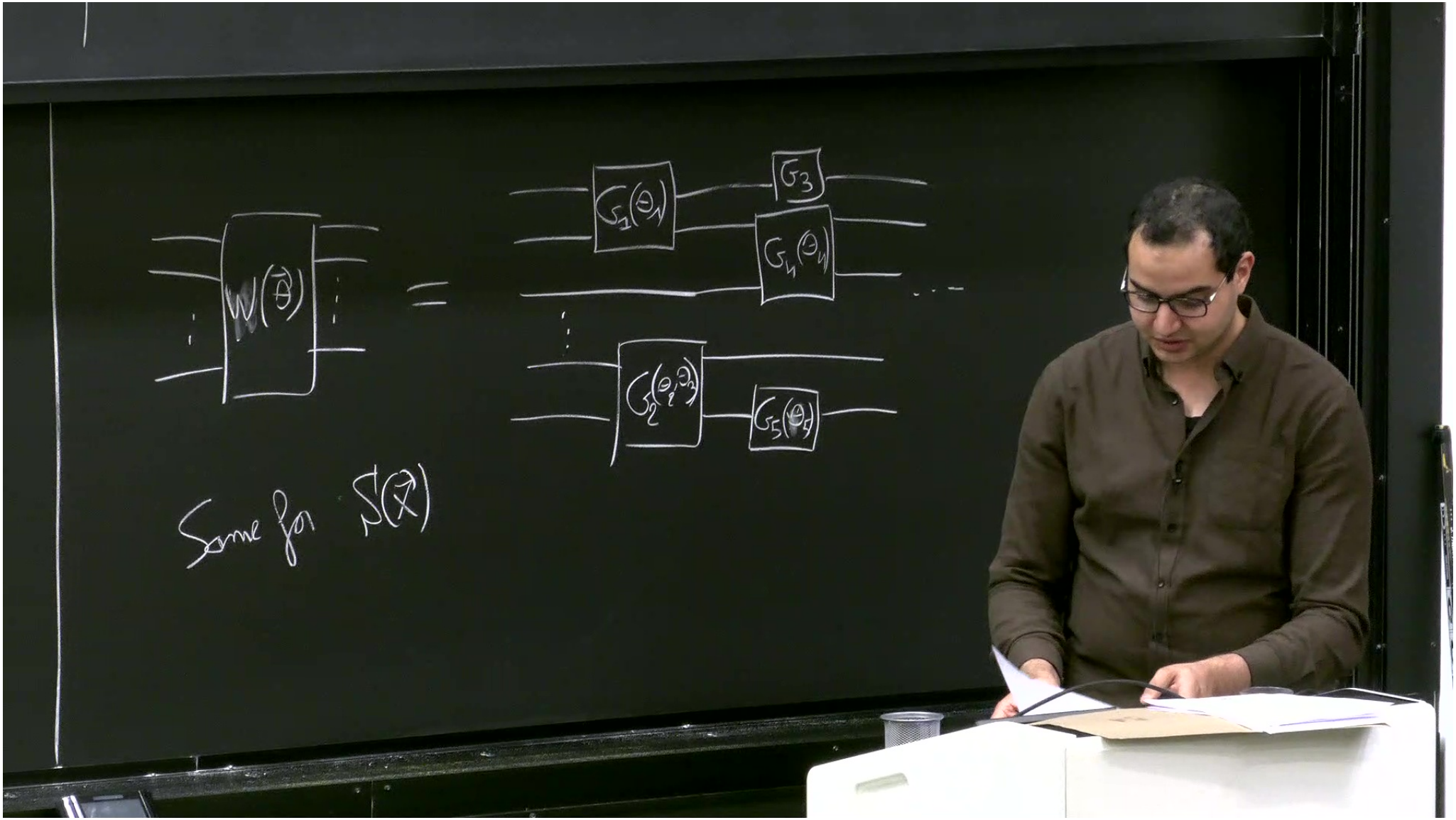
$$|\psi_{out}\rangle = U(\vec{\theta}) \cdot |\psi_{in}\rangle$$



$|\psi_{out}\rangle = U(\vec{x},\vec{\theta})\,|\psi_{in}\rangle$

$U(\vec{x},\vec{\theta}) = \underbrace{W(\vec{\theta})}_{\text{Processing}}\ \underbrace{S(\vec{x})}_{\text{Encoding}}$




W(θ)
G1(θ1)
G3
G4(θ4)
G2(θ2,θ3)
G5(θ5)
Same for S(x)