Generative Models

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ML4FP School 2024

Generative Models in Media

- Learn underlying distribution of data
- Produce realistic new samples
- Recently gained attention for AI art generation (Dall-E 2, Imagen, Midjourney)

GOOGLE
IMAGEN AI
DALL·E 2

particle shower in a calorimeter in the style of egon schiele, Dall-E 2

Classification

High Dim. Data

Classification

High Dim. Data

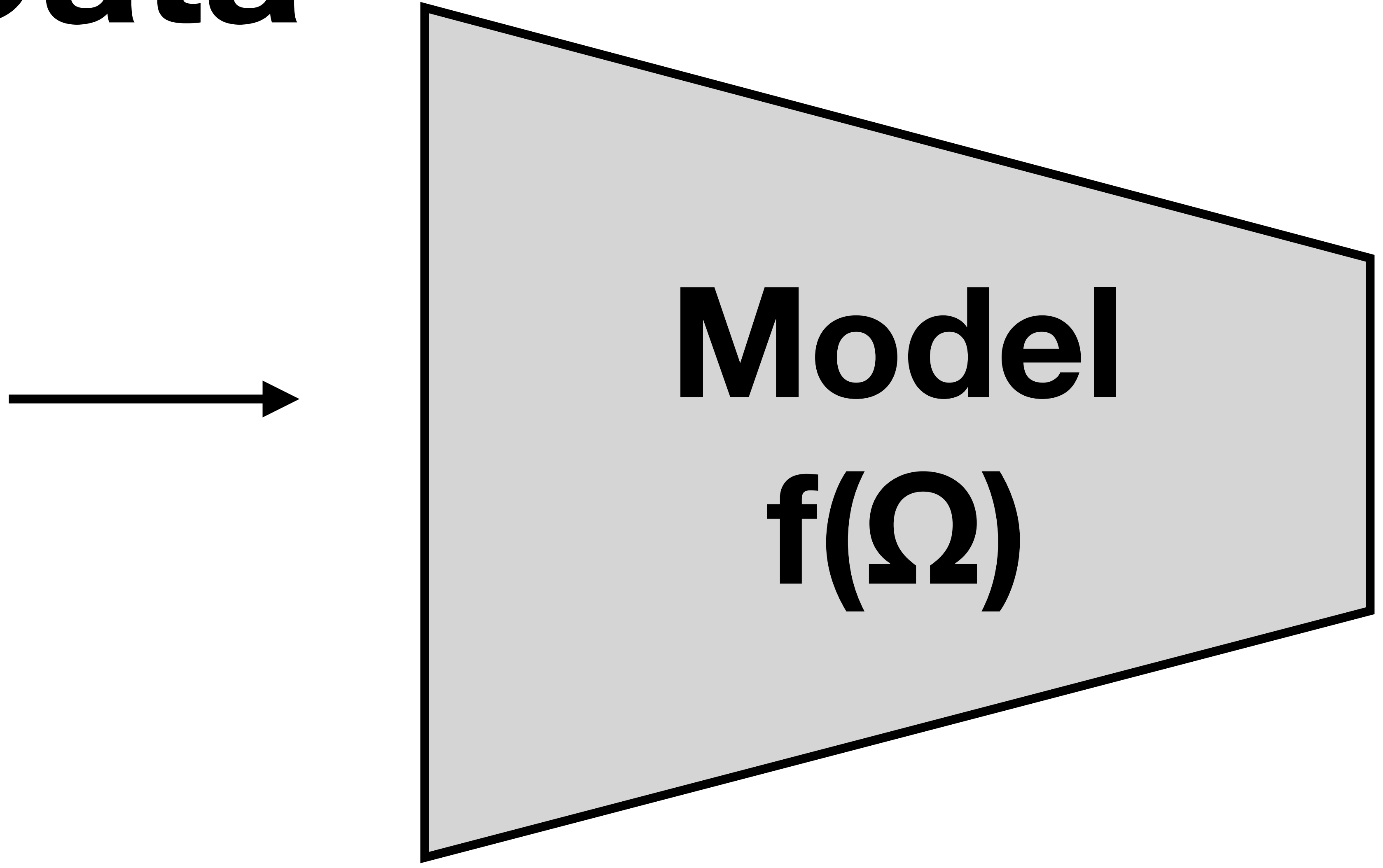
Low Dim. Label

Dog

Cat

Classification

High Dim. Data



Classification

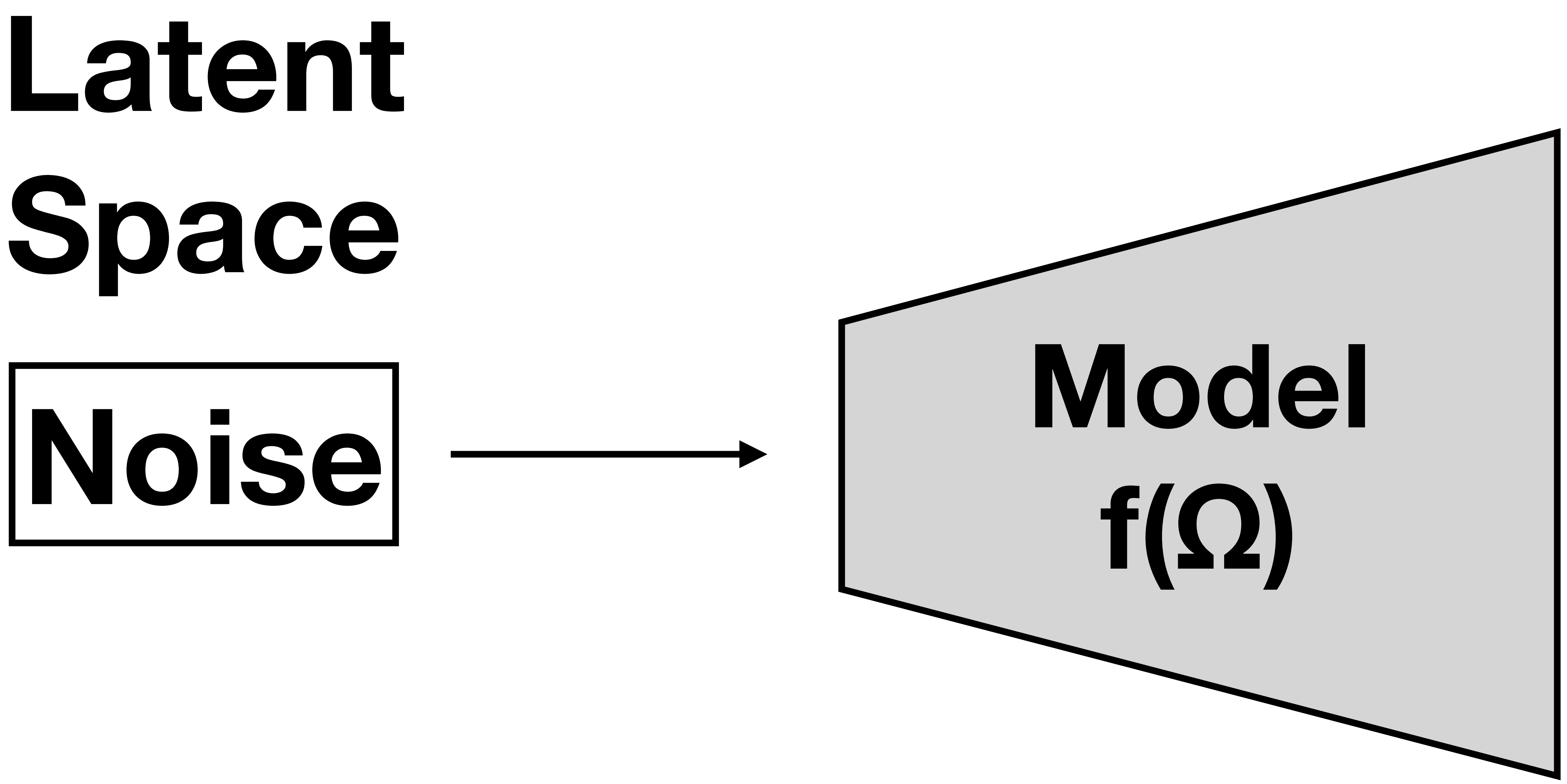
High Dim. Data

Model
f(Ω)

Prediction

Cat/Dog?

Generation



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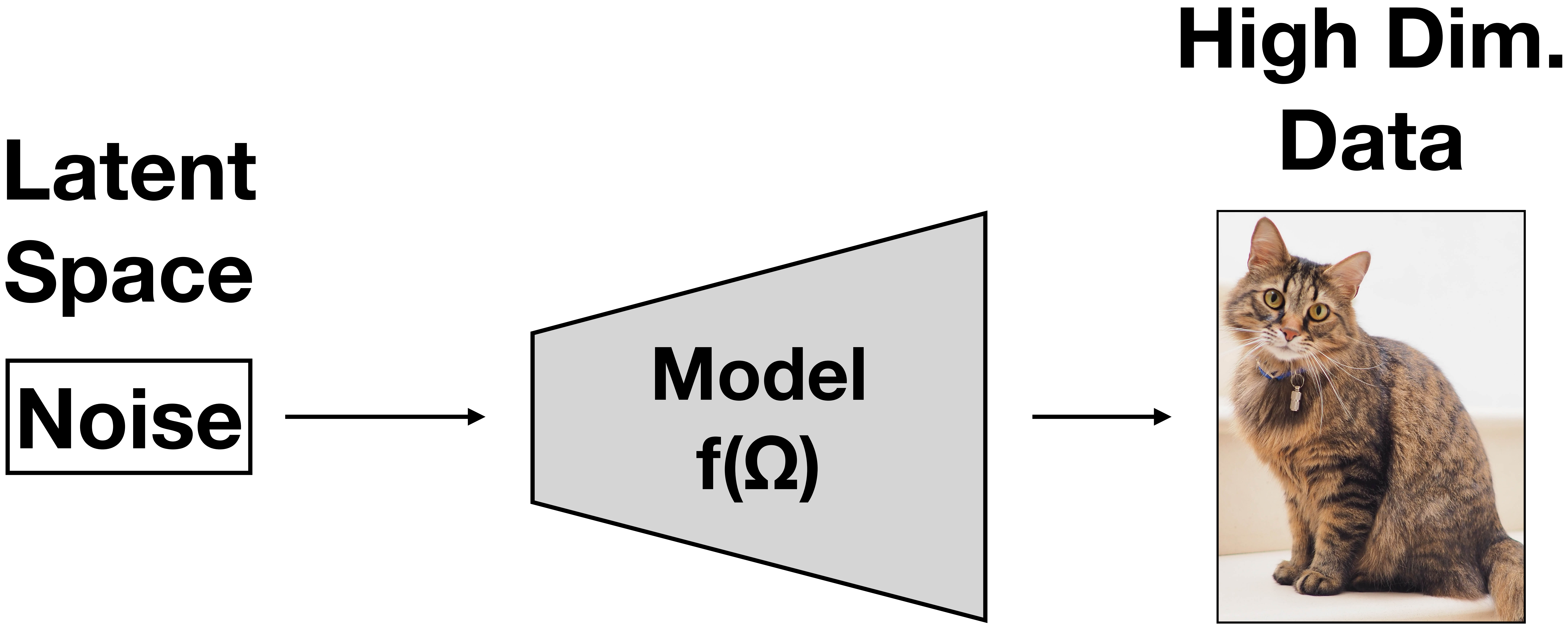

Generation

Training a generative model

1. Start from random noise
2. Use network to transform noise to data
3. Use loss function that gauges quality of generated data

Generation

Training a generative model

1. Start from random noise ✓
2. Use network to transform noise to data ✓
3. Use loss function that gauges quality of generated data

This is where it gets tricky

Classification Loss Functions

- Easy to understand model outputs
  - Predictions for a given data sample
  - Accuracy, Area Under Curve, directly measure network performance

Classification Loss Functions

- Easy to understand model outputs
  - Predictions for a given data sample
  - Accuracy, Area Under Curve, directly measure network performance
  - Directly compare network output to true prediction
  - Wide range of available loss functions
    - Mean Squared Error
    - Cross-Entropy

Generative Loss Functions

- How do you measure the model performance?
- How is this expressed mathematically (and differentiable)

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http://thesecatsdonotexist.com

Generative Difficulties

- Image Set:
  - Does the new set have the same properties as the data?

Training Data:

Generative Difficulties

- Image Set:
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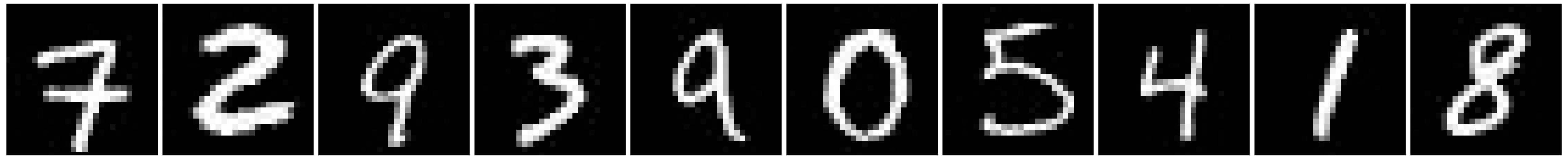
Training Data:

Generated Data:

Generative Difficulties



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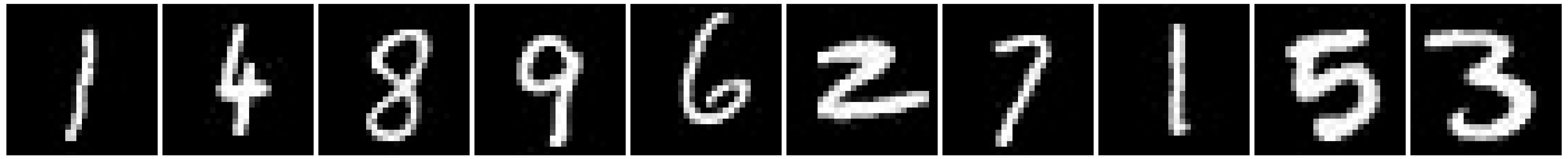
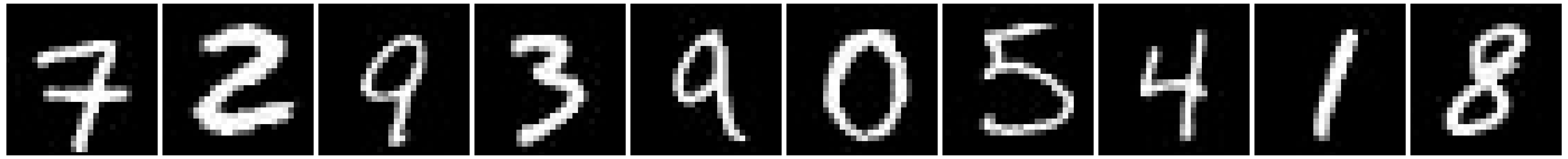


Ideal generative outcome

Generative Difficulties



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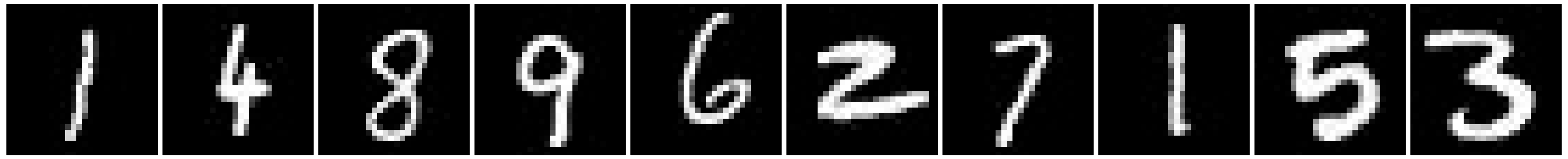

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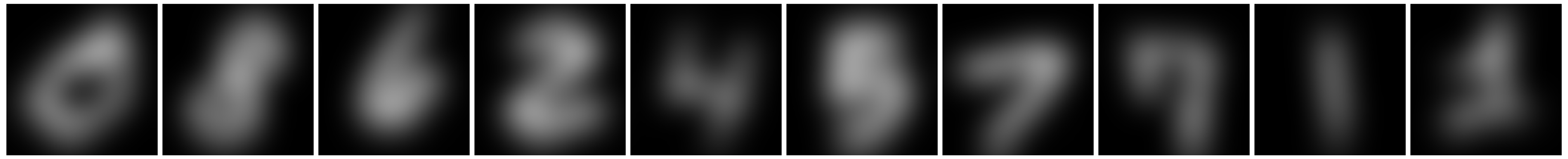
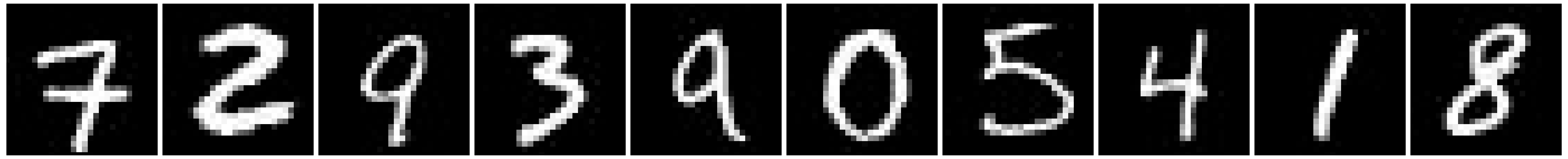


Low sample quality

Generative Difficulties



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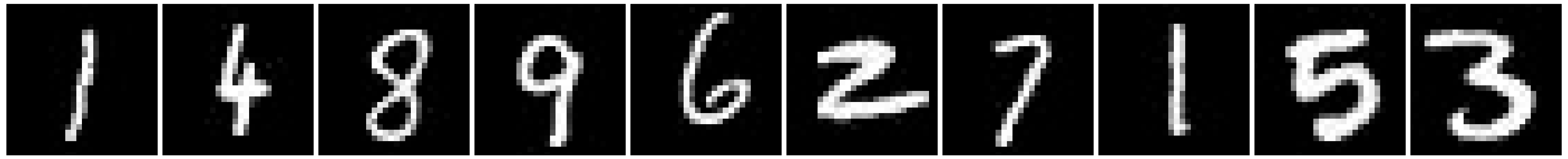

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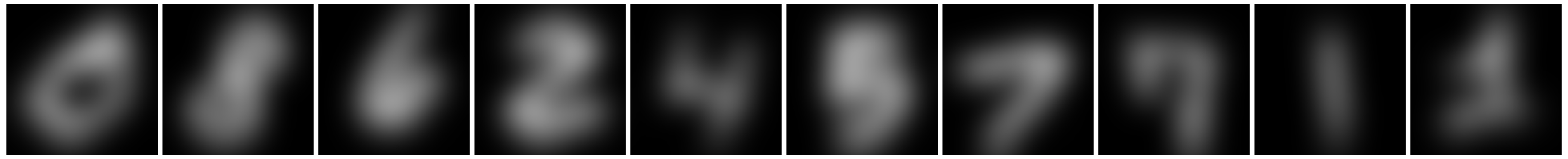

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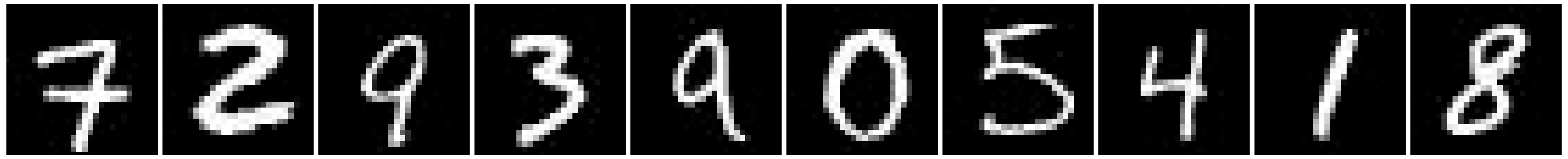
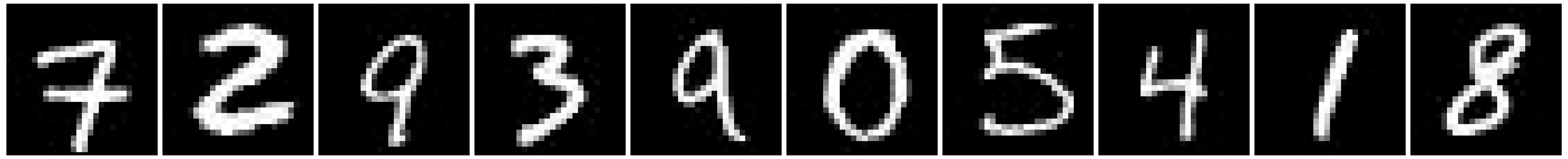


Overfitting

Generative Difficulties



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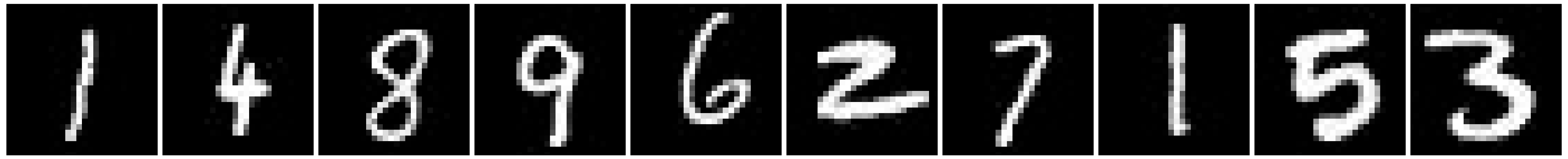

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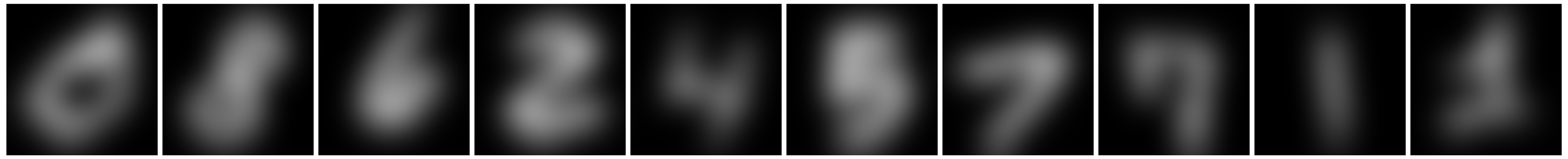

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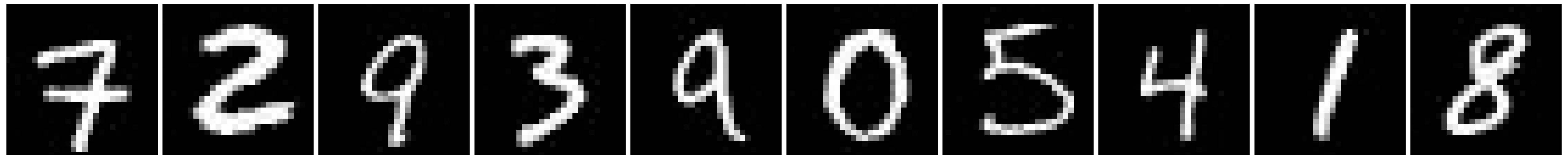

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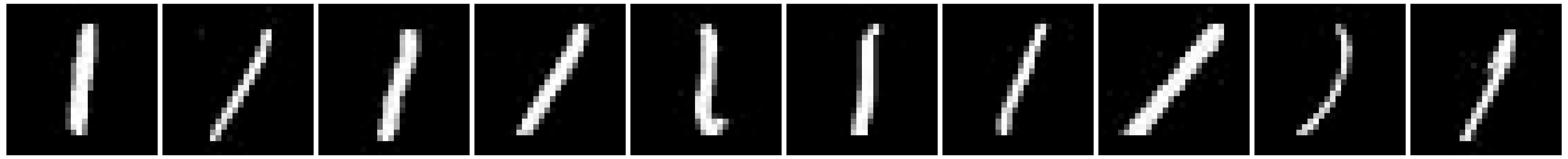
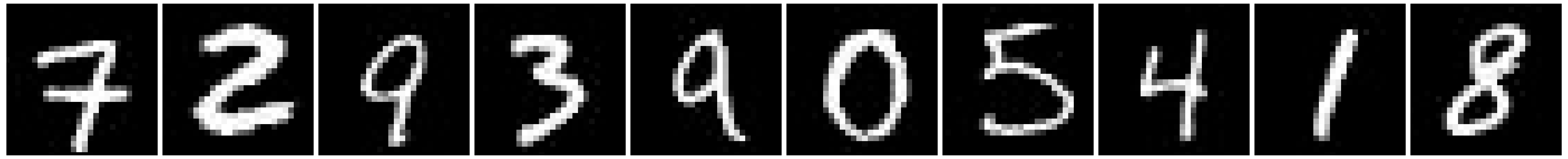


Mode collapse

Generative Difficulties



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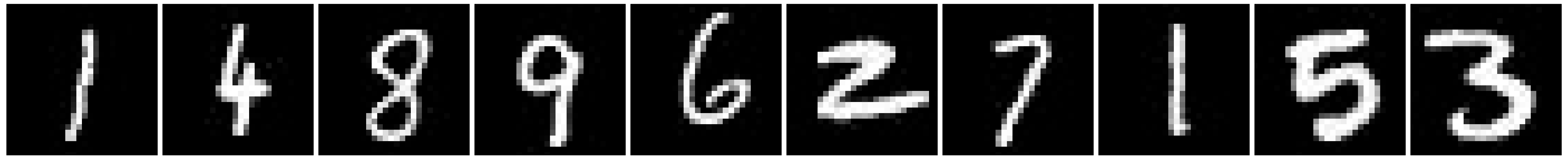

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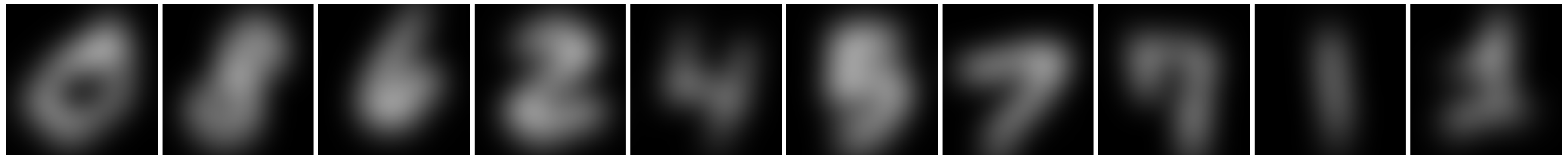

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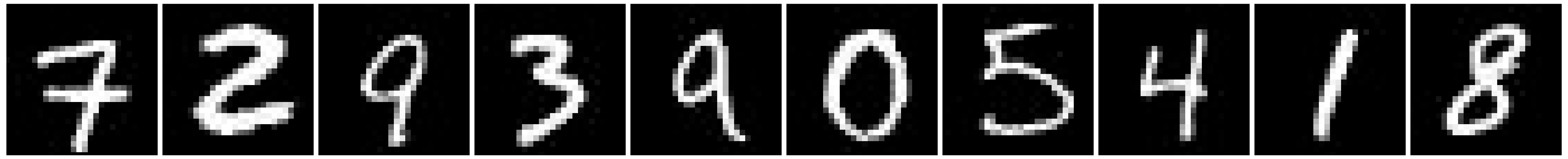

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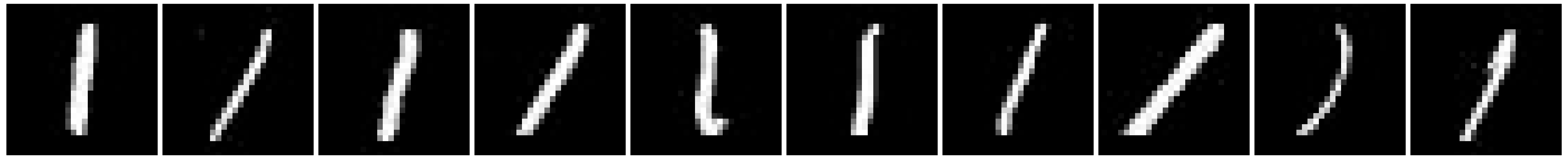

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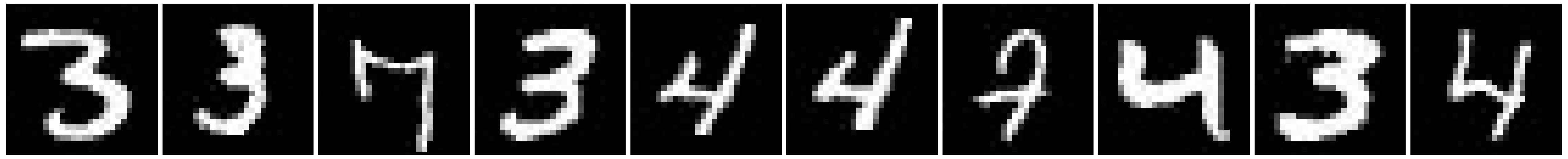


Incorrect composition

Generative Difficulties

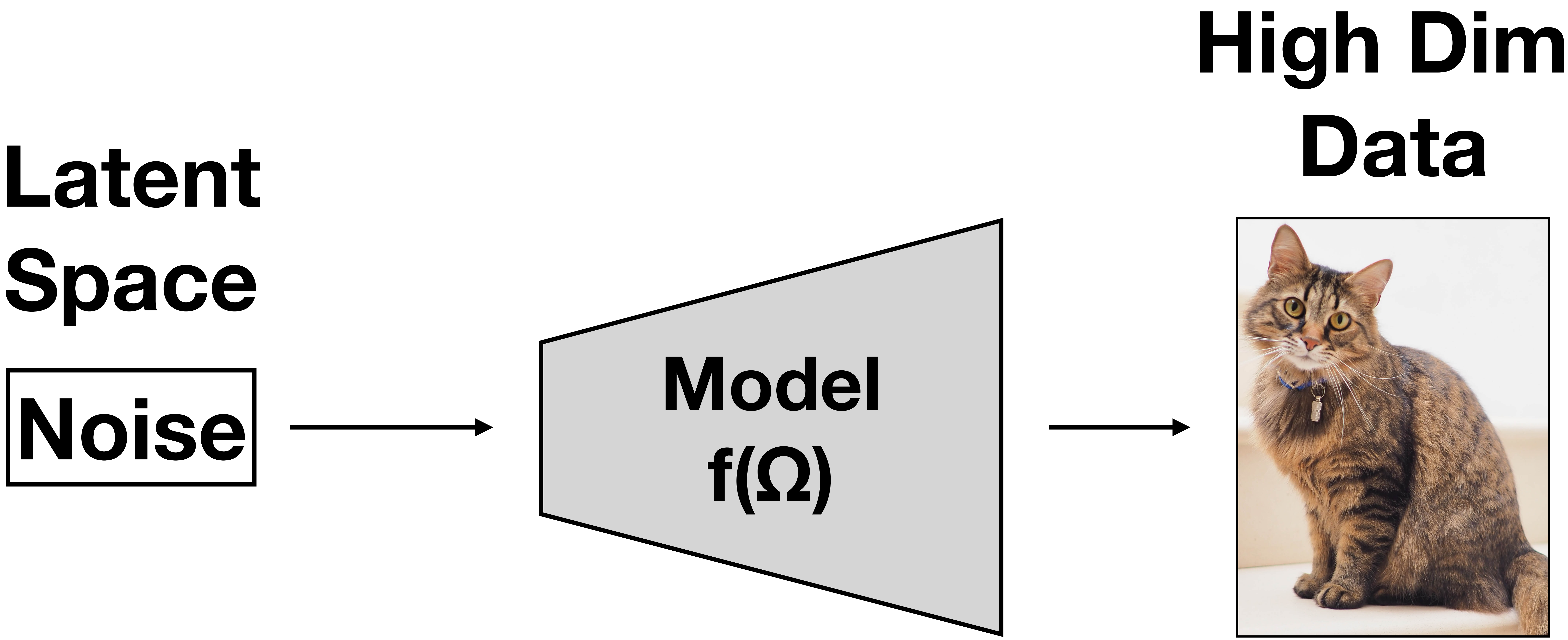
GANs
Generative Adversarial Networks

Score-based

NFs
Normalizing Flows

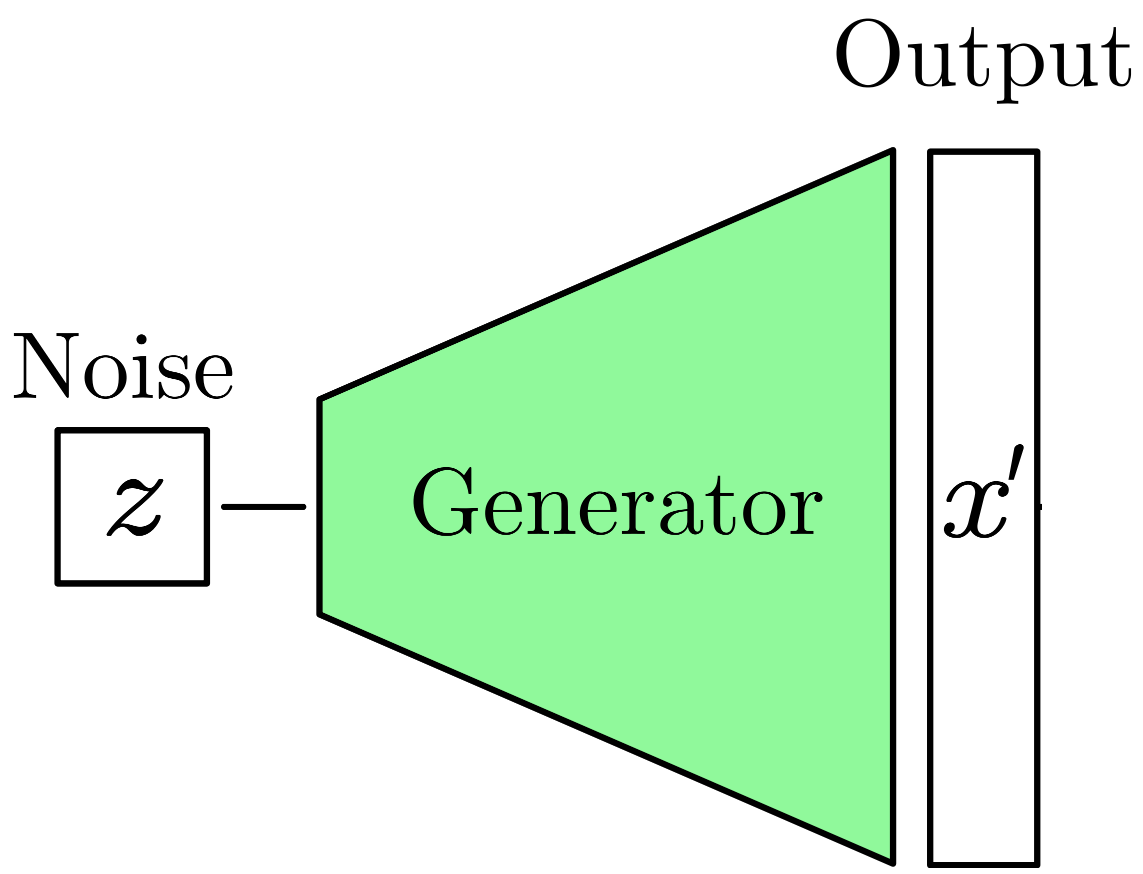
VAEs
Variational Autoencoders

Generative Adversarial Network



Generative Adversarial Network

- Generator Network G(z)=x
  - Maps noise Z to Data X



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- Generator Network G(z)=x
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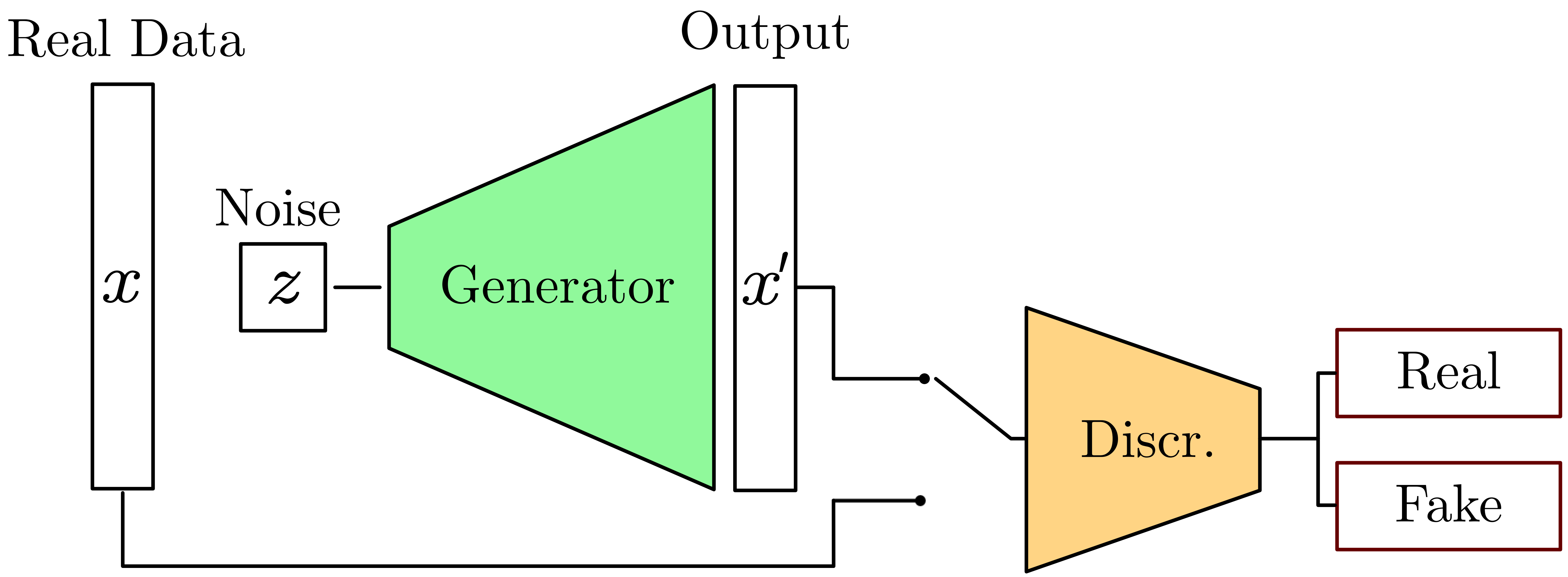
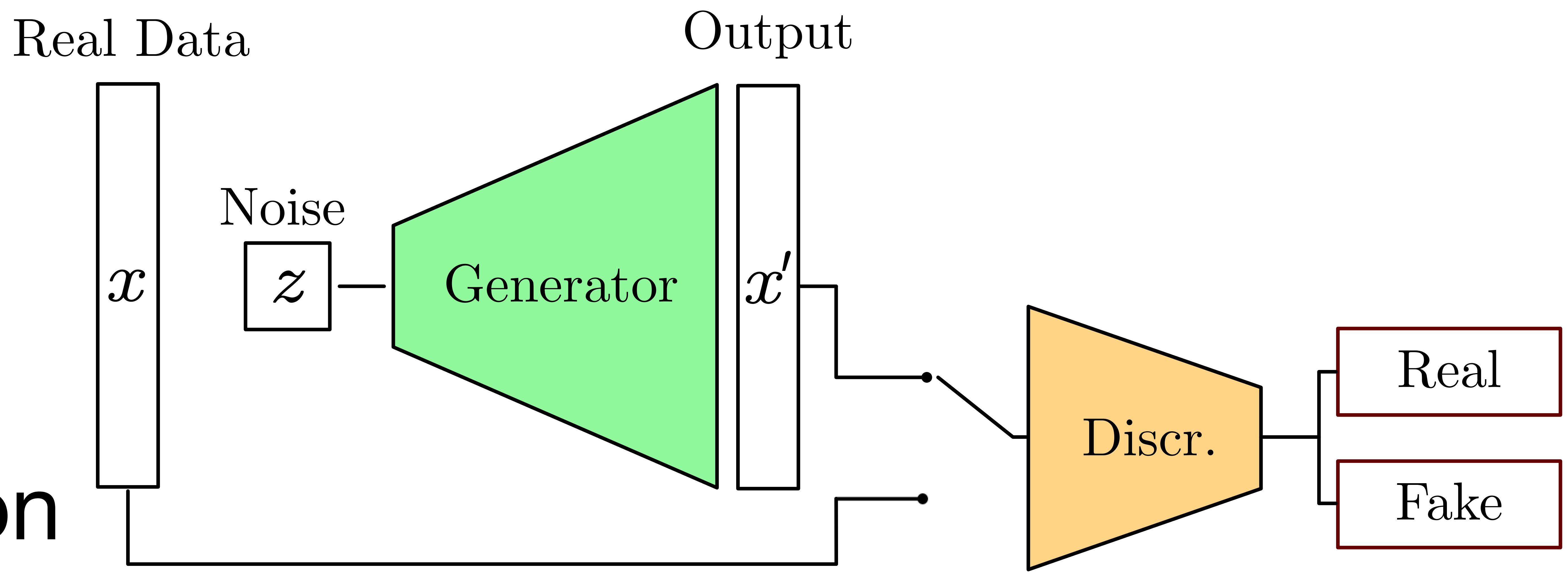
- Discriminator D(G(z)) and D(x)
  - Learns difference between real and fake



Generative Adversarial Network

- Generator Network G(z)=x
  - Maps noise Z to Data X
- Discriminator D(G(z)) and D(x)
  - Learns difference between real and fake
- D(G(z)) is differentiable function measuring performance
- Use D(G(z)) as loss to update G



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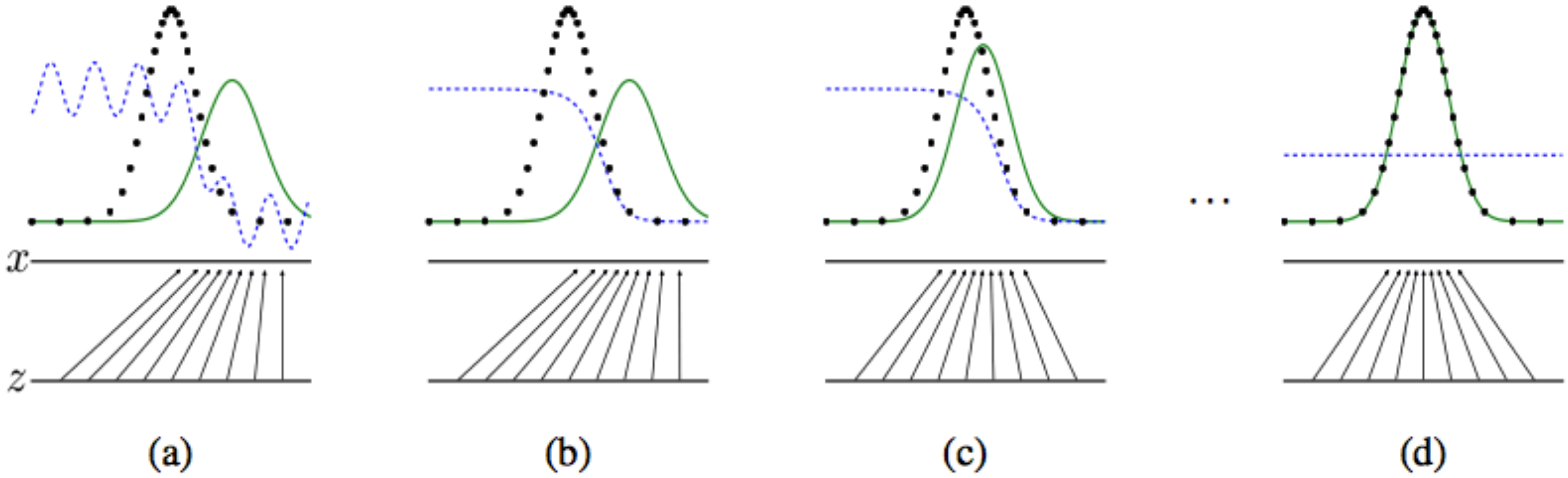


Goodfellow et al.- arXiv:1406.2661

- Discriminator of GAN approximates Jensen Shannon Divergence
- Guides Generated distribution to match real distribution

Generative Adversarial Network

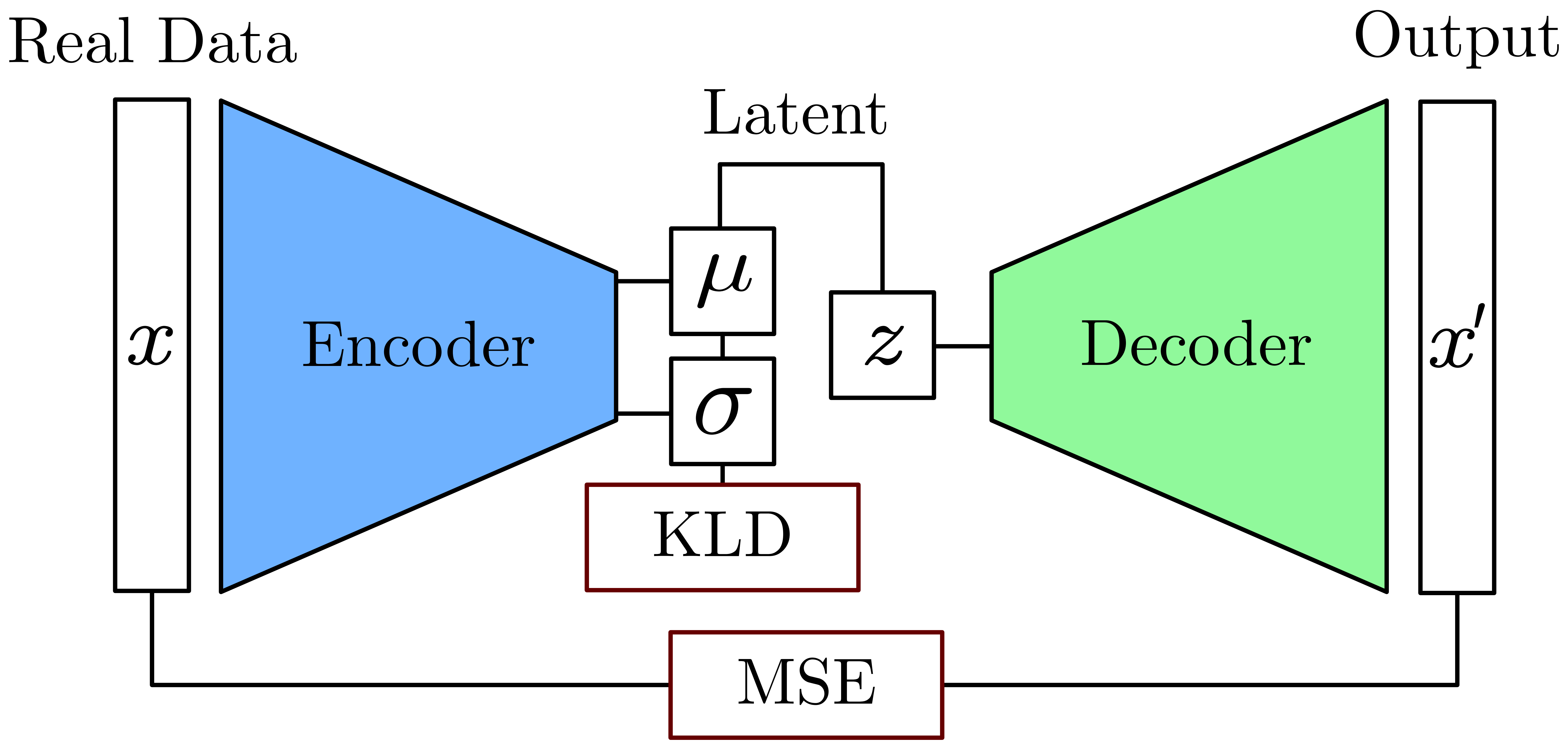
Upsides

- Intuitive approach
- Easy to introduce additional constraints
- Well explored with several improvements (WGANs, normalisations)

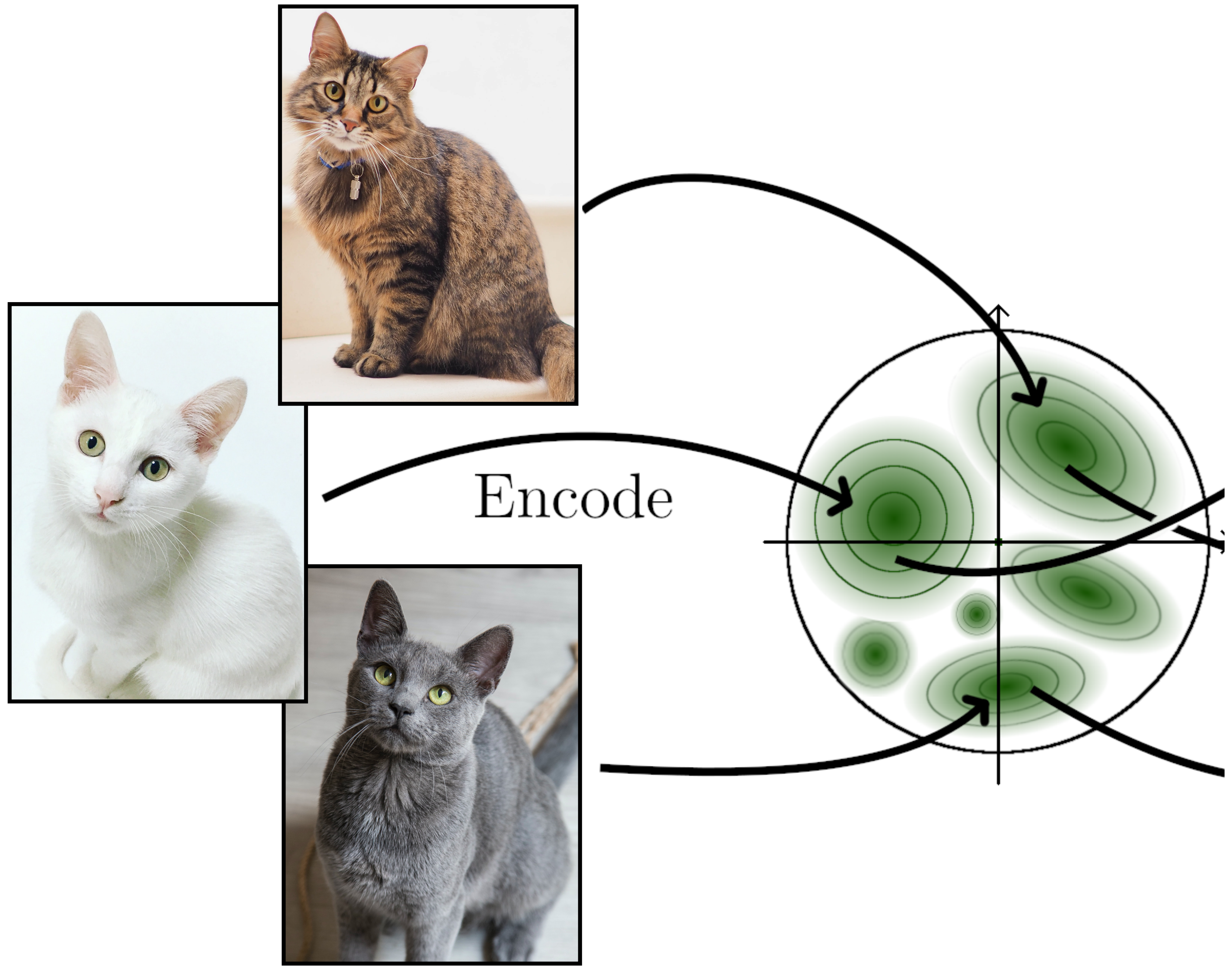
Difficulties

- Difficult to train
- Gen. and disc. needs to be balanced
- Can fail to converge
- Prone to mode collapse

Variational AutoEncoder



AutoEncoder



- Encoding function E(x)=z map high dimensional data X to low dimensional latent space Z

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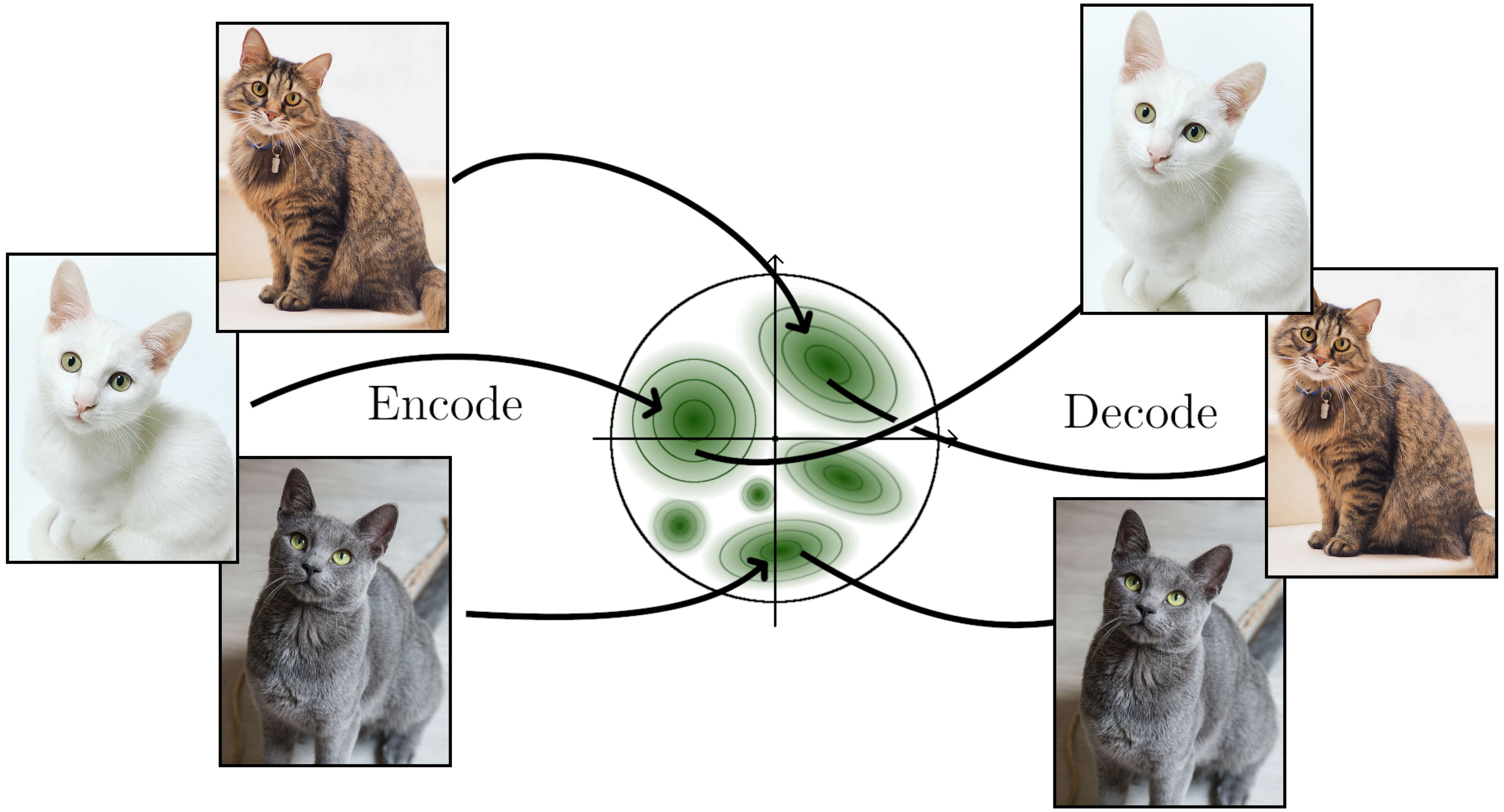

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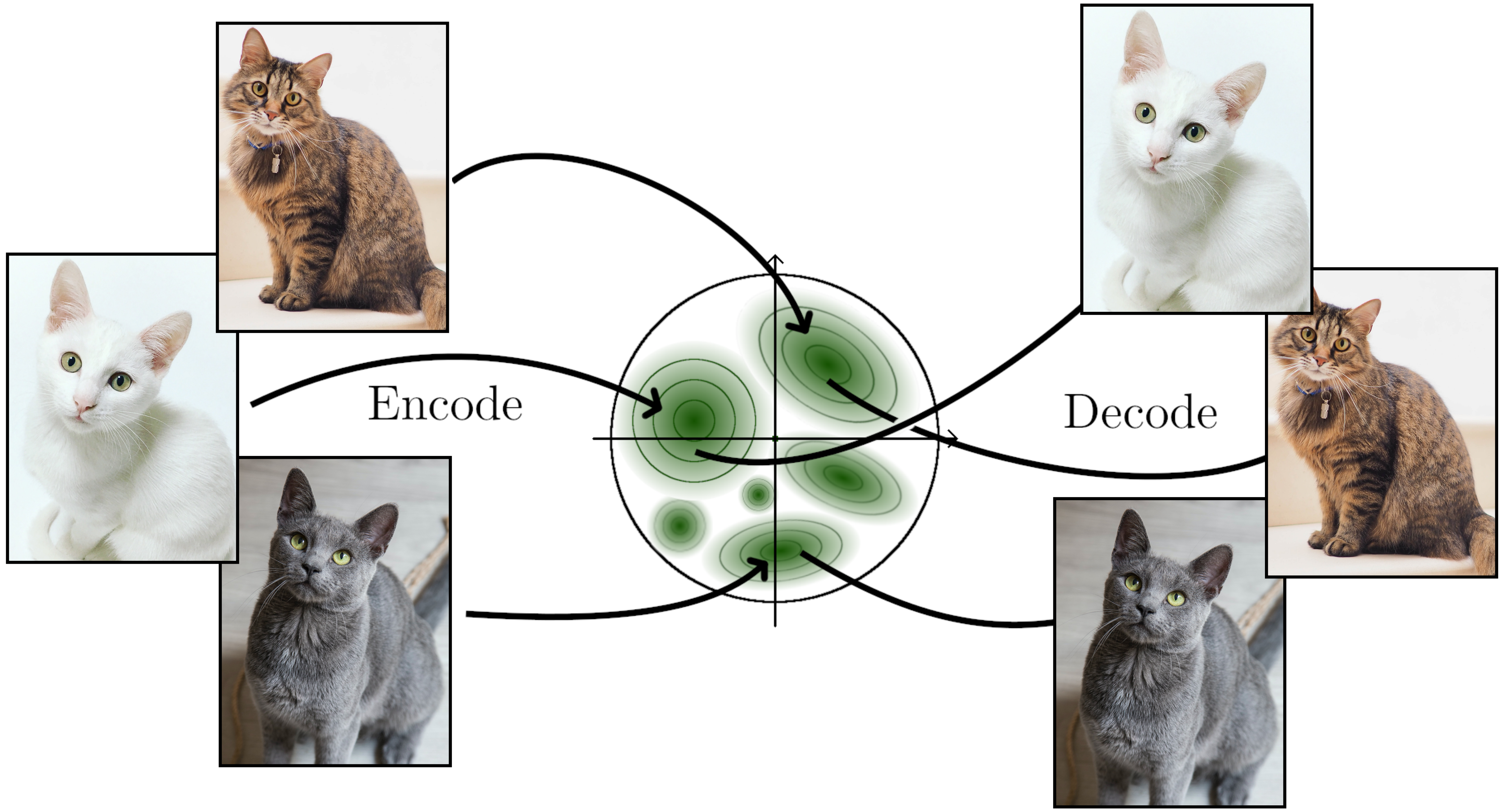

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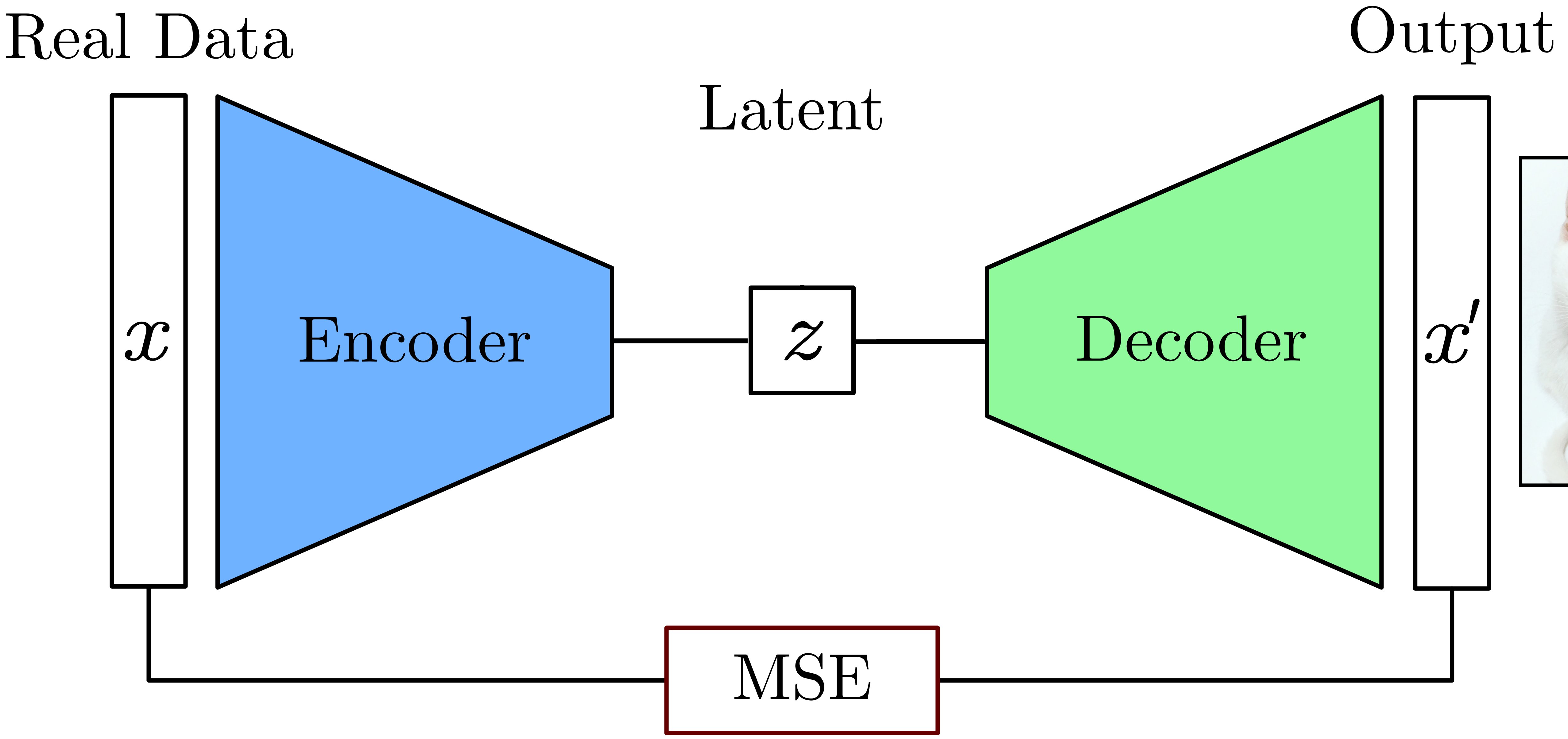
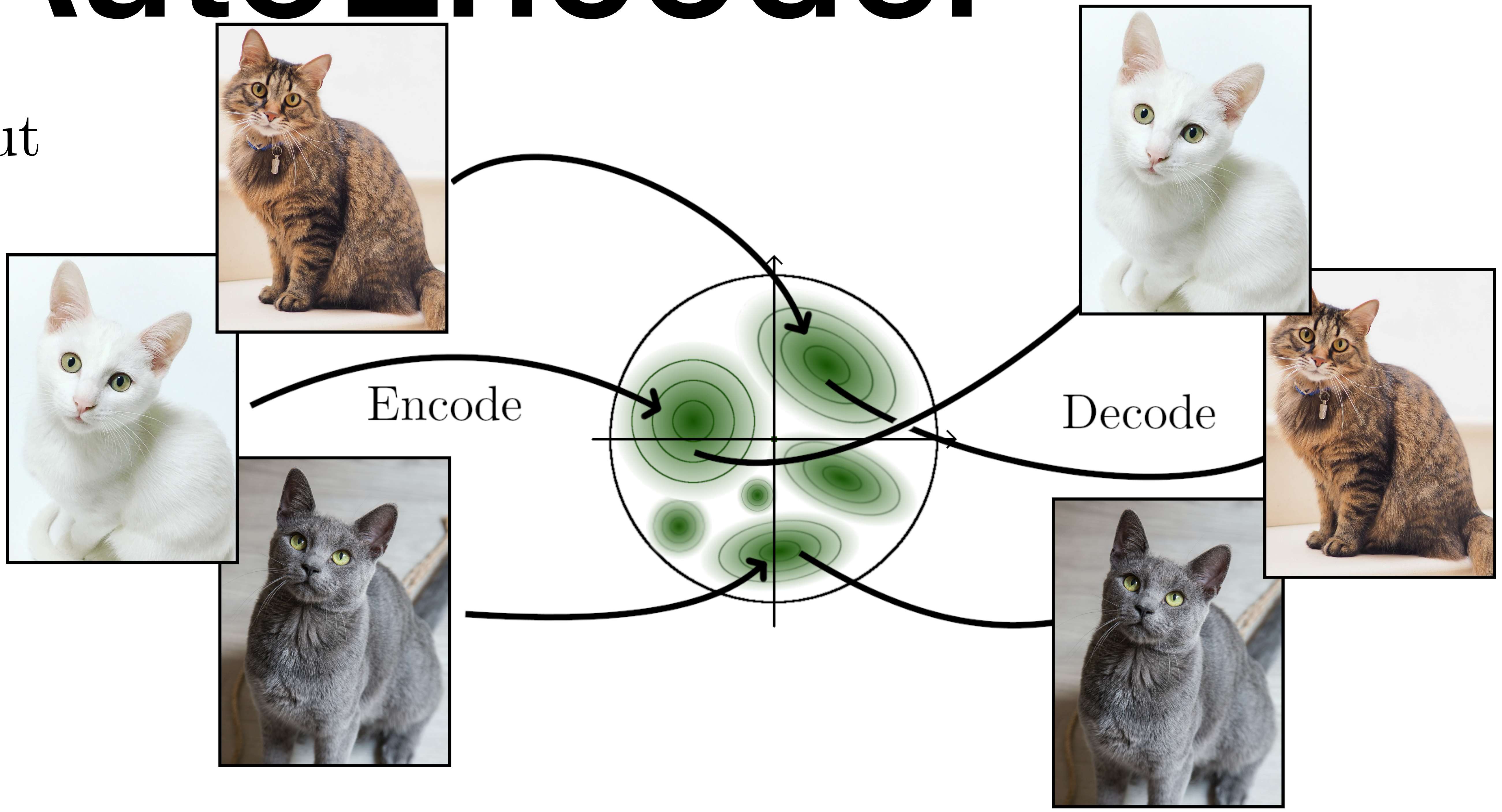
- Compare Input and Output pixel by pixel with mean squared error

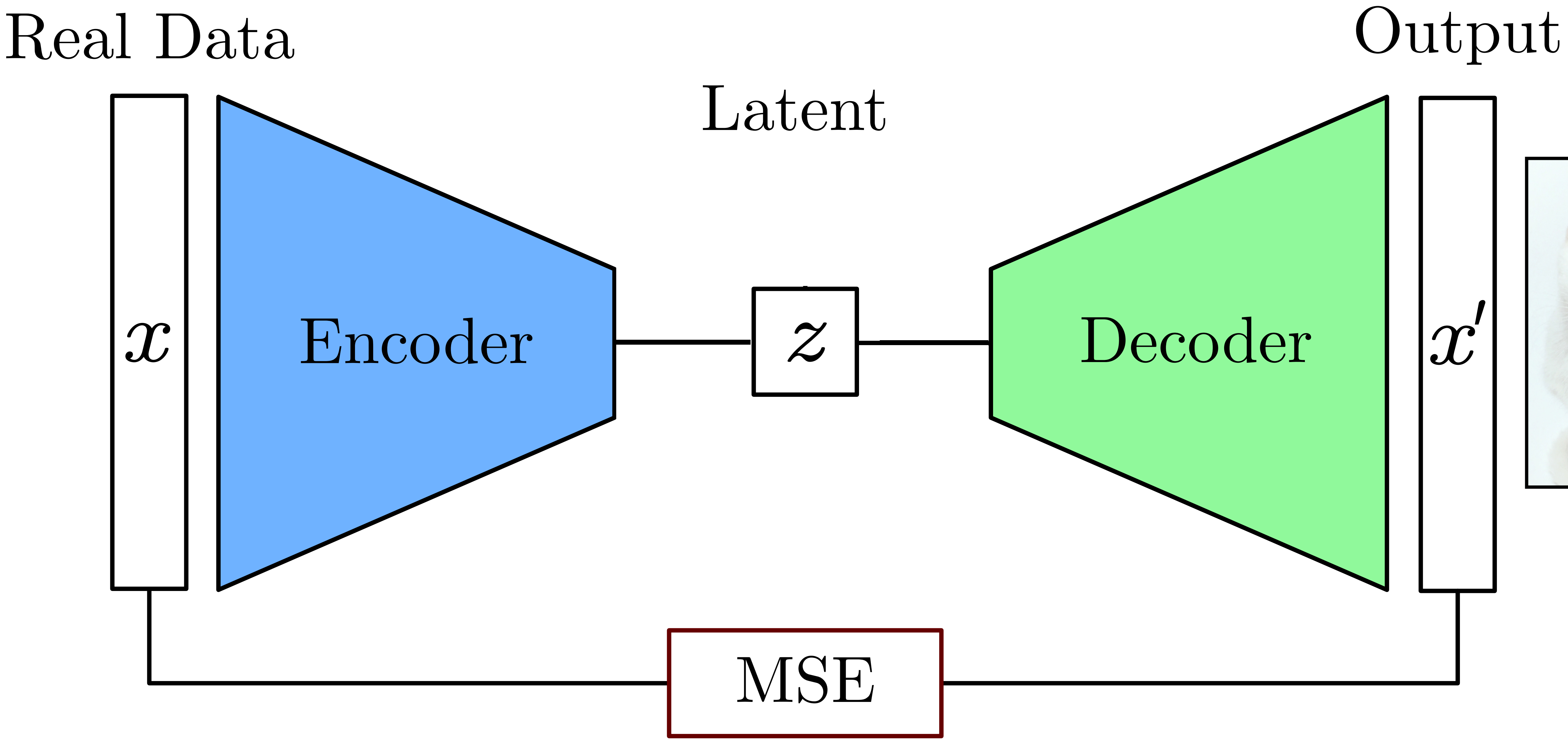
Variational AutoEncoder

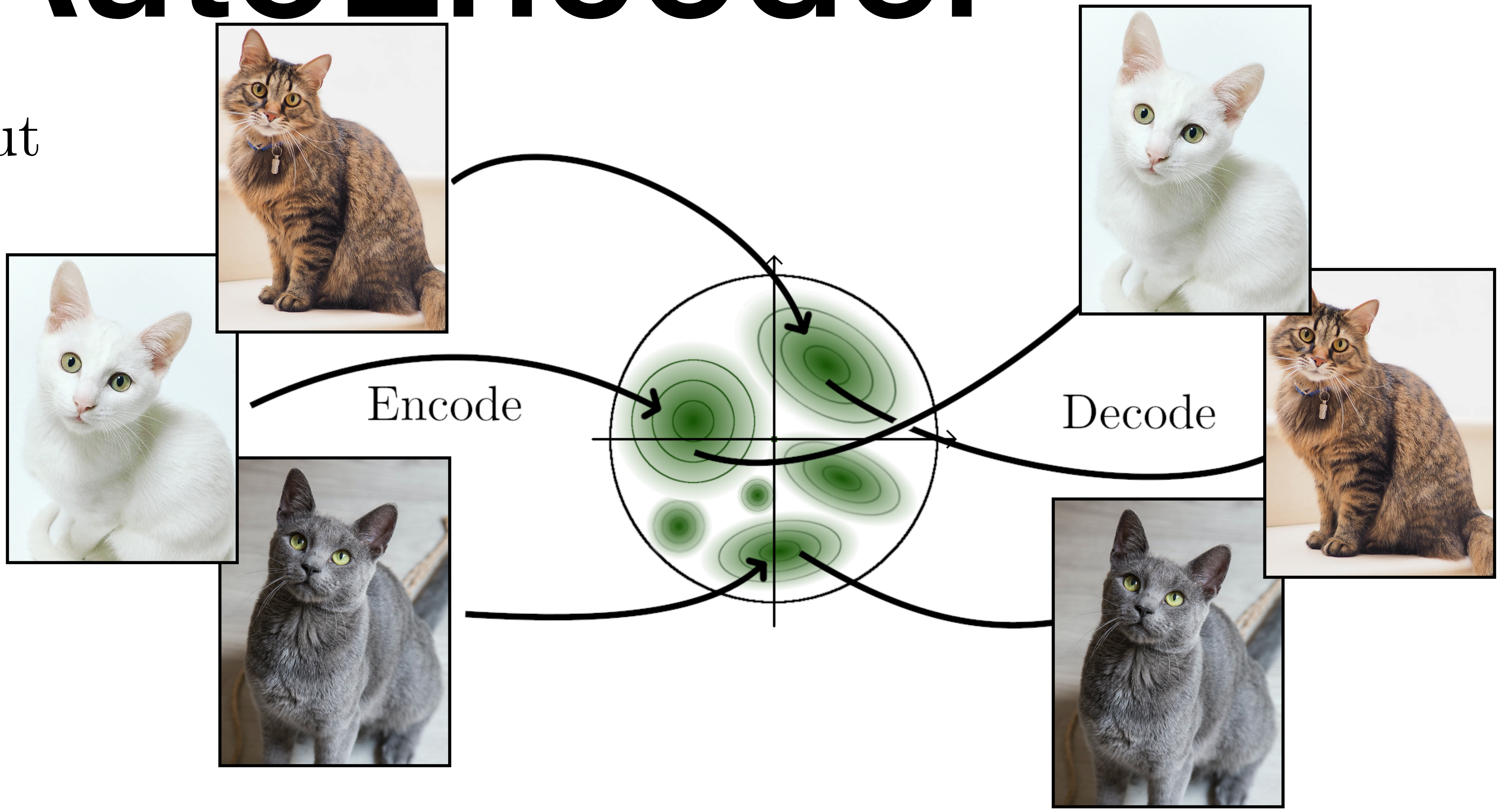




- Sample for Z and pass it to D(Z) ➡ Generate new samples

Variational AutoEncoder

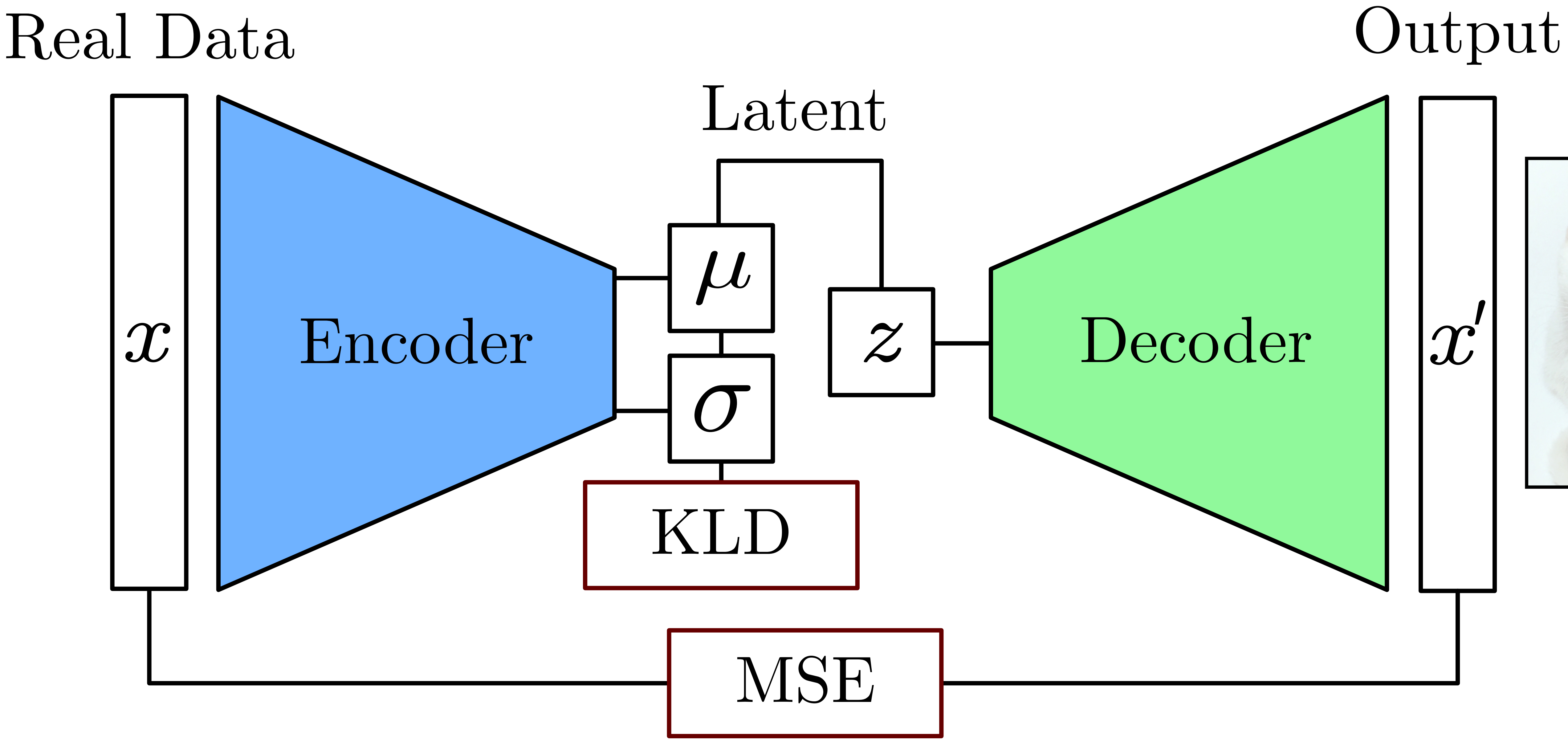


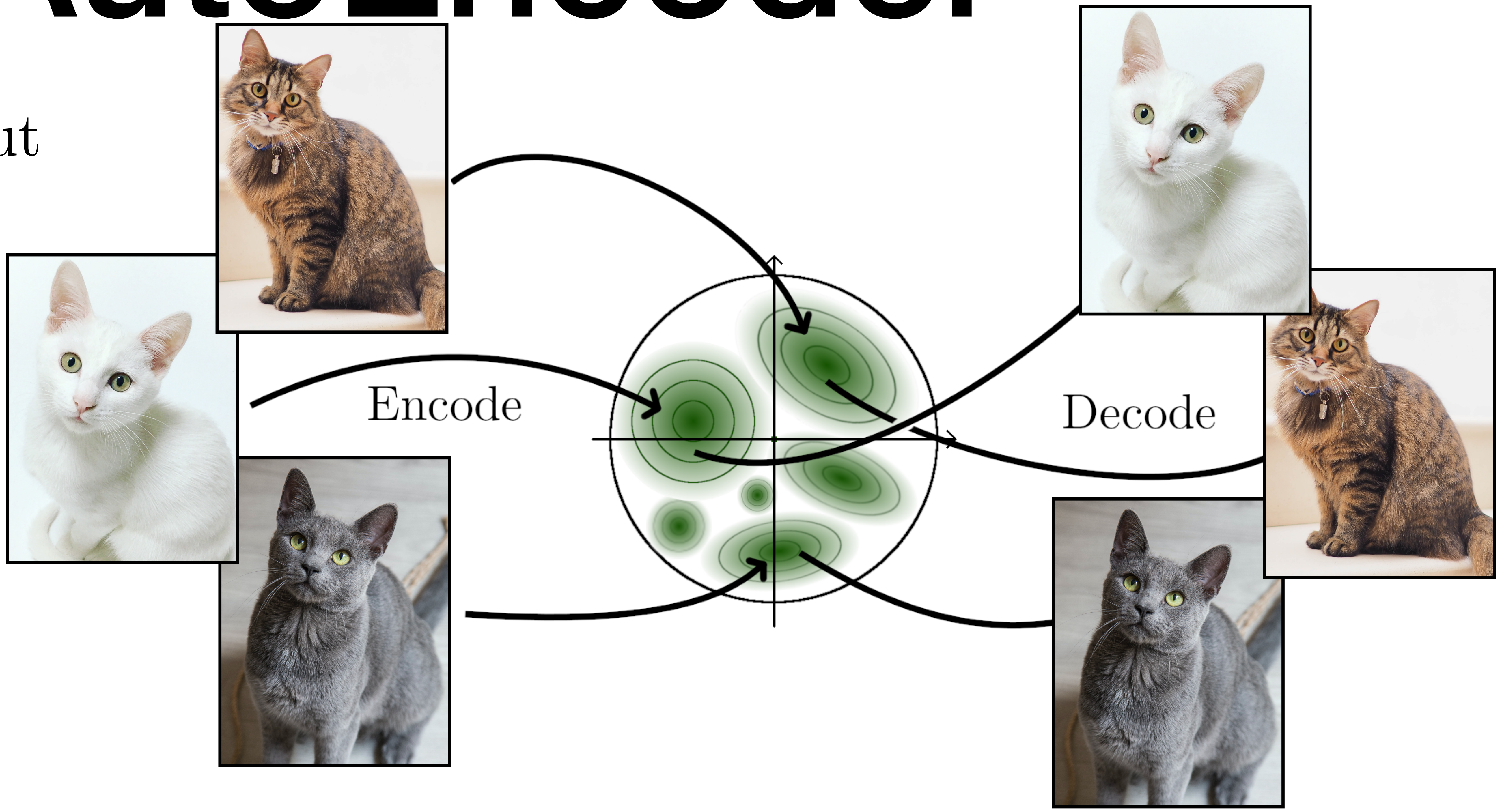


- Sample for Z and pass it to D(Z) ➡ Generate new samples
- Problem: Need regularised later space to sample form

➡ Variational AutoEncoder

Variational AutoEncoder





- Latent space: Series of Gaussians, regularised match N(μ=0, σ=1)
  - Using Gaussians lets us use Kullback–Leibler divergence

$$\sum_{i=1}^{n} \sigma_i^2+\mu_i^2-\log(\sigma_i)-1$$

  - Compare Input and Output again using MSE

Variational AutoEncoder

Upsides

- Directly evaluates log likelihood
- Stable in training

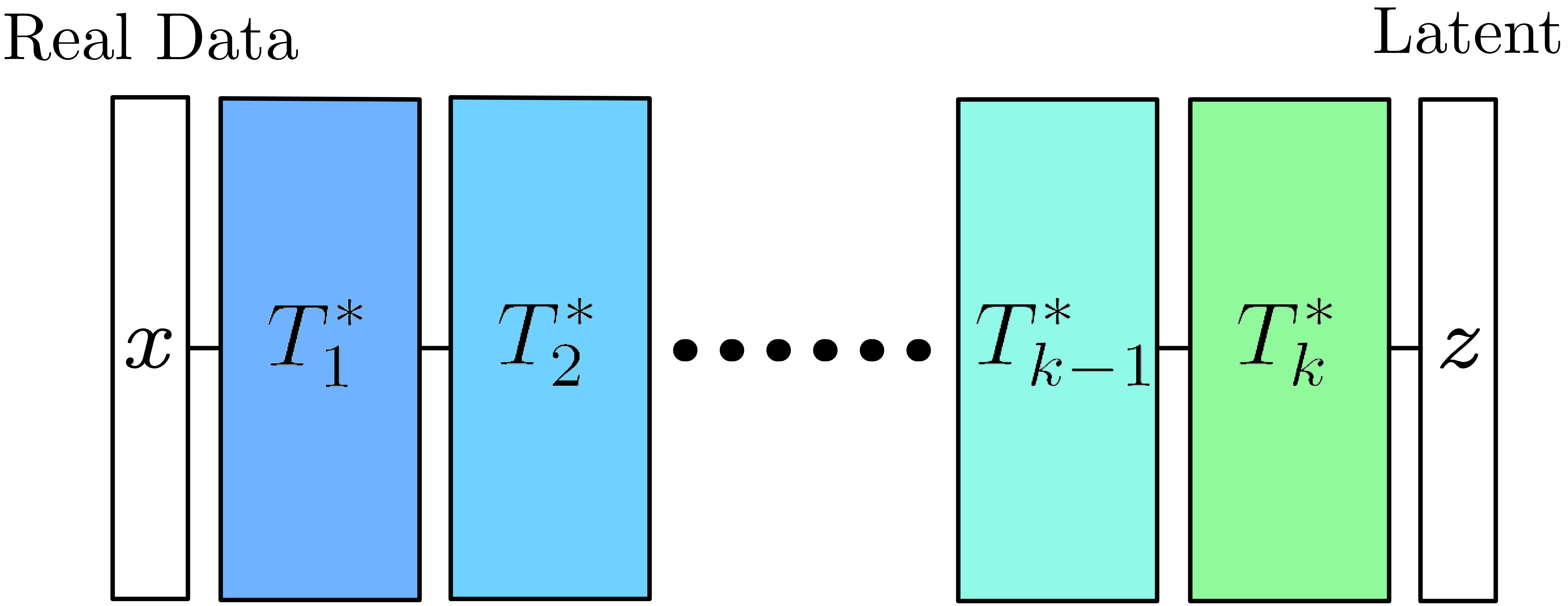
Difficulties

- MSE loss insufficient for certain data sets
- Needs to balance KLD and MSE loss terms

Normalizing Flows

- Variational AutoEncoder: map data to normal distribution and back using two networks
- Can we do this with a single network instead?

➡ Normalising Flow



Normalizing Flows

- Train invertible model T^{*-1} to map data to Normal distribution
- Well understood loss function:

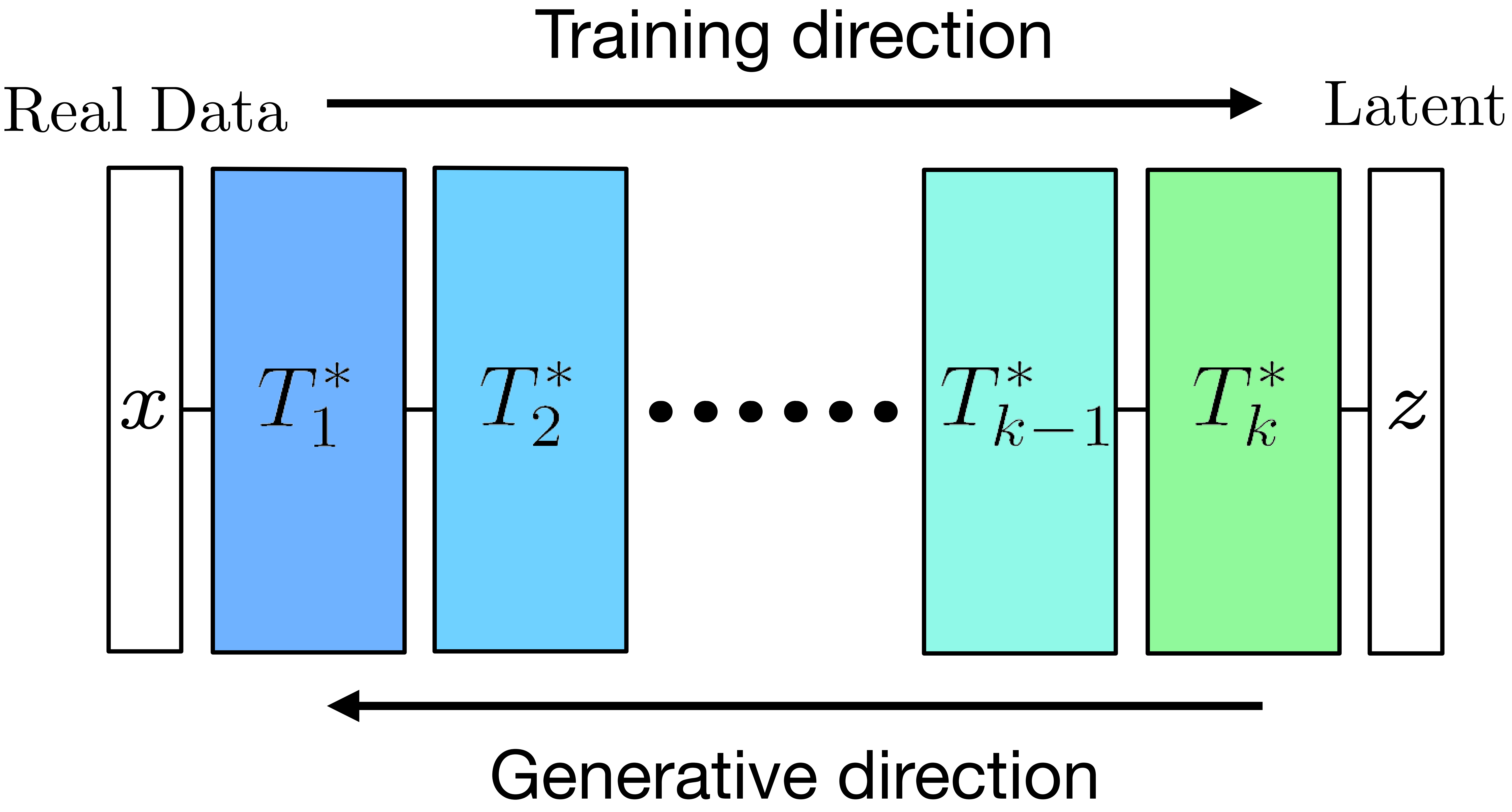
$$\mathcal{L}_{\text{Flow}} = \frac{1}{N}\sum_{n=1}^{N} \boxed{\log(p_z(T^{*-1}(\mathbf{x_n}, \theta)))} + \boxed{\log(|\det J_{T^{-1}}(\mathbf{x_n}, \theta)|)}$$

Latent Normal distribution

How well does the transformed sample match the latent distribution

Jacobean of transformation

Normalizing Flows



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Latent Normal distribution

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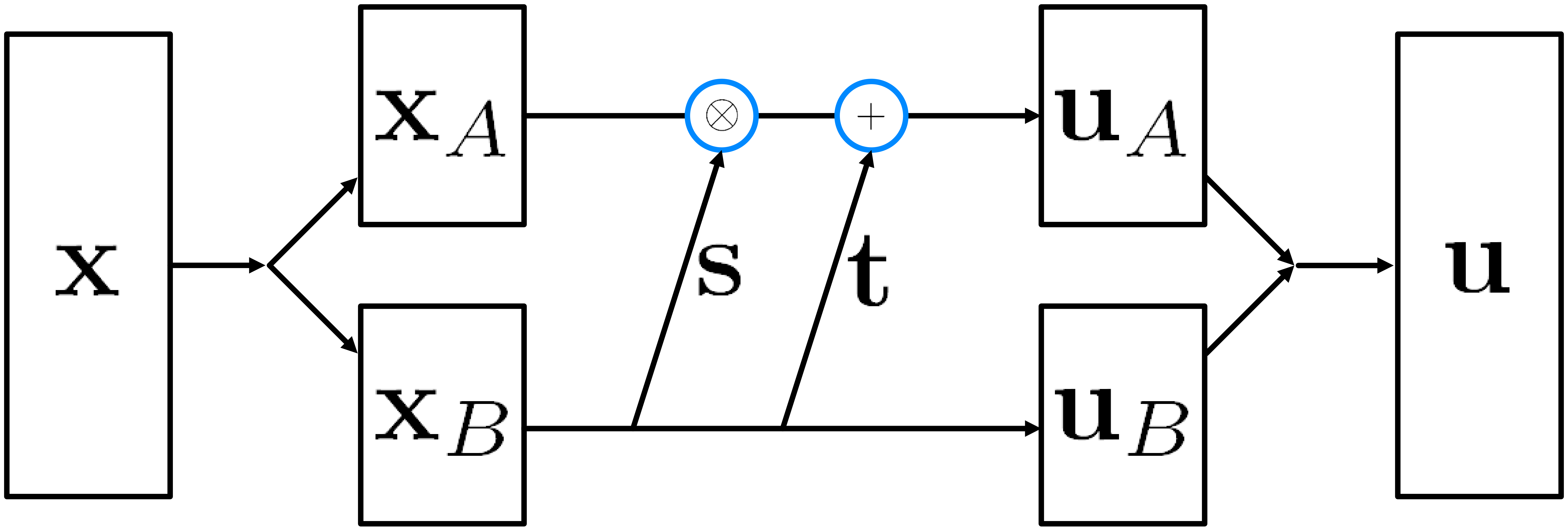
Jacobean of transformation

Invertible Neural Networks

- Dense layer: matrix multiplication
- Invertible if square matrix with det > 0
- Difficult in practice, use Coupling layers instead



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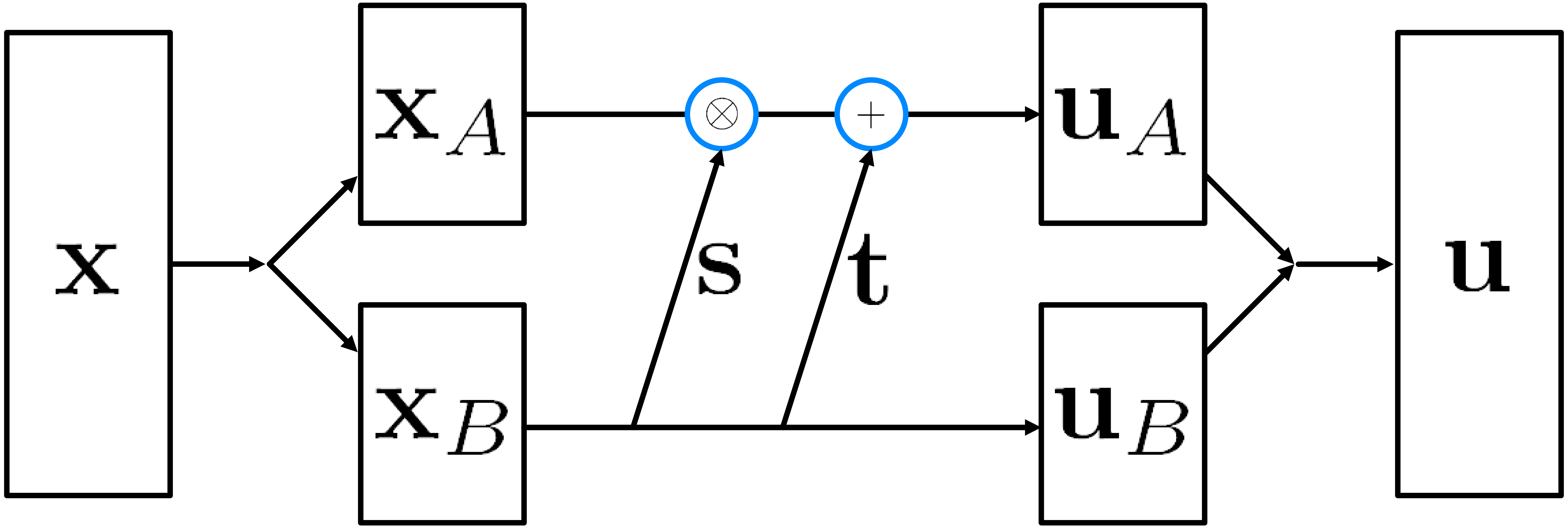
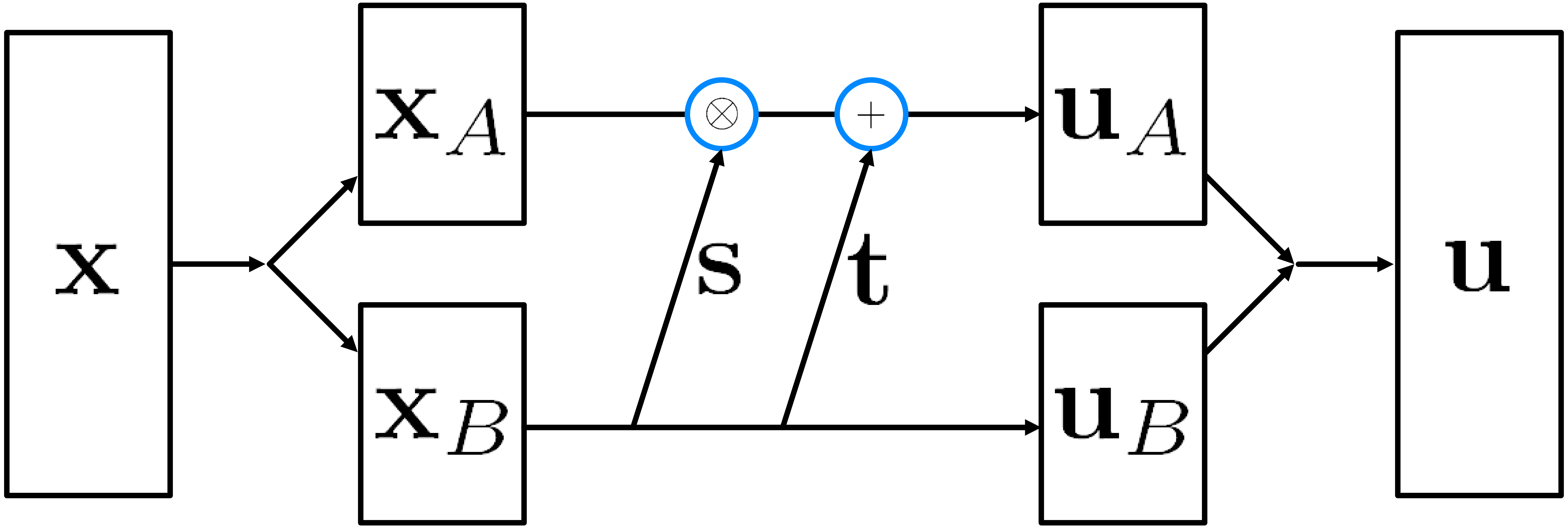


$$\mathbf{u}_A = \mathbf{x}_A \otimes \mathbf{s}(\mathbf{x}_B) + \mathbf{t}(\mathbf{x}_B)$$

$$\mathbf{u}_B = \mathbf{x}_B$$

Invertible Neural Networks



$$\mathbf{u}_A = \mathbf{x}_A \otimes \mathbf{s}(\mathbf{x}_B) + \mathbf{t}(\mathbf{x}_B)$$

$$\mathbf{u}_B = \mathbf{x}_B$$

$$\mathbf{x}_A = \frac{\mathbf{u}_A - \mathbf{t}(\mathbf{u}_B)}{\mathbf{s}(\mathbf{u}_B)}$$

$$\mathbf{x}_B = \mathbf{u}_B$$

Normalizing Flows

Upsides

- Directly evaluates log likelihood
- Stable in training
- High generative quality
- Easy to train and use

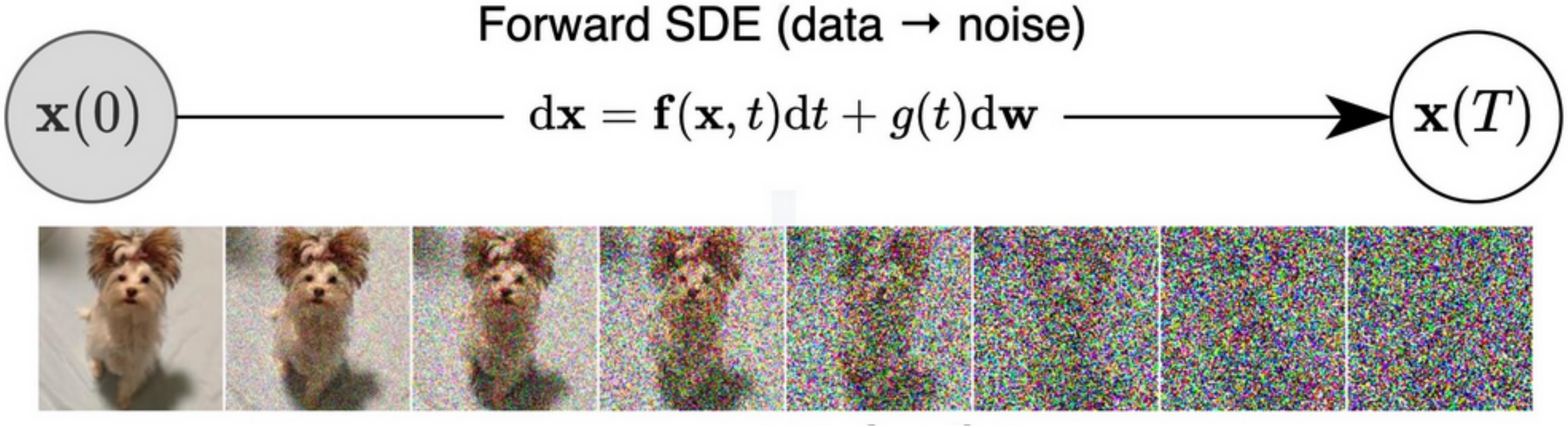
Difficulties

- Fixed dimensionality through entire flow
- Slow generation times for large models/data

Score-Based Models

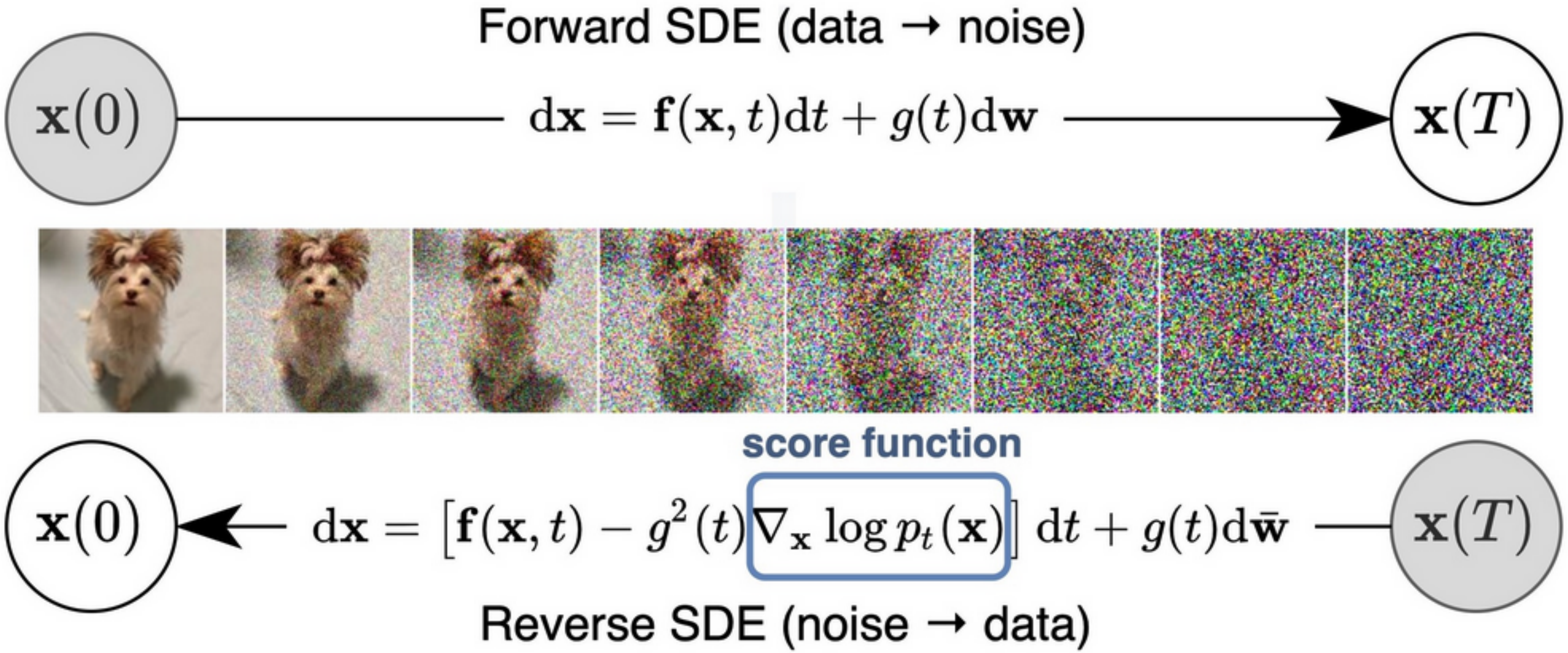
- Normalizing Flow: learn map of data to Normal distribution
- Do we need to explicitly learn this?
- Map data to Normal distribution by repeatedly adding noise

➔ Diffusion Models



Score-Based Models

- Repeatedly add noise to data point
- Learn to undo noise at every step
- Possible using Stochastic Differential Equation and score function



Score-Based Models

- Approximating the score function of the data
- Equivalent to approximating the score function of a smearing func.

Score func.

$$\frac{1}{2}\mathbb{E}_{p(\mathbf{x})}\left[\|\mathbf{s}_\theta(\mathbf{x},t) - \nabla_\mathbf{x} \log p(\mathbf{x})\|_2^2\right].$$

Score func. of smearing

$$\frac{1}{2}\mathbb{E}_t\mathbb{E}_{p_t(x)}\left[\lambda(t)\,\|\mathbf{s}_\theta(\mathbf{x_t},t) - \nabla_{\mathbf{x_t}} \log p_t(x_t|x_0)\|_2^2\right]$$

For gaussian smearing

$$\nabla_{\tilde{\mathbf{x}}} \log p_\sigma(\tilde{\mathbf{x}}|\mathbf{x}) = \frac{\mathbf{x}-\tilde{\mathbf{x}}}{\sigma^2} \sim \frac{\mathcal{N}(0,1)}{\sigma}$$

Score-Based Models

Upsides

- Superior generation quality
- State of the Art for generative models

Difficulties

- Conceptually complex
- Difficult to train for non-standard data-sets

Physics Use Cases

Generative Models can

- Learn underlying distribution from a given dataset
- Quickly sample from learned distribution

What HEP uses can such models have?

- Fast simulation

Physics Use Cases

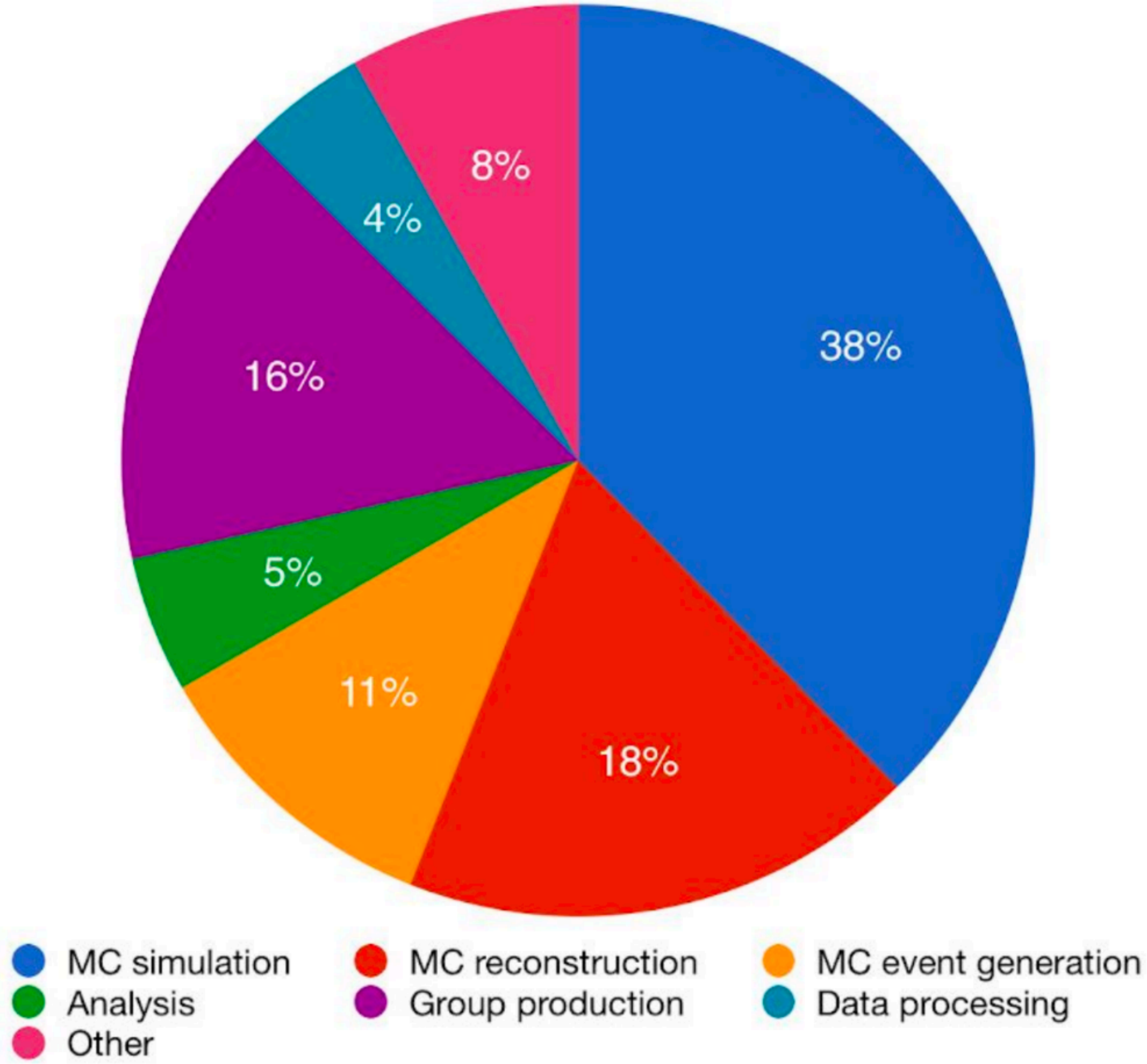
Generative Models can

- Learn underlying distribution from a given dataset
- Quickly sample from learned distribution

What HEP uses can such models have?

- Fast simulation
- Anomaly detection
- Many more!

Generative Simulation



- MC simulation large part of computing
- Speed up:
  - Train ML model on small dataset
  - Draw majority of samples form ML model

    ➔ Amplify original data set

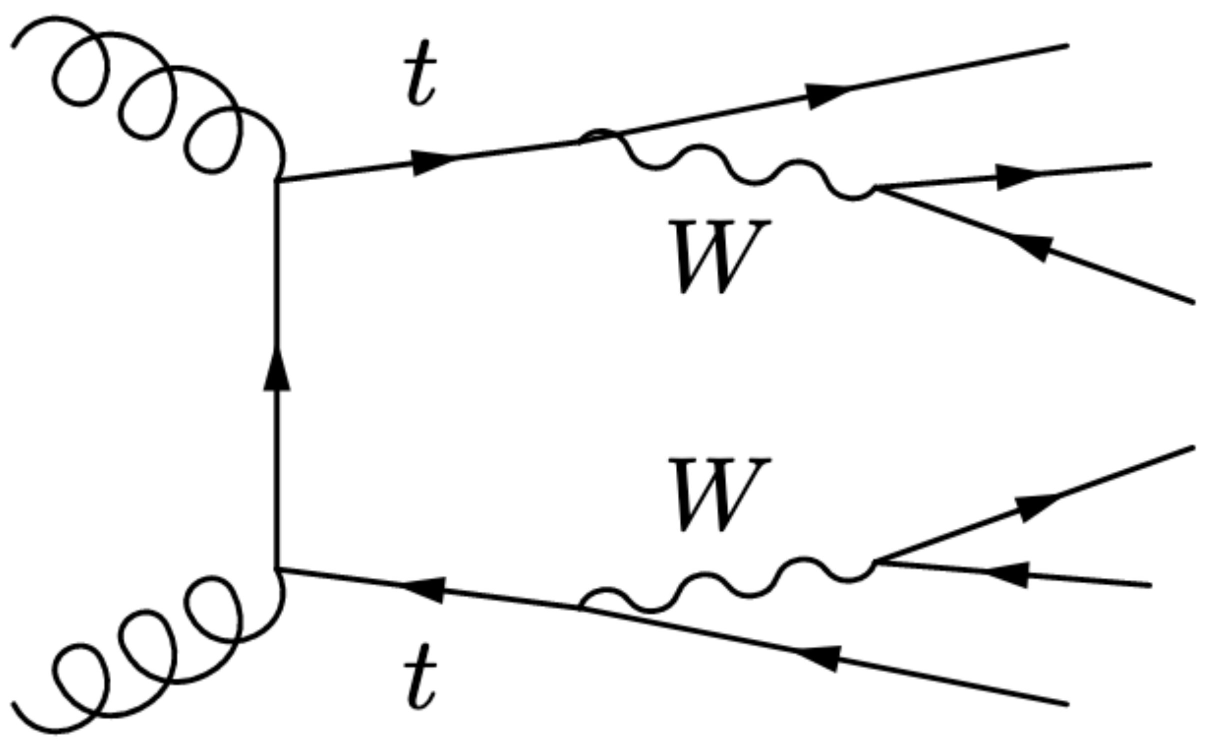
    ➔ Significantly faster

Catmore et. al. **ATLAS HL-LHC Computing Conceptual Design Report,** [CERN-LHCC-2020-015 ; LHCC-G-178]()

Butter et al.: **Amplifying Statistics using Generative Models:** NeurIPS ML4PS 2020, [2008.06545]()

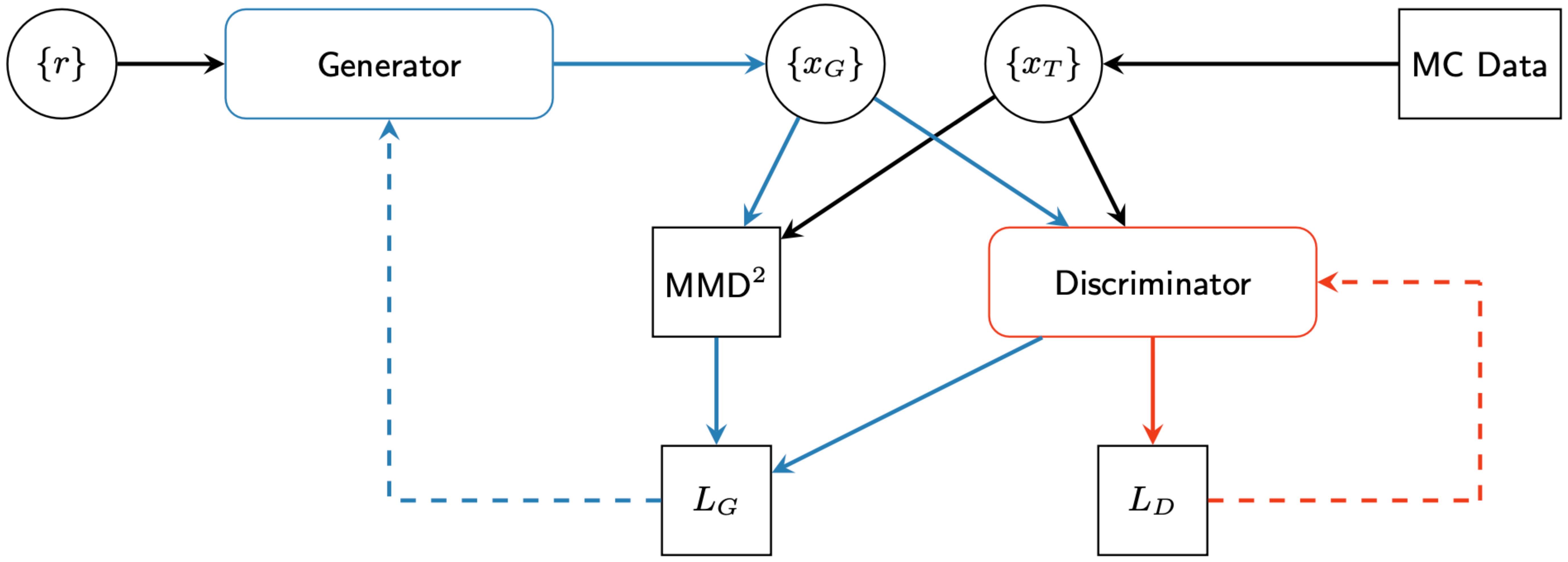
Generative Simulation

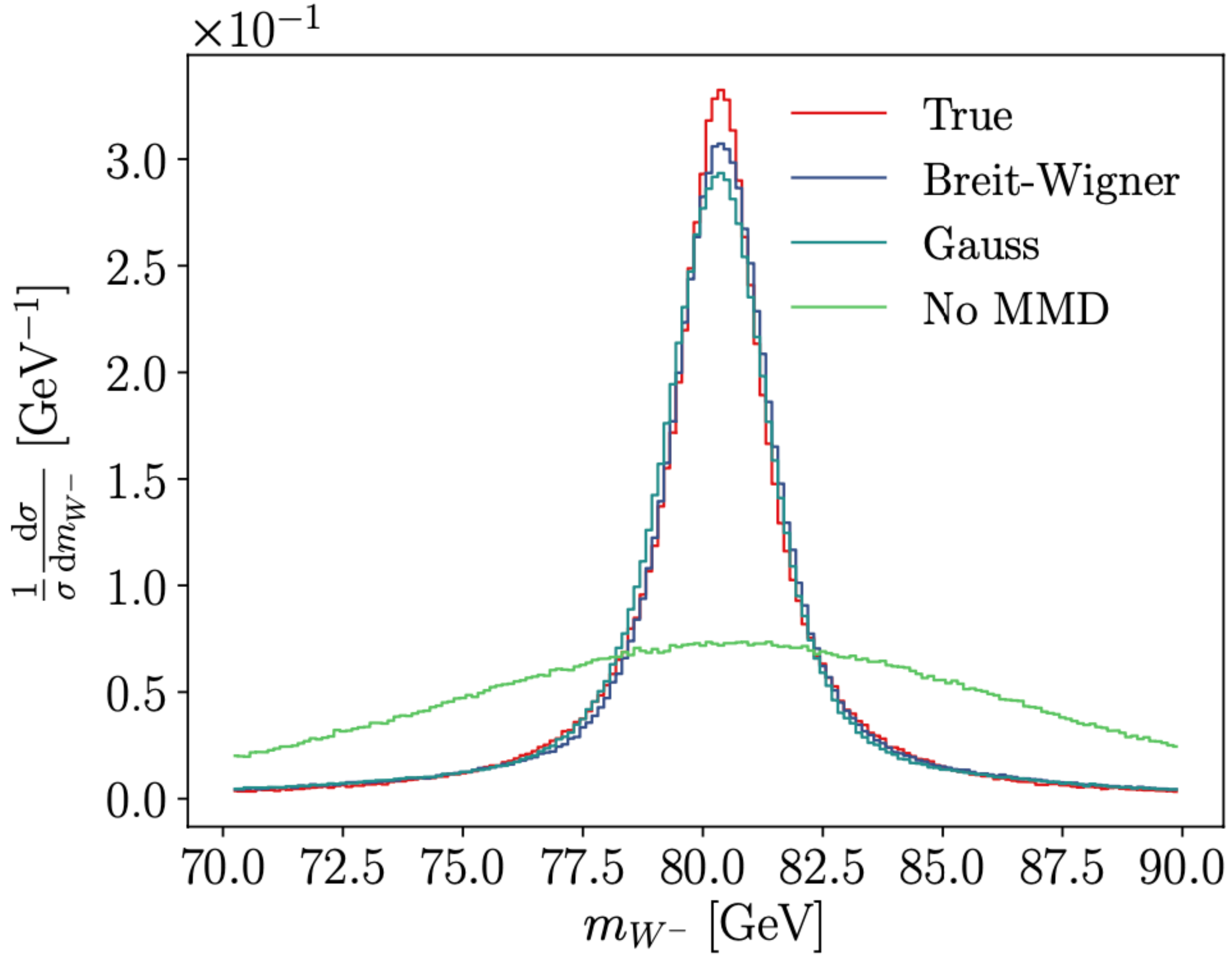
Event Generation



Event Generation

- Generation of event 4-momenta, ordered list, O(10) dimensions
- Using GAN model with additional MMD loss for mass peaks

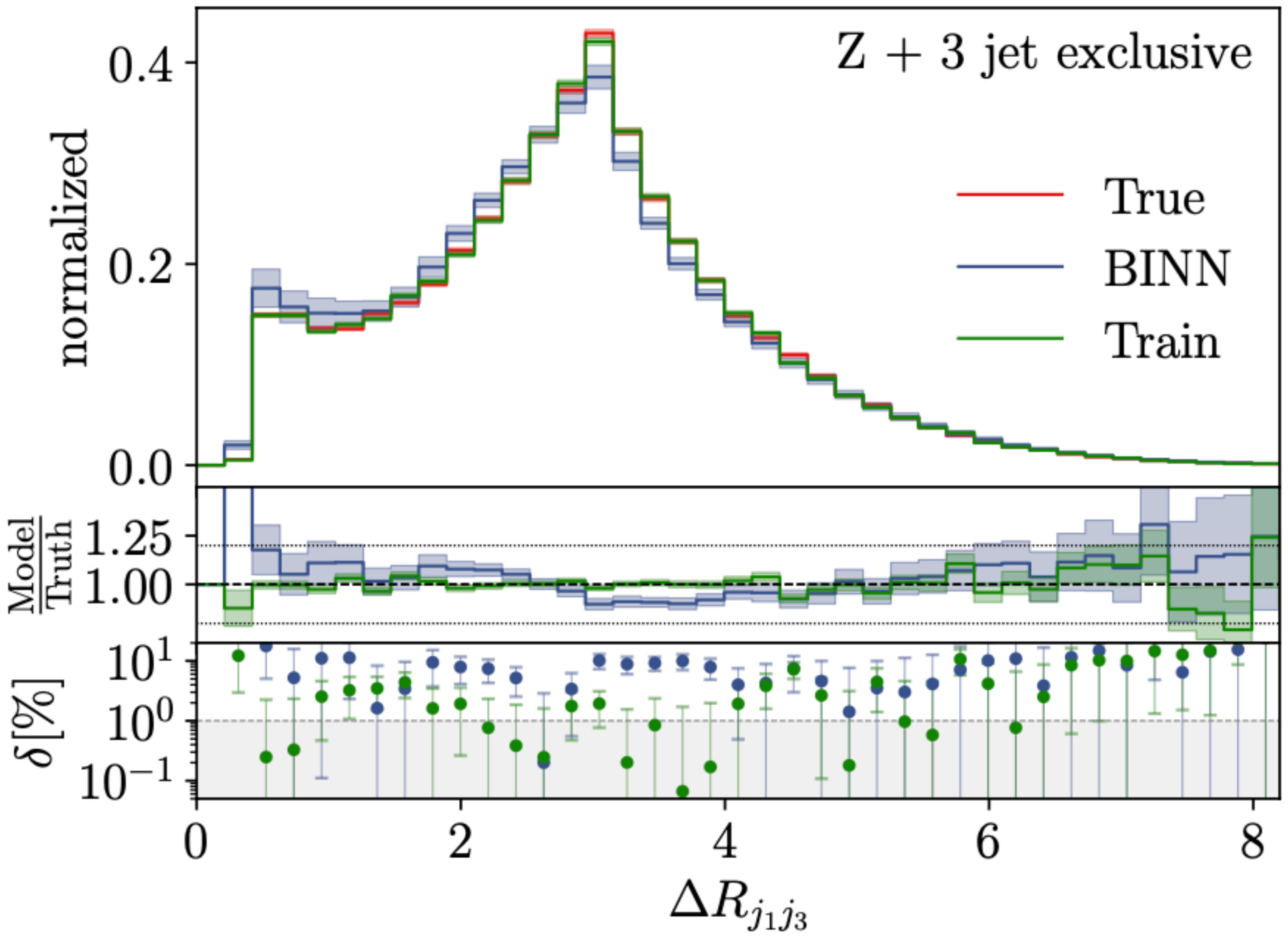


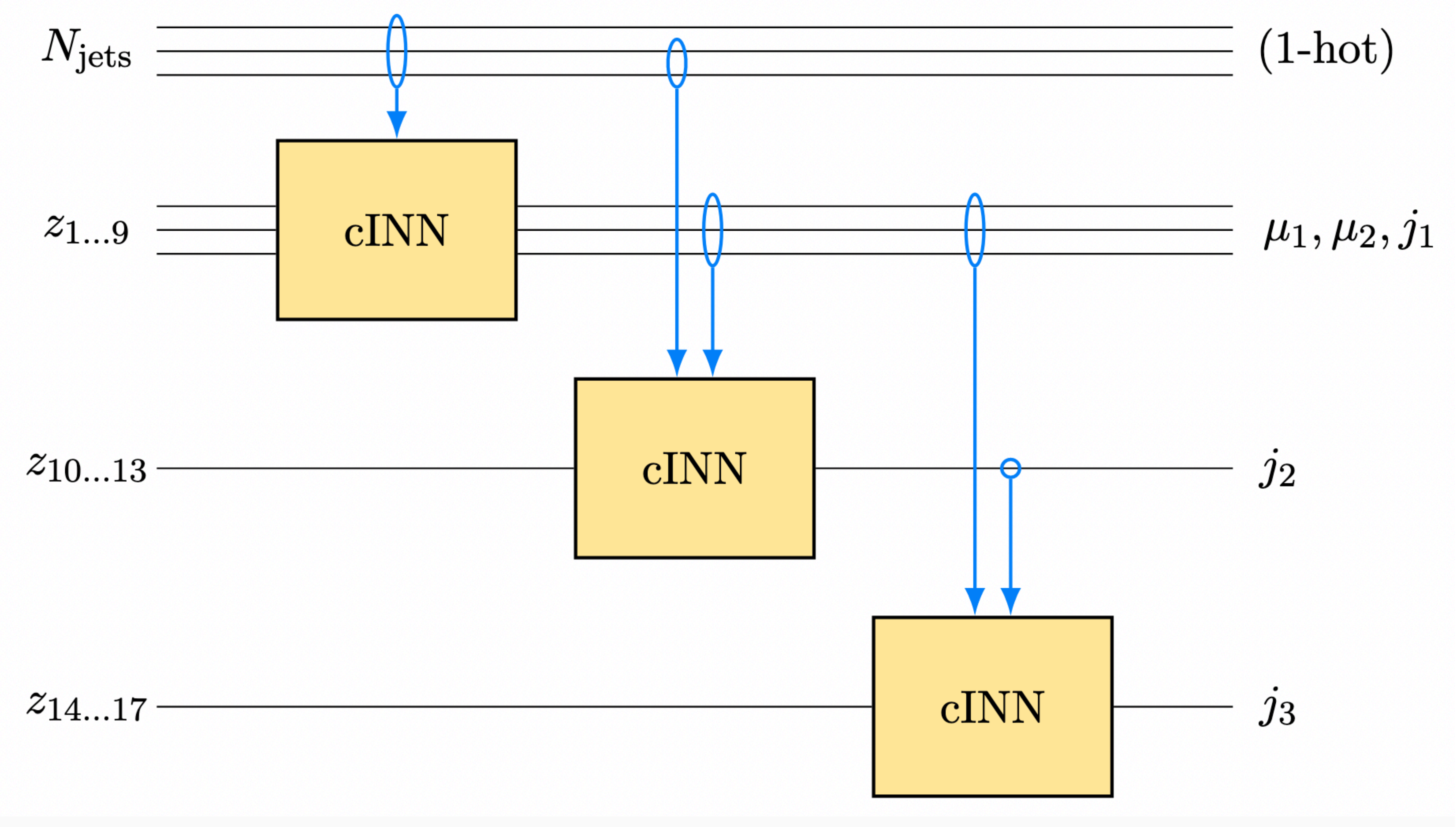


Butter et al.: **How to GAN LHC Events:** (2019), [1907.03764]

Event Generation

- Normalizing flow approach improves precision
- Bayesian network enables uncertainty estimation

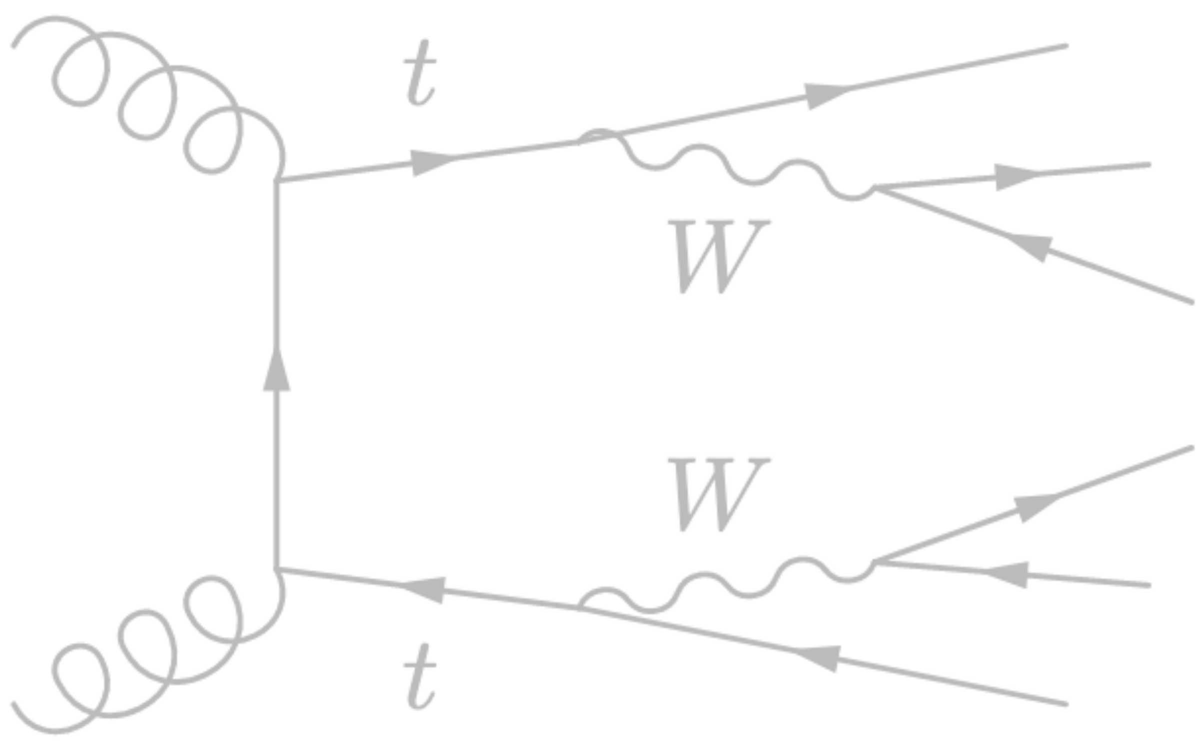




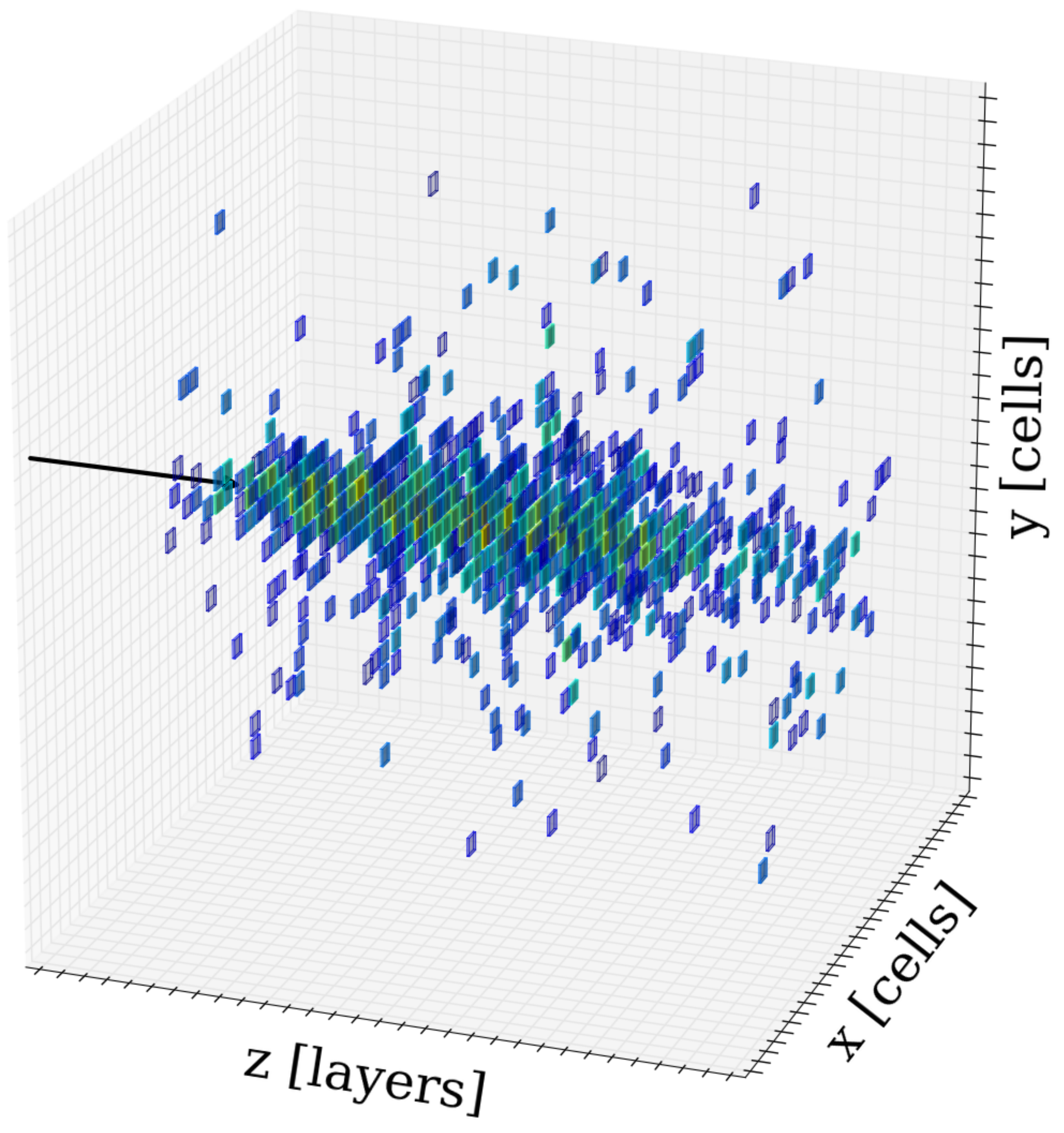
Butter et al.: **Generative Networks for Precision Enthusiasts** (2021), 2110.13632

Generative Simulation

Event Generation

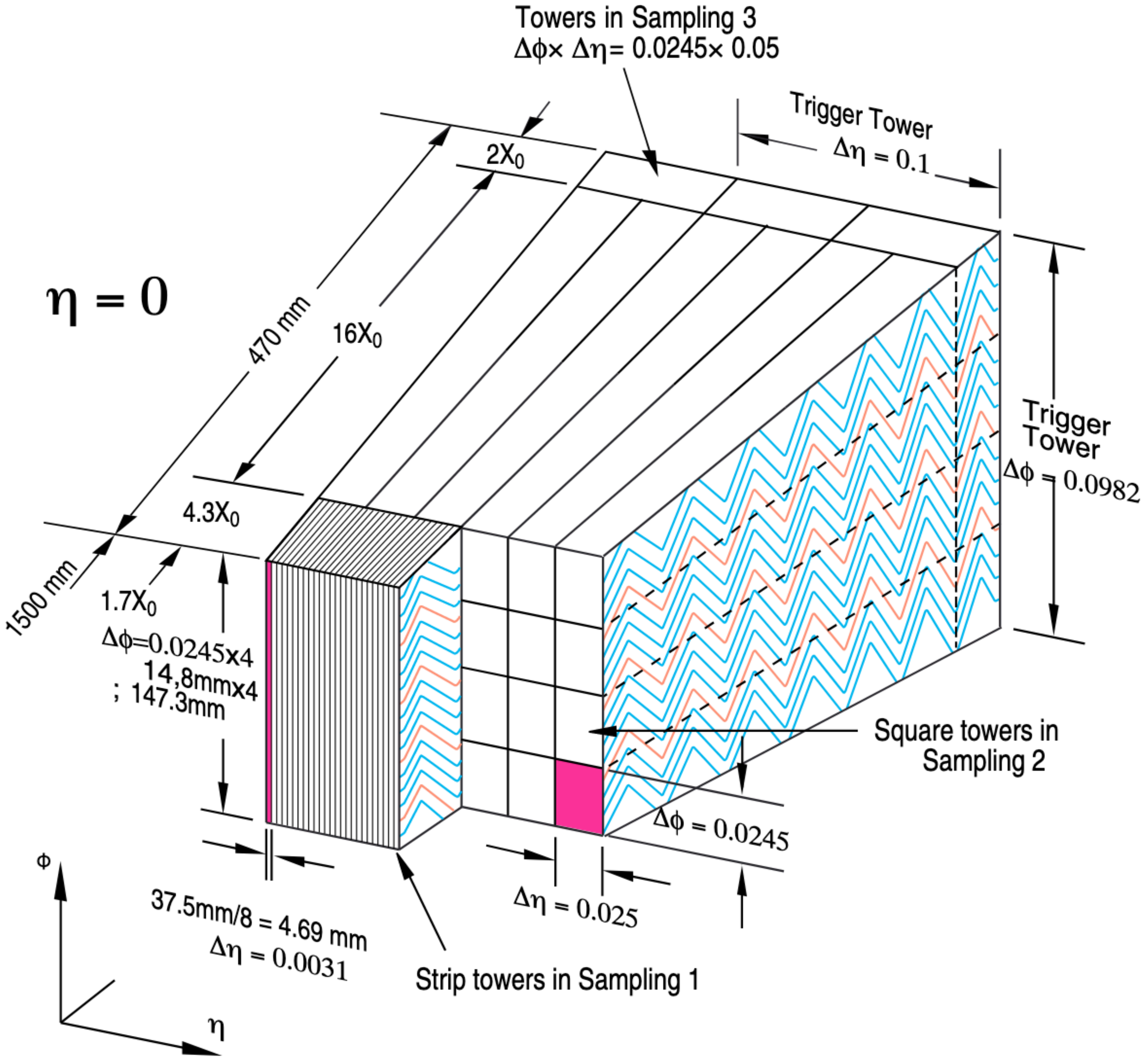


Detector Simulation



Detector Simulation

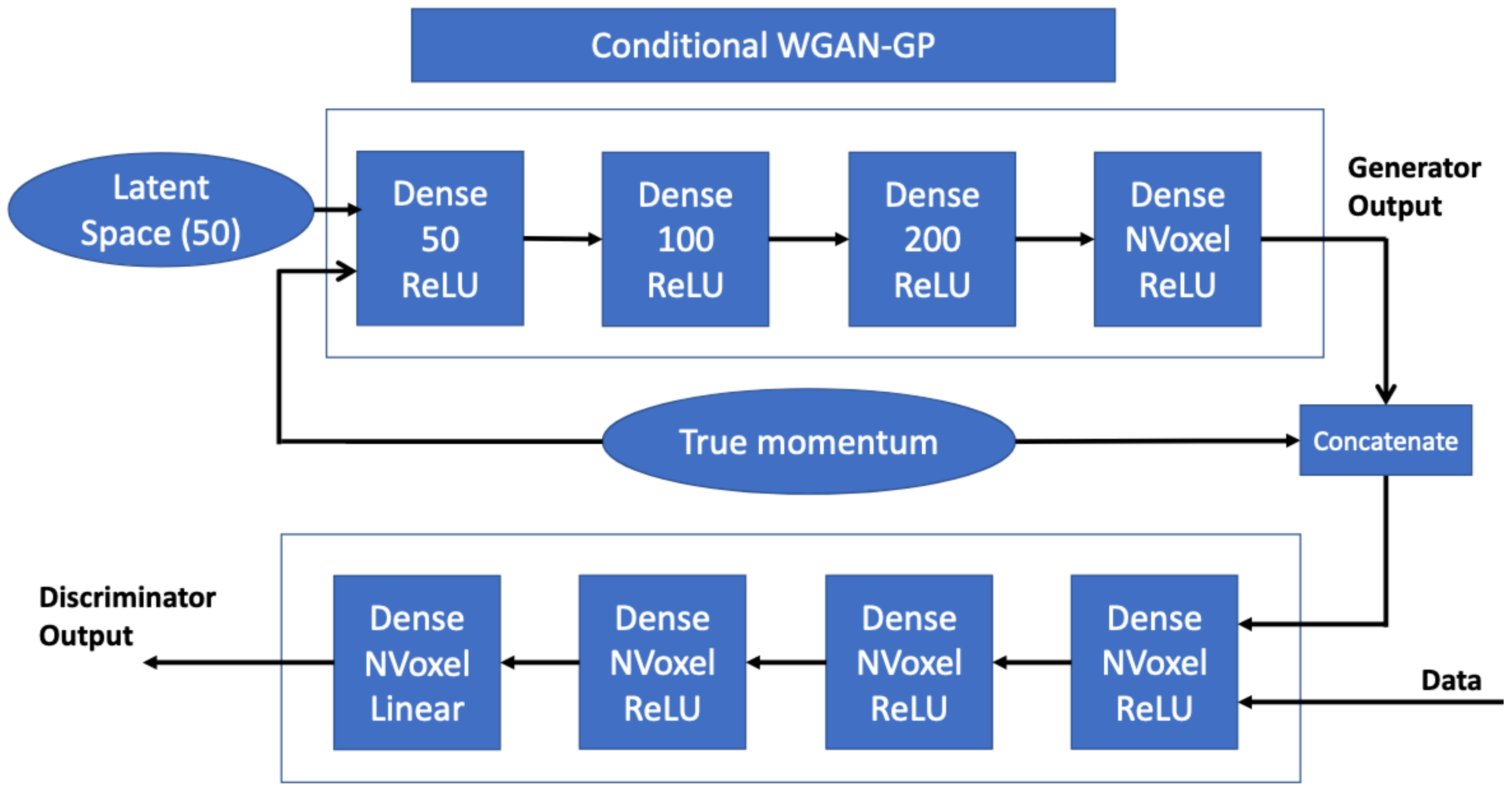
- Fixed output geometry O(100-10,000) dimensions
- Common in detector simulation, e.g. ATLAS FastCaloGAN
- Already in use for fast simulation of calorimeter showers

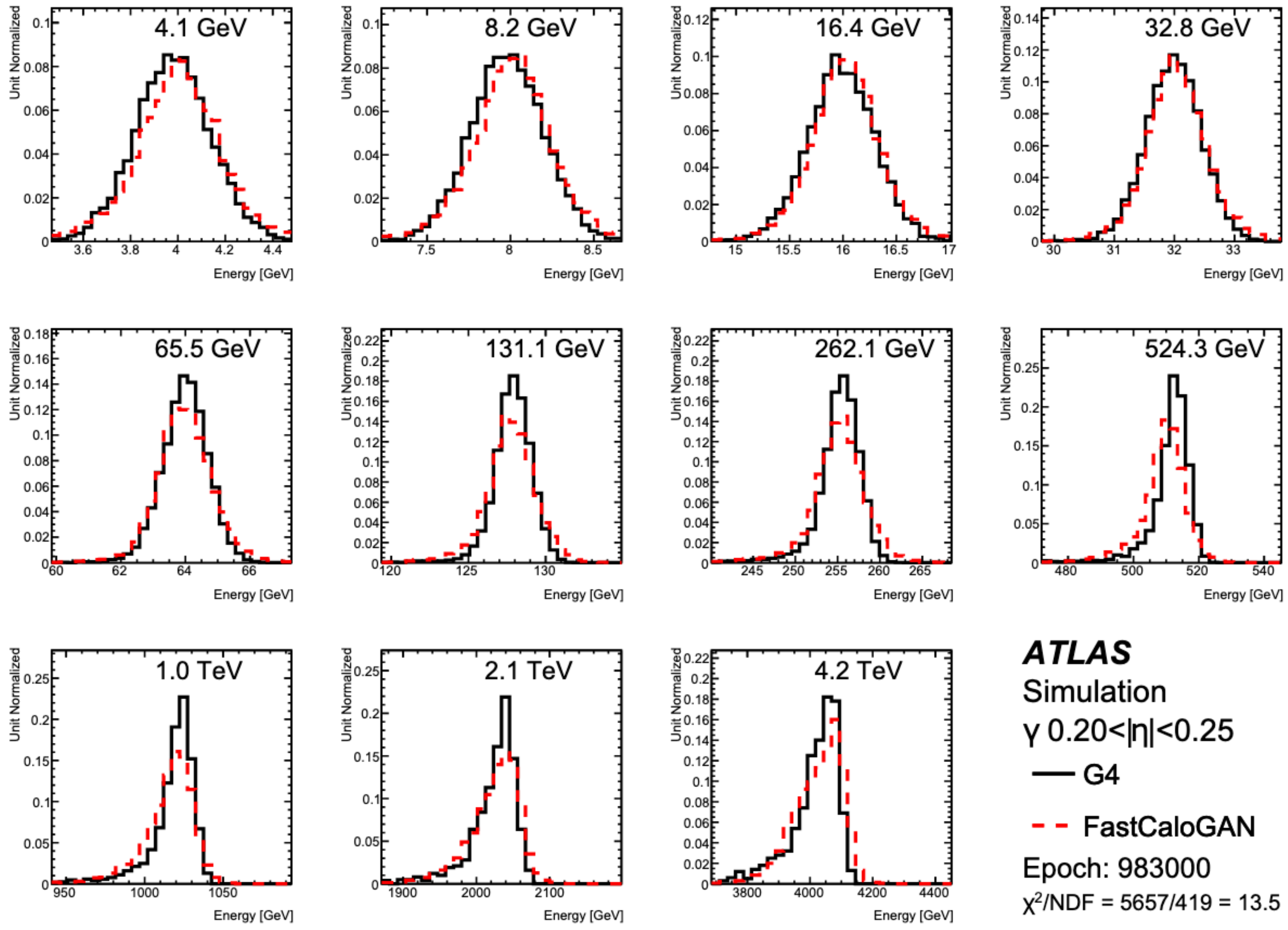


ATLAS Collaboration, **AtlFast3: the next generation of fast simulation in ATLAS** (2021), [2109.02551]

Detector Simulation

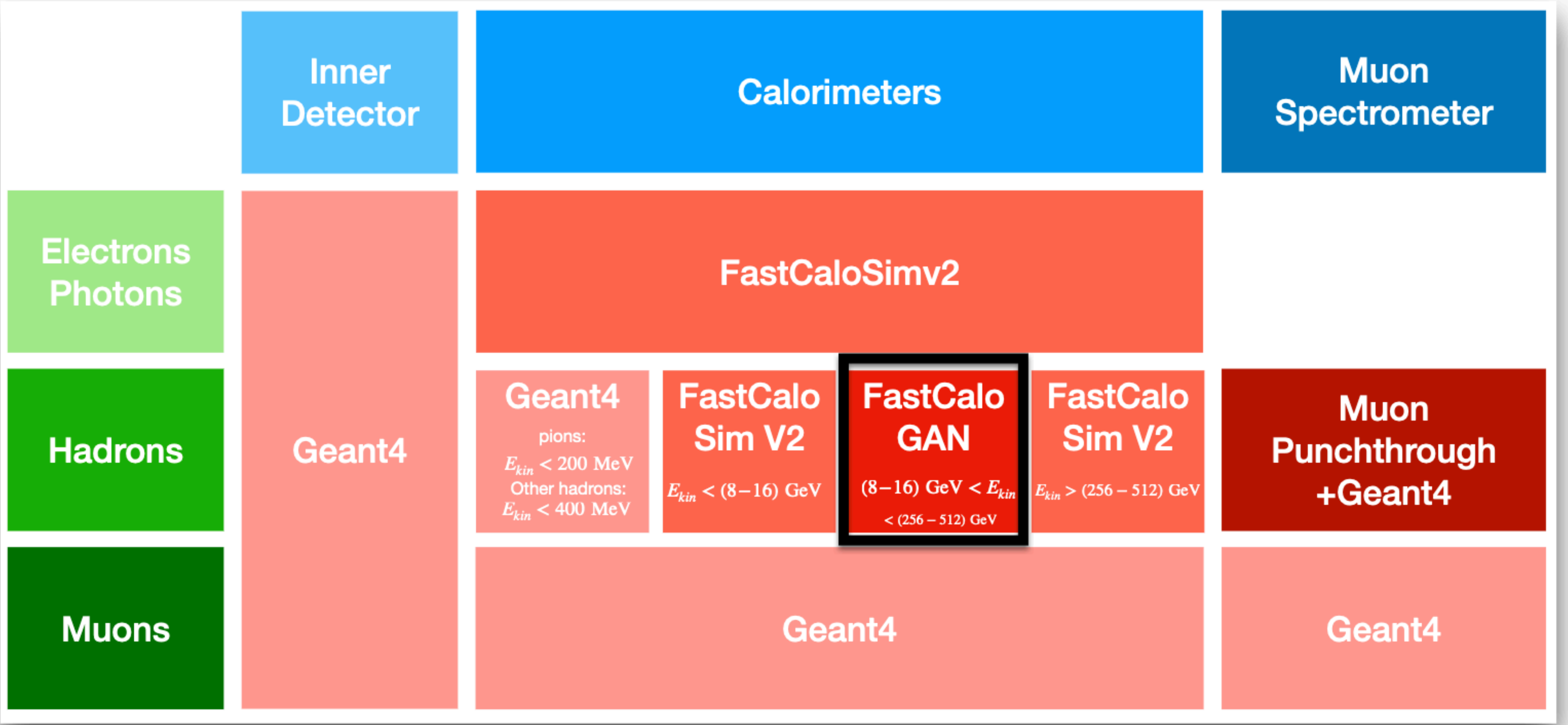
- ATLAS FastCaloGAN
- 300 total networks for particle types and η slices





ATLAS Collaboration, **AtlFast3: the next generation of fast simulation in ATLAS** (2021), [2109.02551](2109.02551)

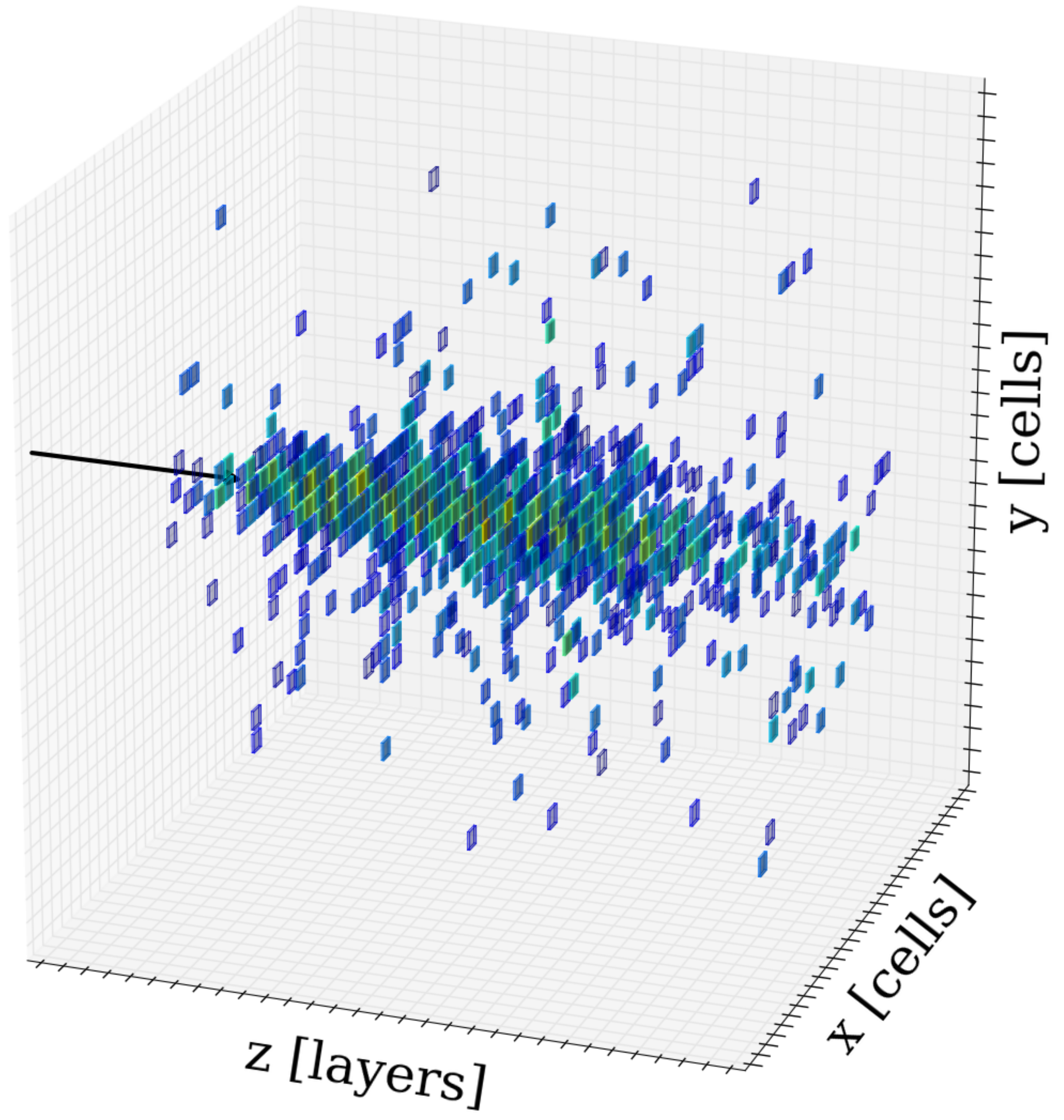
Detector Simulation



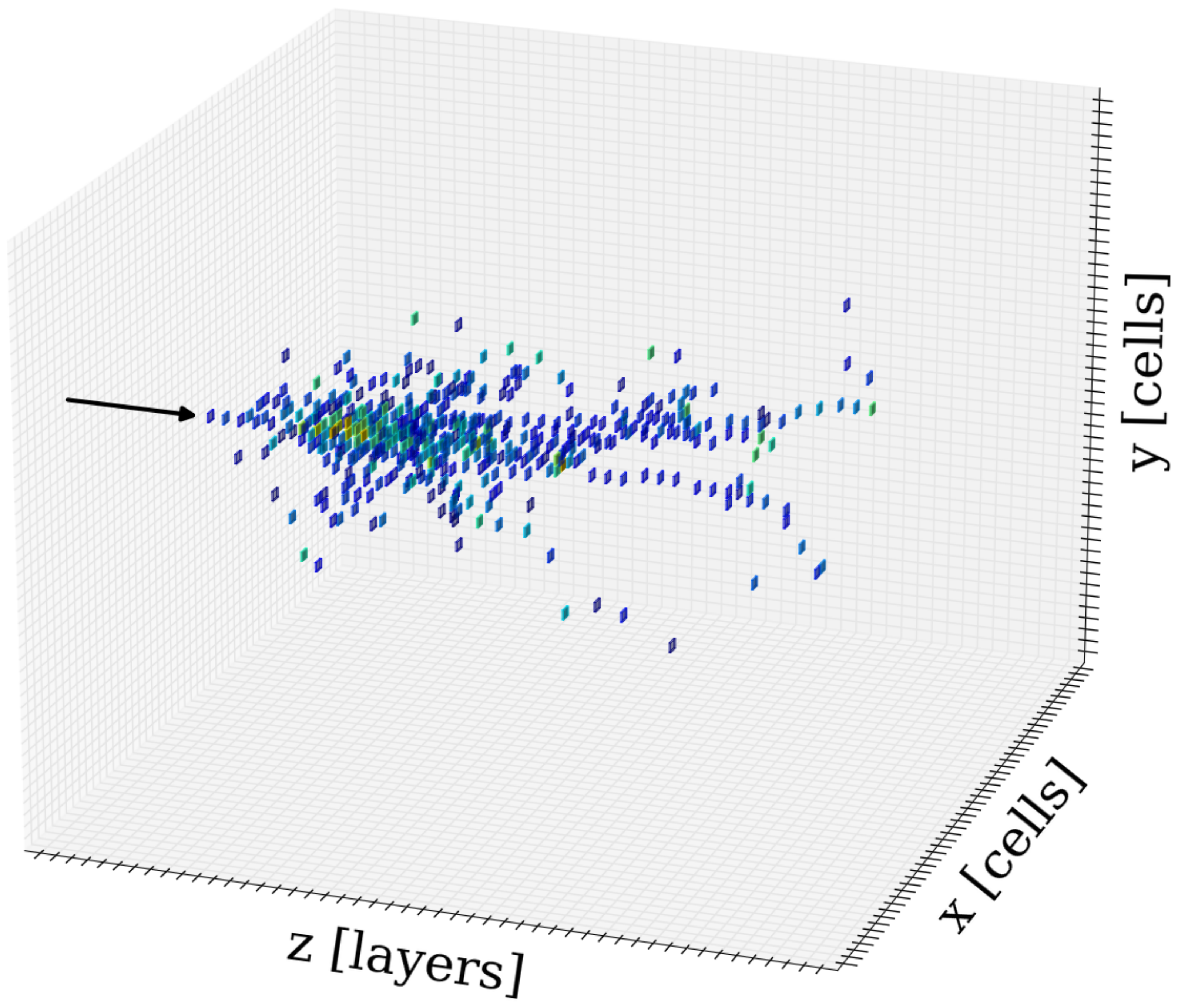
ATLAS Collaboration, **AtlFast3: the next generation of fast simulation in ATLAS** (2021), 2109.02551

High Granularity Calorimeter

Photon shower



Charged pion shower



Training data:

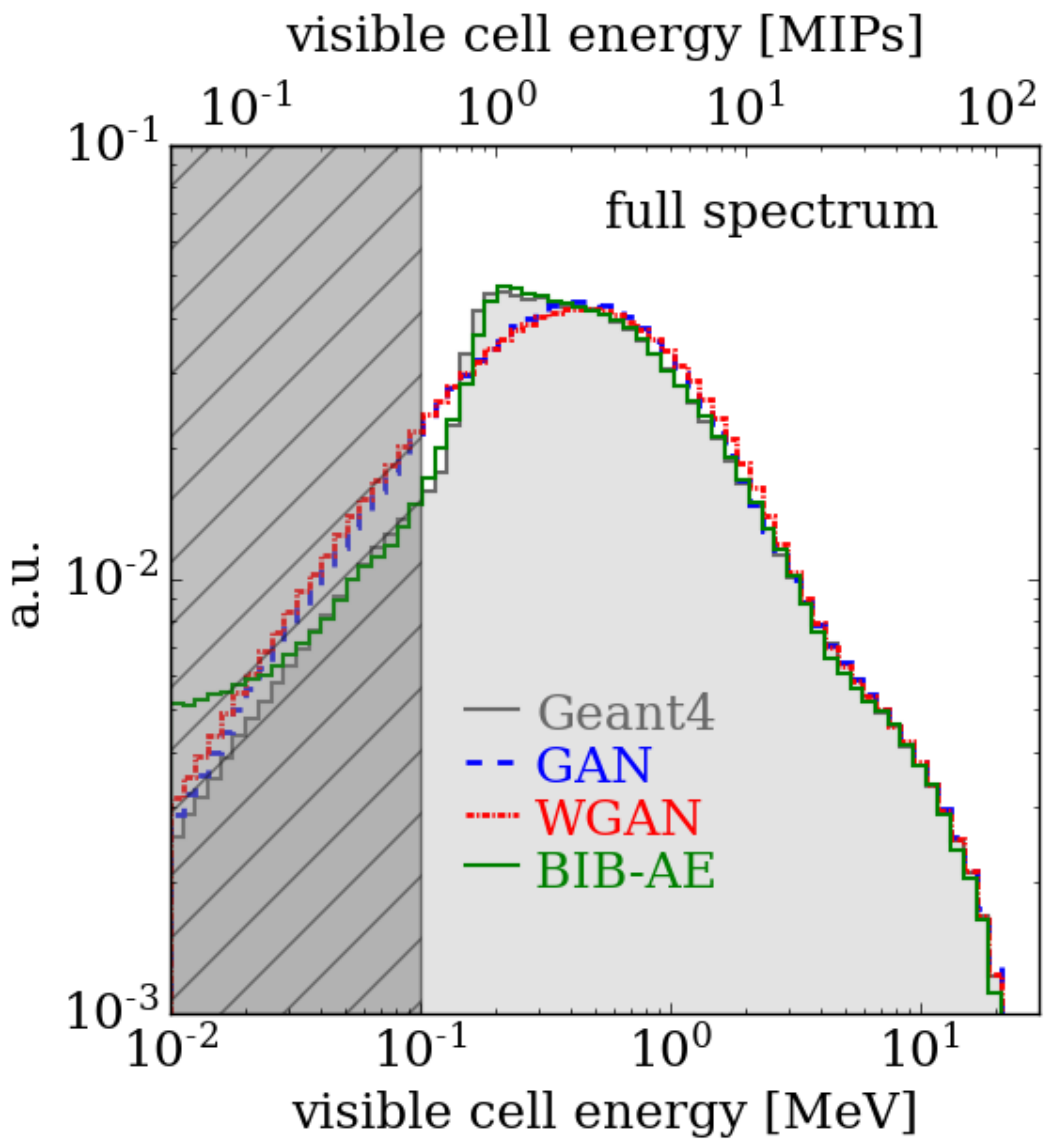
- Photons / charged Pions
- 1 million / 500k showers
- 10 to 100 GeV
- Fixed incident point & angle
- Project to grid
- 30×30×30 / 25×25×48

Buhmann et al.: **Getting High: High Fidelity Simulation of High Granularity Calorimeters with High Speed** (2020) 2005.05334

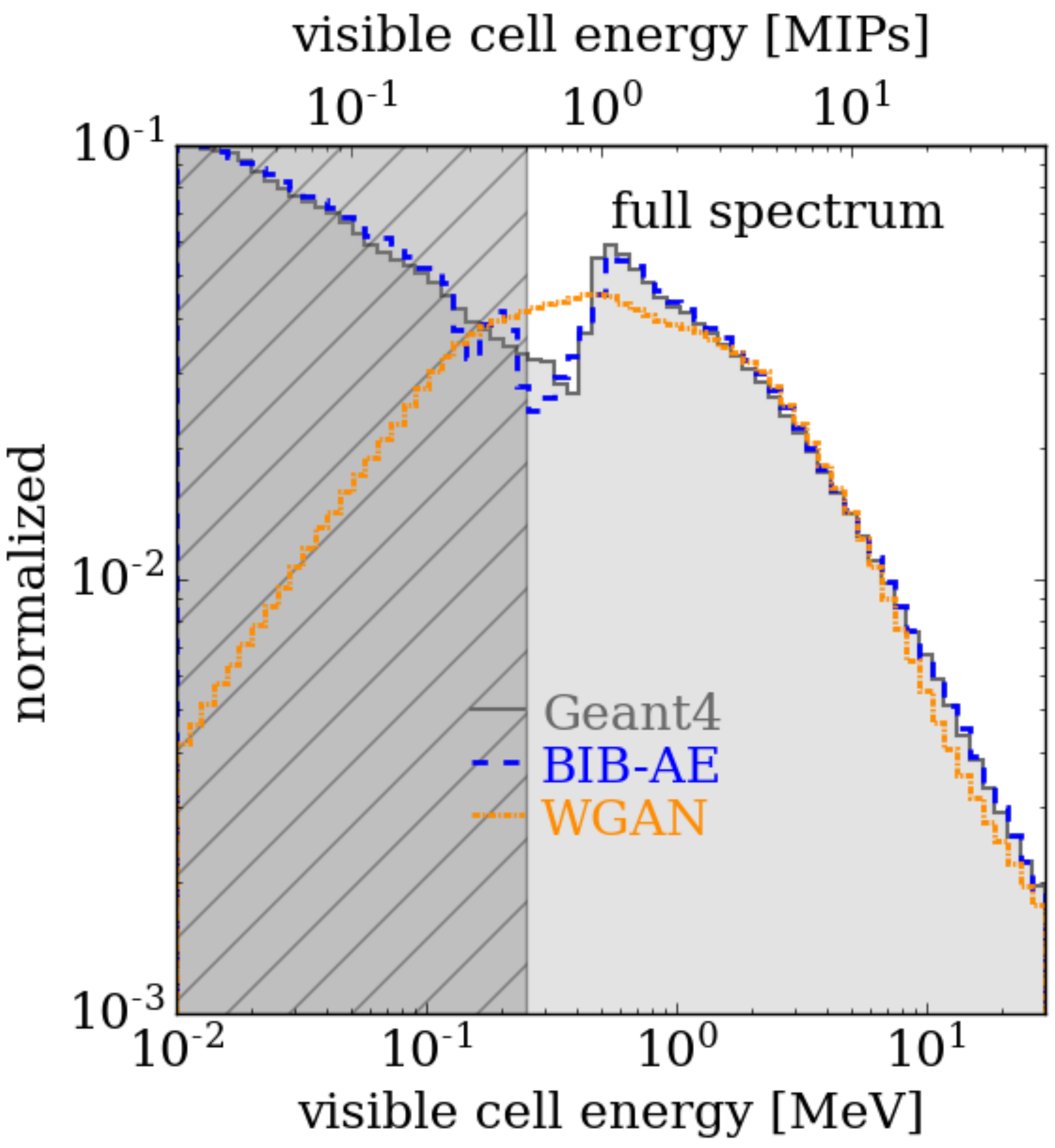
Buhmann et. al. **Hadrons, Better, Faster, Stronger:** (2021) 2112.09709

High Granularity Calorimeter

Photons



Pions



Anomaly Detection

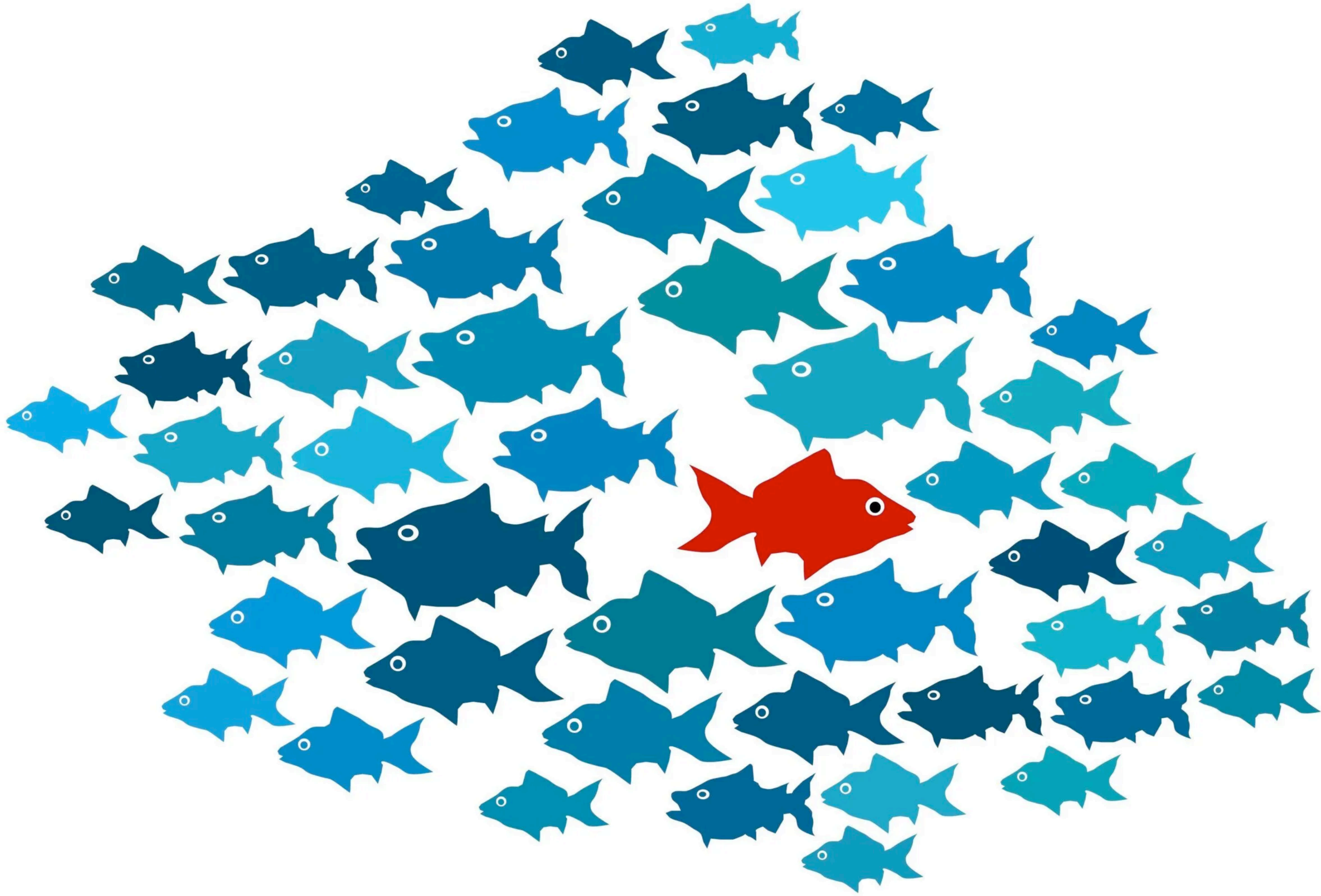
So far: no new discoveries of particles beyond the Standard Model

- Maybe not enough data

  → Previous ML methods

- Not looking for the right theory

  → Anomaly detection

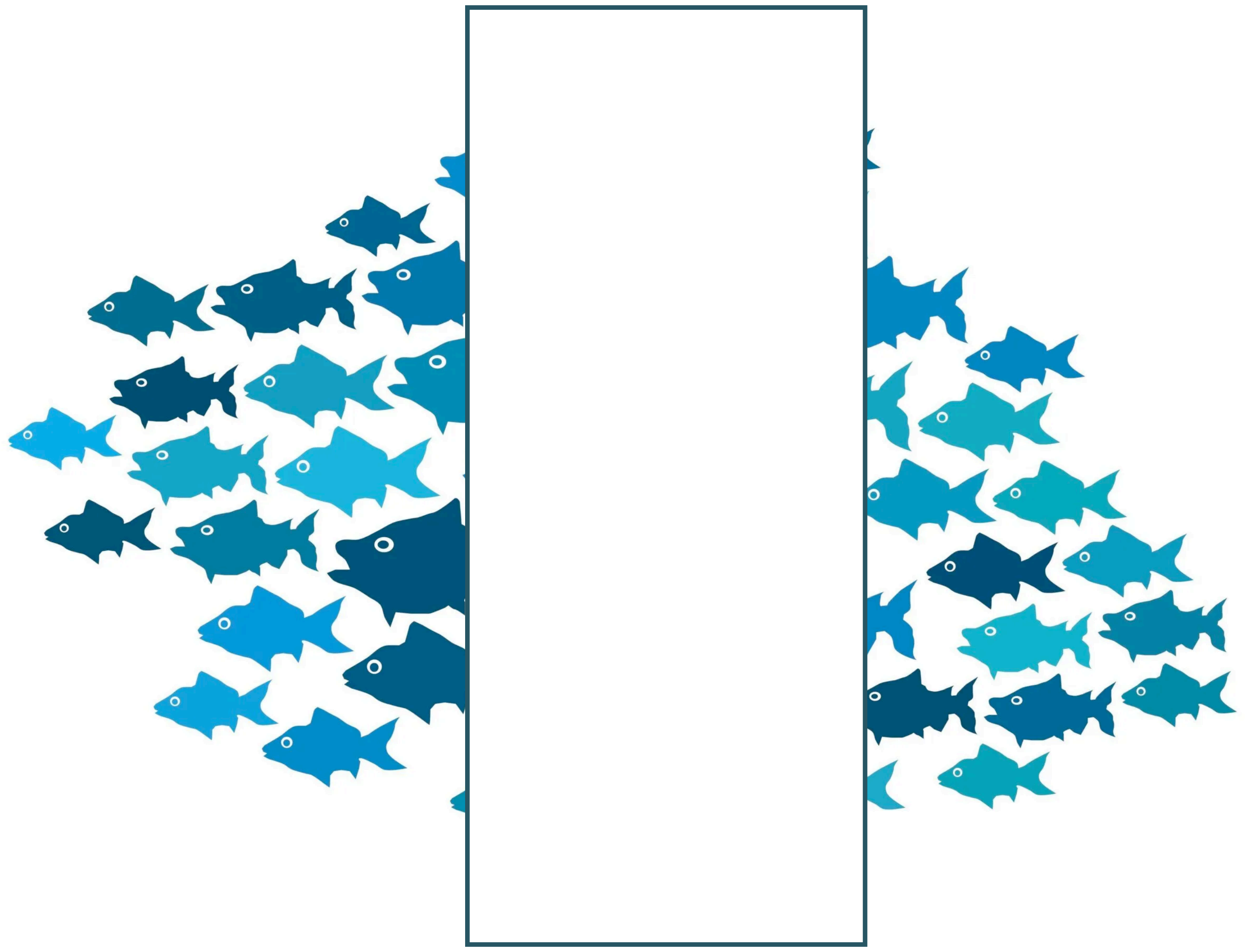


https://www.tatvic.com/blog/detecting-real-time-anomalies-using-r-google-analytics-360-data/

Anomaly Detection

Semi-Supervised AD:

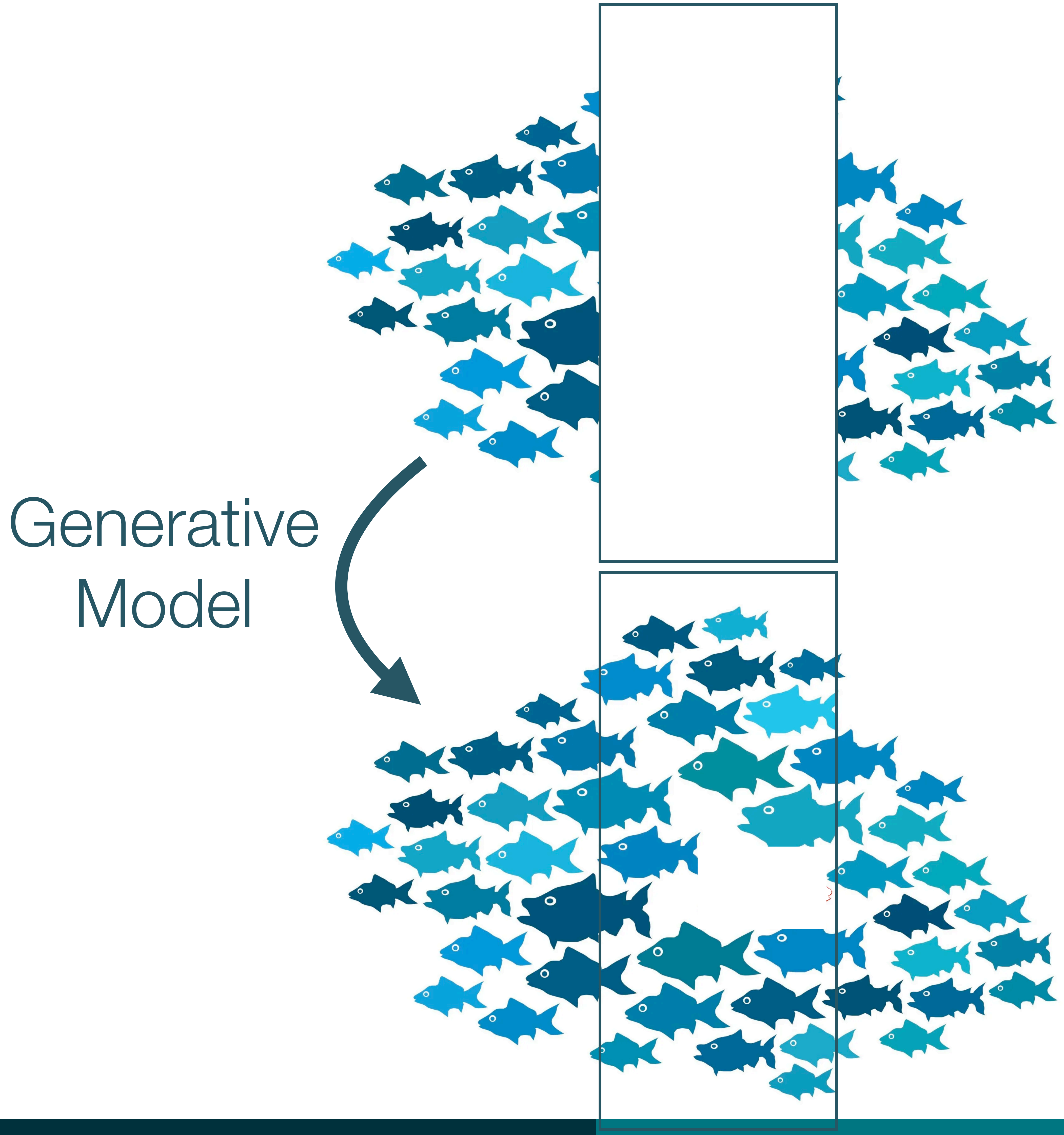
- Find unexpected samples
- Cut out part of data
- Use generative model to learn data



Anomaly Detection

Semi-Supervised AD:

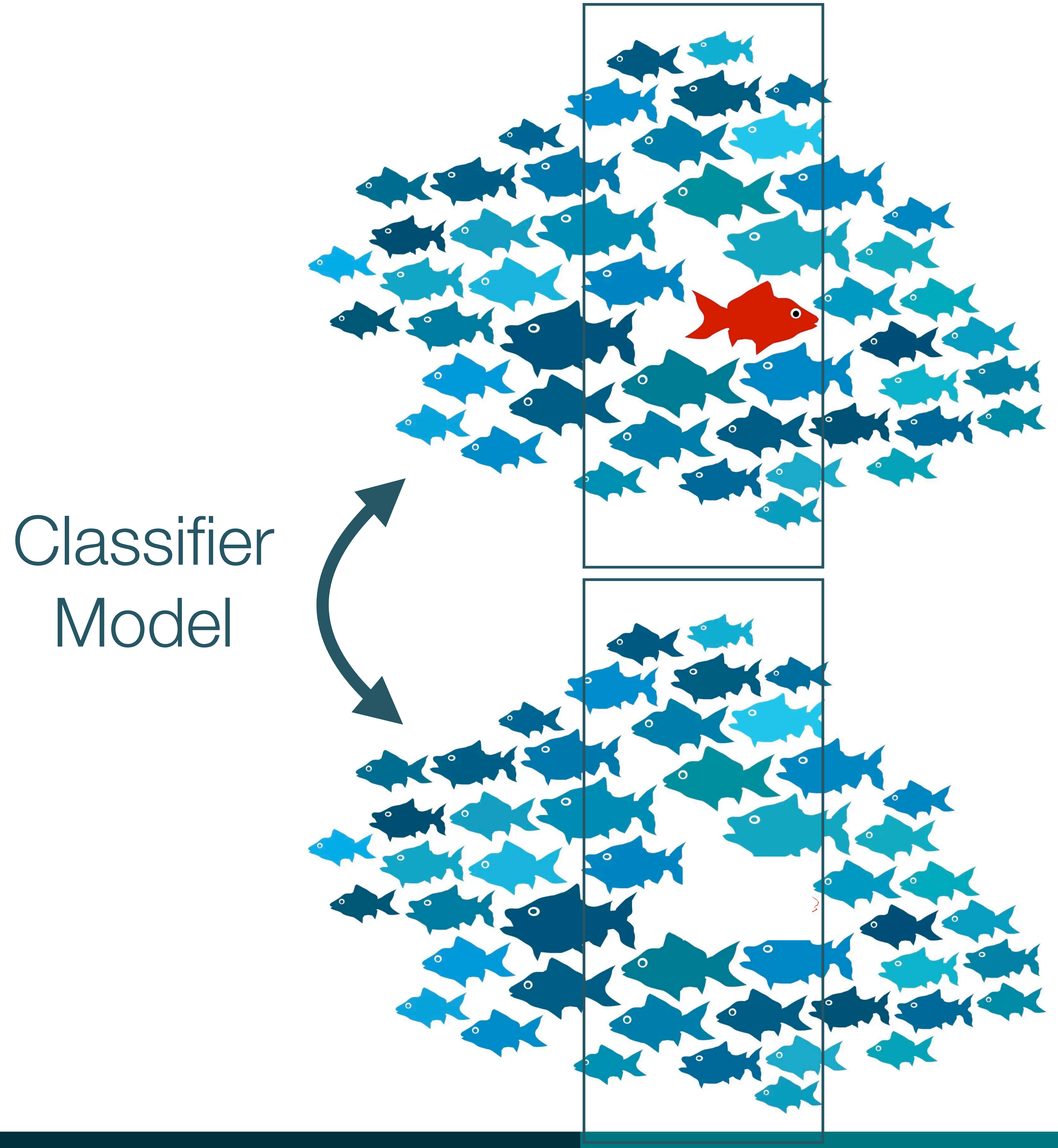
- Find unexpected samples
- Cut out part of data
- Use generative model to learn data
- Predict cut out part



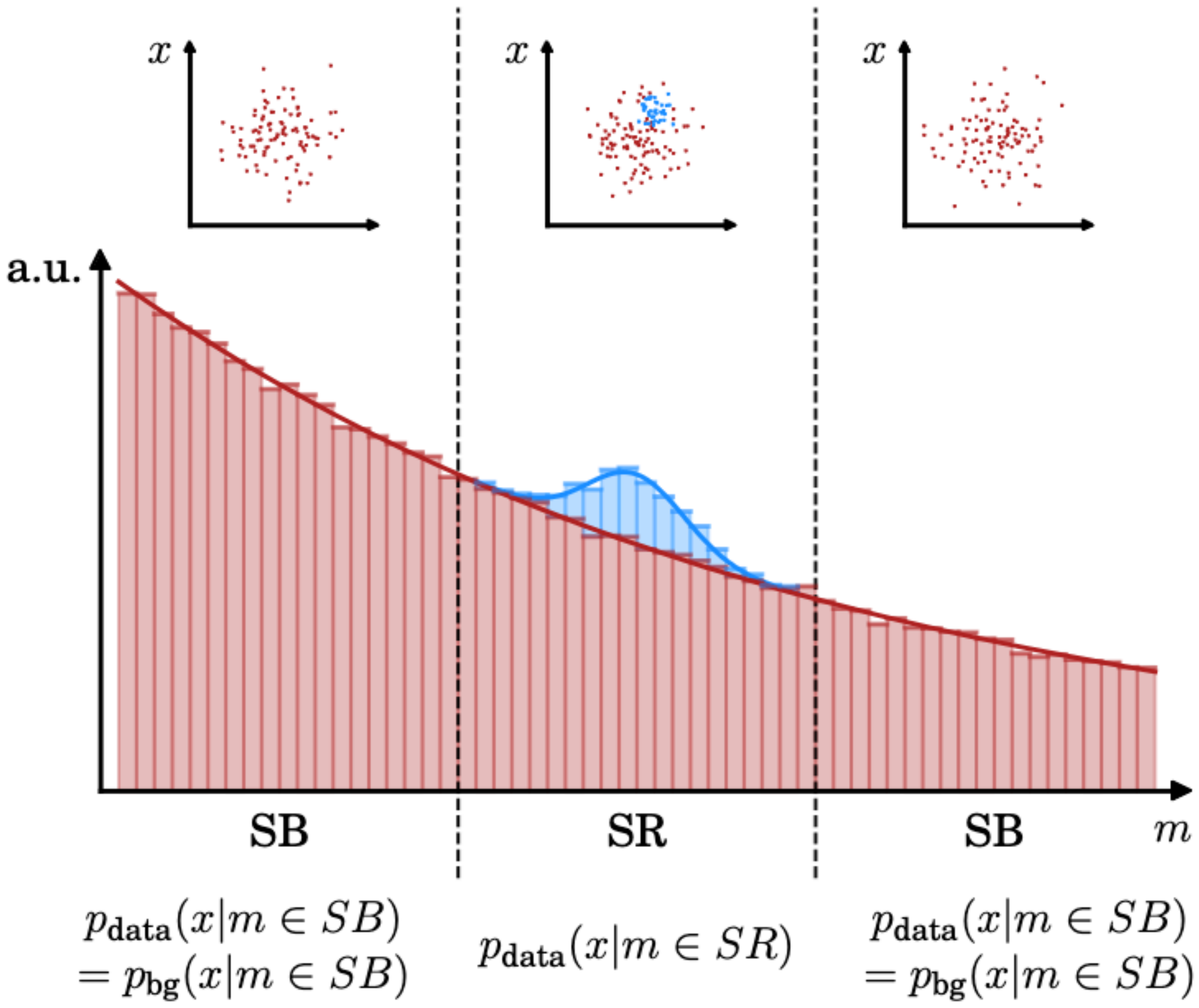
Anomaly Detection

Semi-Supervised AD:

- Find unexpected samples
- Cut out part of data
- Use generative model to learn data
- Predict cut out part
- Compare prediction and cut out



Anomaly Detection

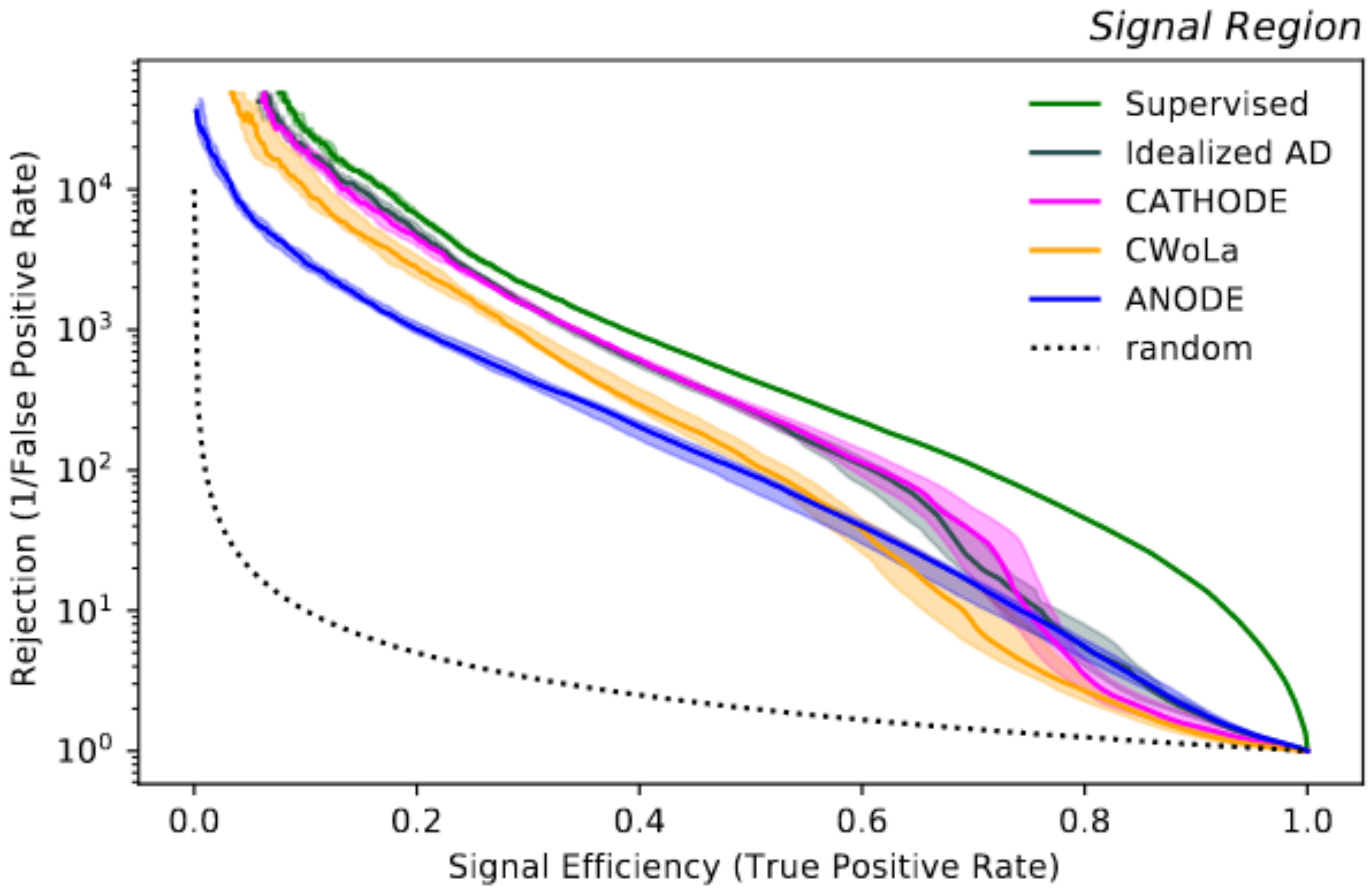


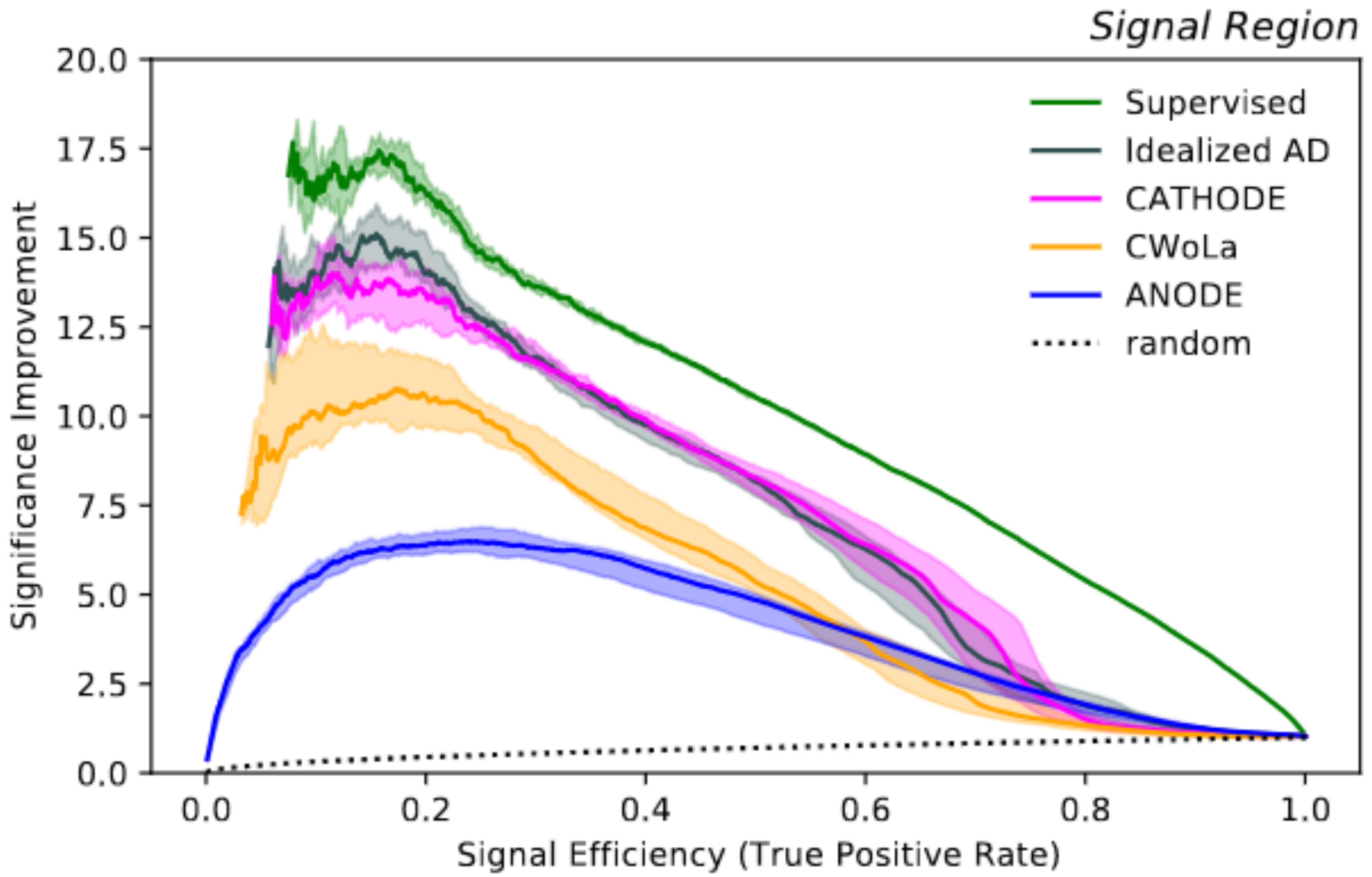
Classifying Anomalies THrough Outer Density Estimation (CATHODE)

- Divide data into Signal Region (SR) and Side Bands (SB)
- SR contains suspected signal (is scanned over in real search
- Train Normalizing Flow on SB
- Extrapolate into SR

Hallin et. al. **Classifying Anomalies THrough Outer Density Estimation (CATHODE),** [2109.00546](https://arxiv.org/abs/2109.00546)

Anomaly Detection

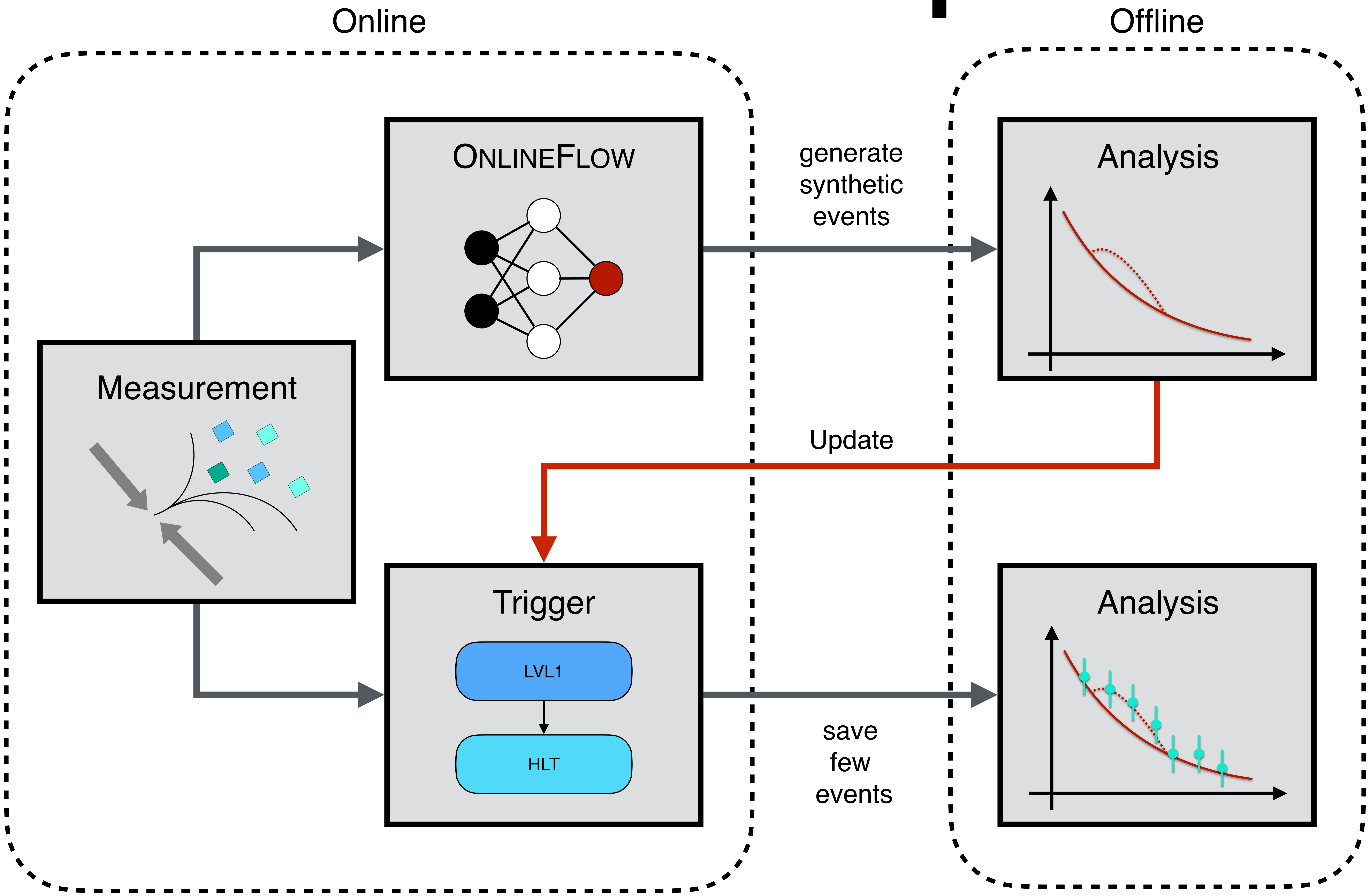




- Train Classifier on real SR vs. extrapolates SR
- Learns to find signal events

Hallin et. al. **Classifying Anomalies THrough Outer Density Estimation (CATHODE),** [2109.00546](2109.00546)

Online Data Compression



Hands-On Tutorial

https://github.com/ml4fp/2024-lbnl

git clone https://github.com/ml4fp/2024-lbnl.git

Or (if already cloned)

```
git add -u
git commit -m ‘past tutorials’
git pull
```

Introduction

Common point of criticism: Information in new samples

- Assume generative model trained on N events
- Used to generate M >> N new events

Info (N real points) = Info (M new points)

Little advantage to be gained from generative model

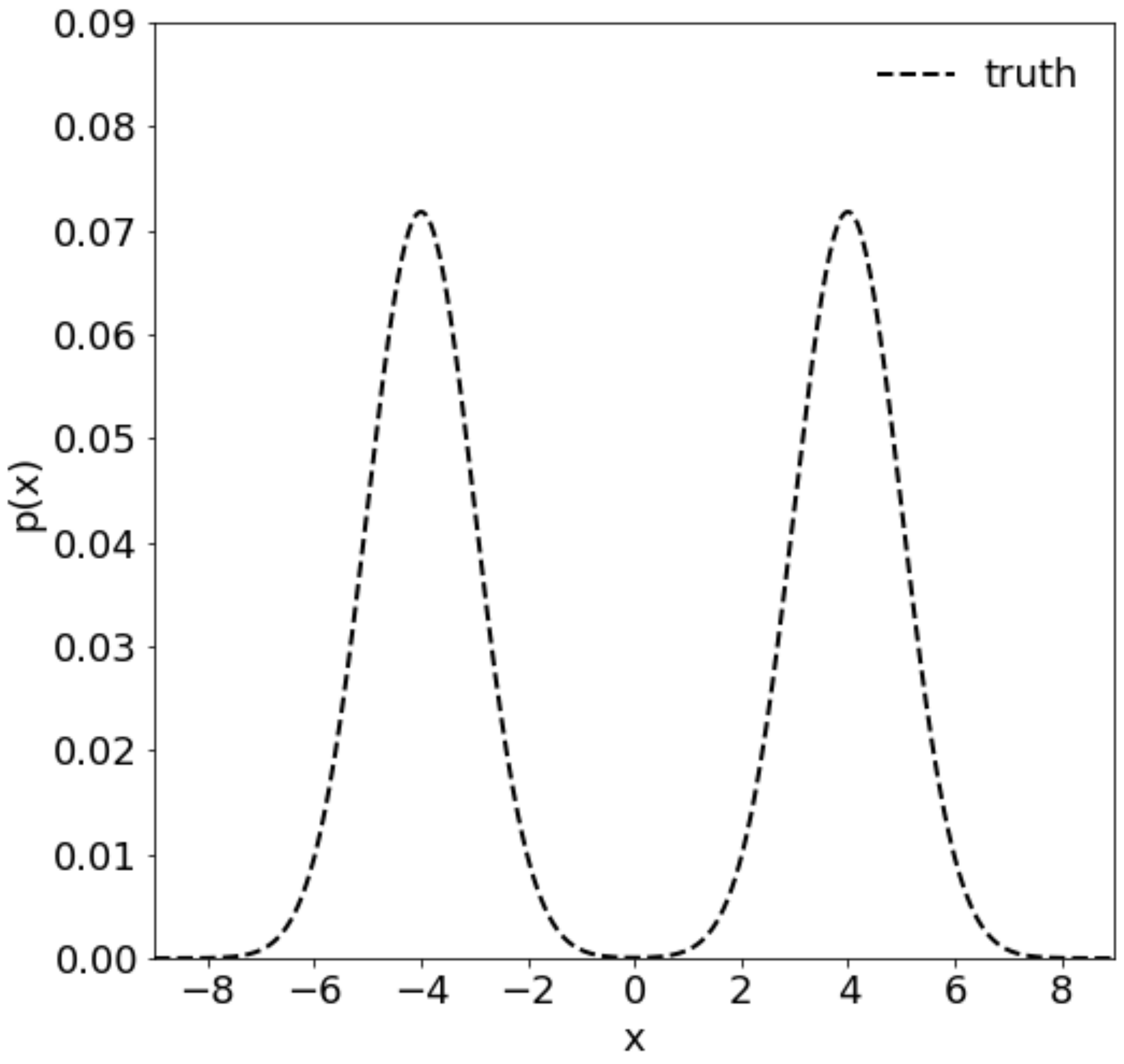
Info (N real points) < Info (M new points)

generative model can speed up simulations

1-D Toy Model

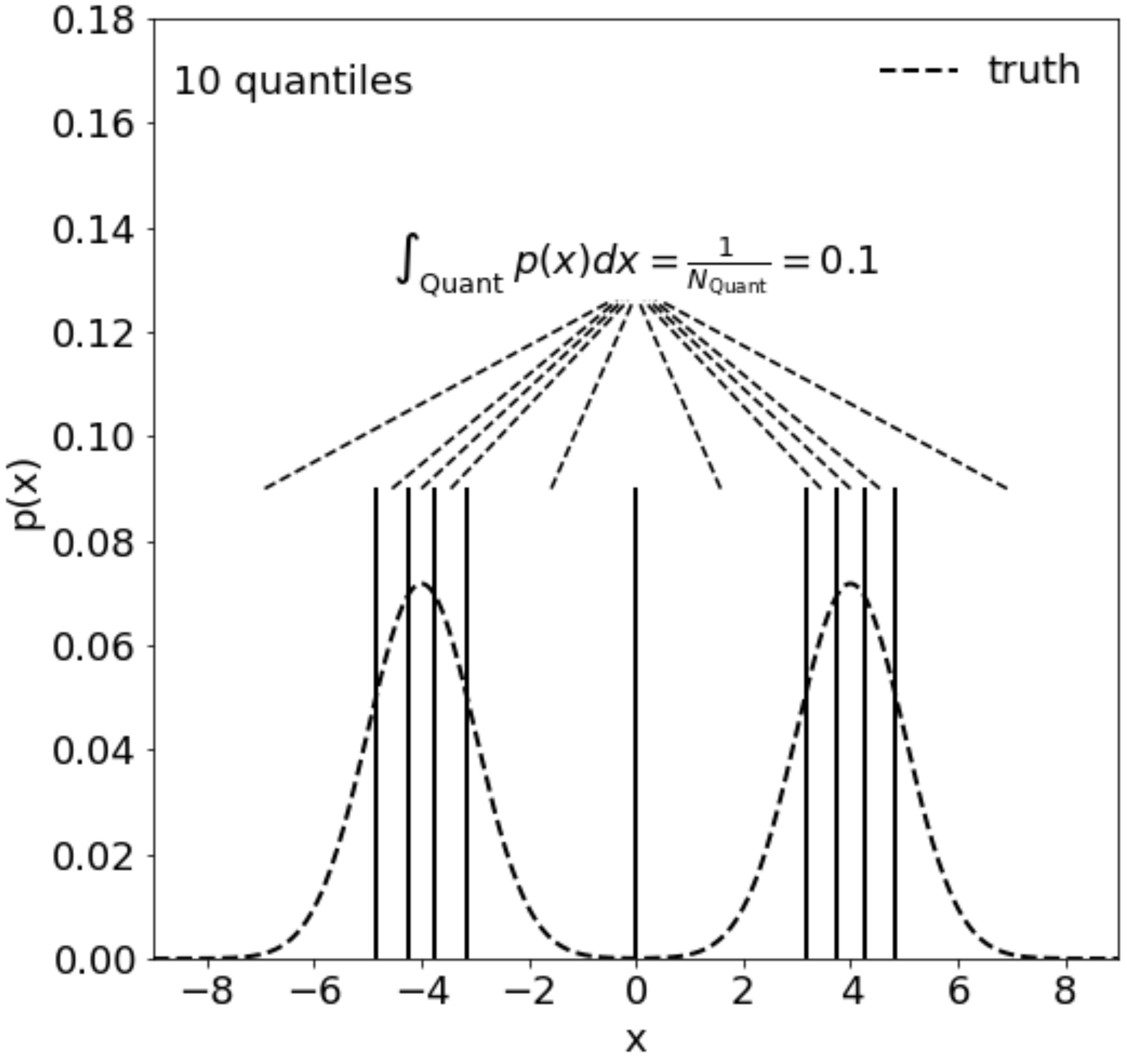
- Camel back function: double peak Gaussian

$$p(X) = \frac{1}{2}(N_{-4,1}(x) + N_{4,1}(x))$$



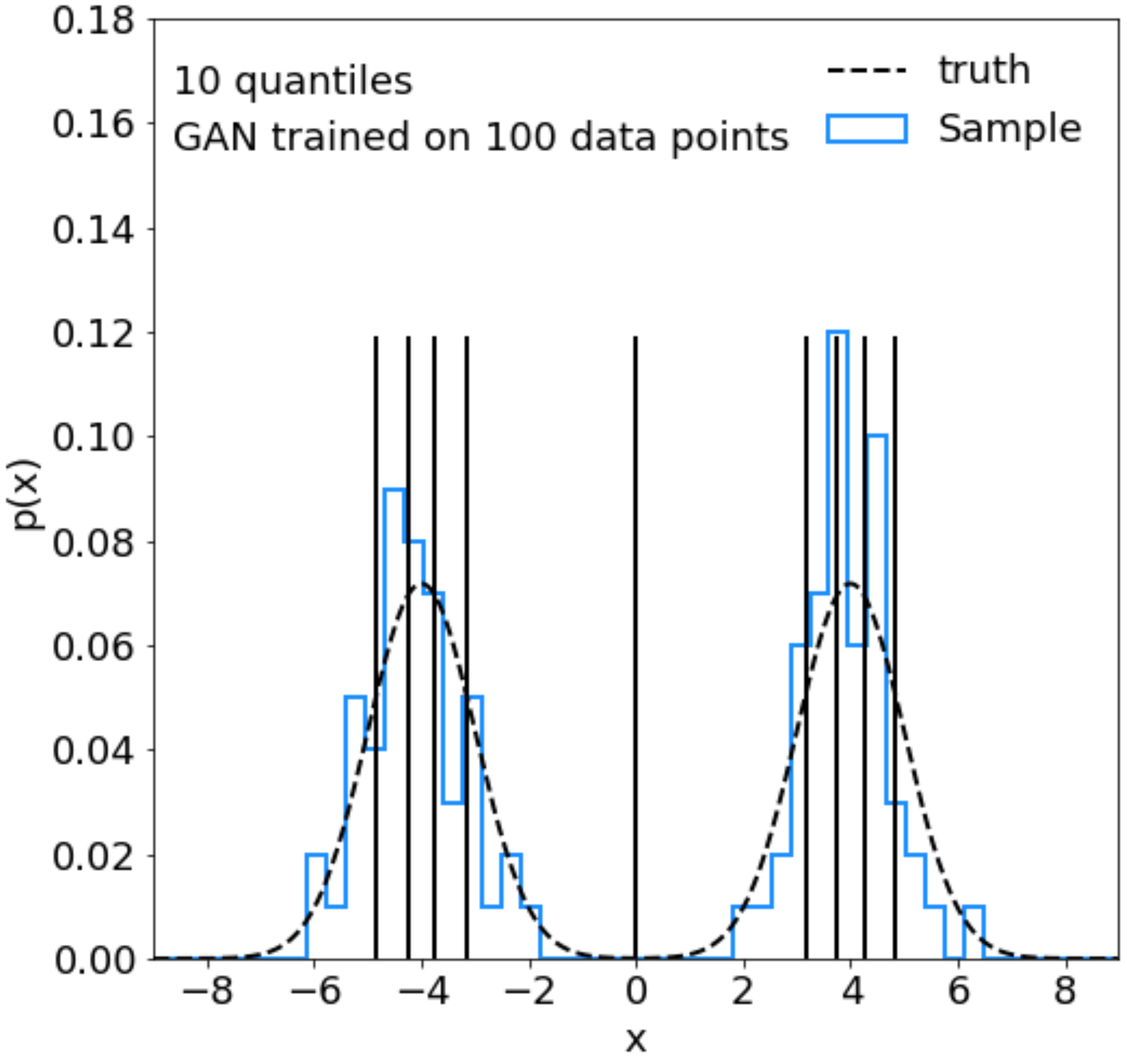
Quantiles

- Measurement how well function is described
- Define N quantiles on true distribution
- Each quantile contains equal probability

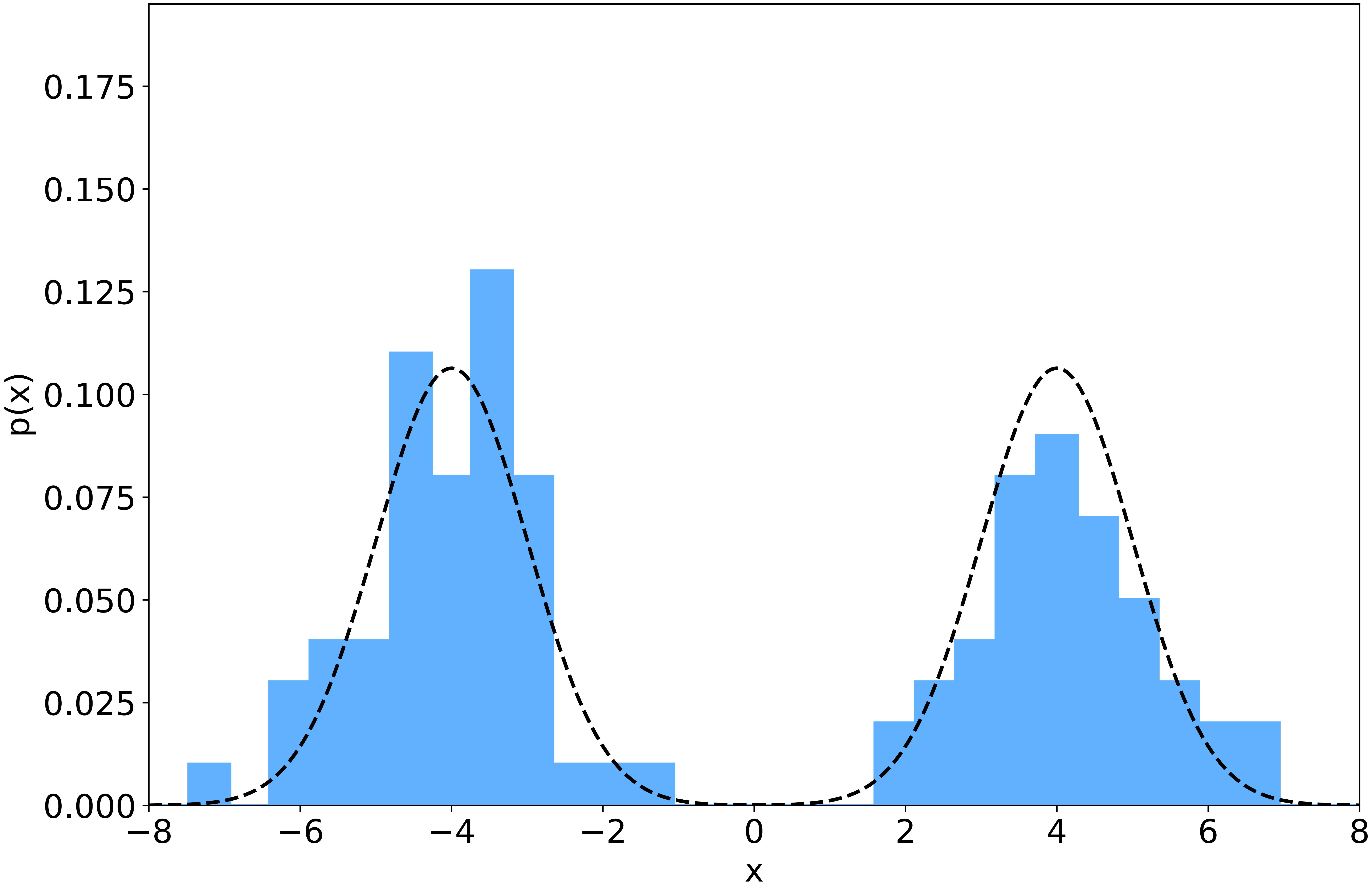


Training Sample

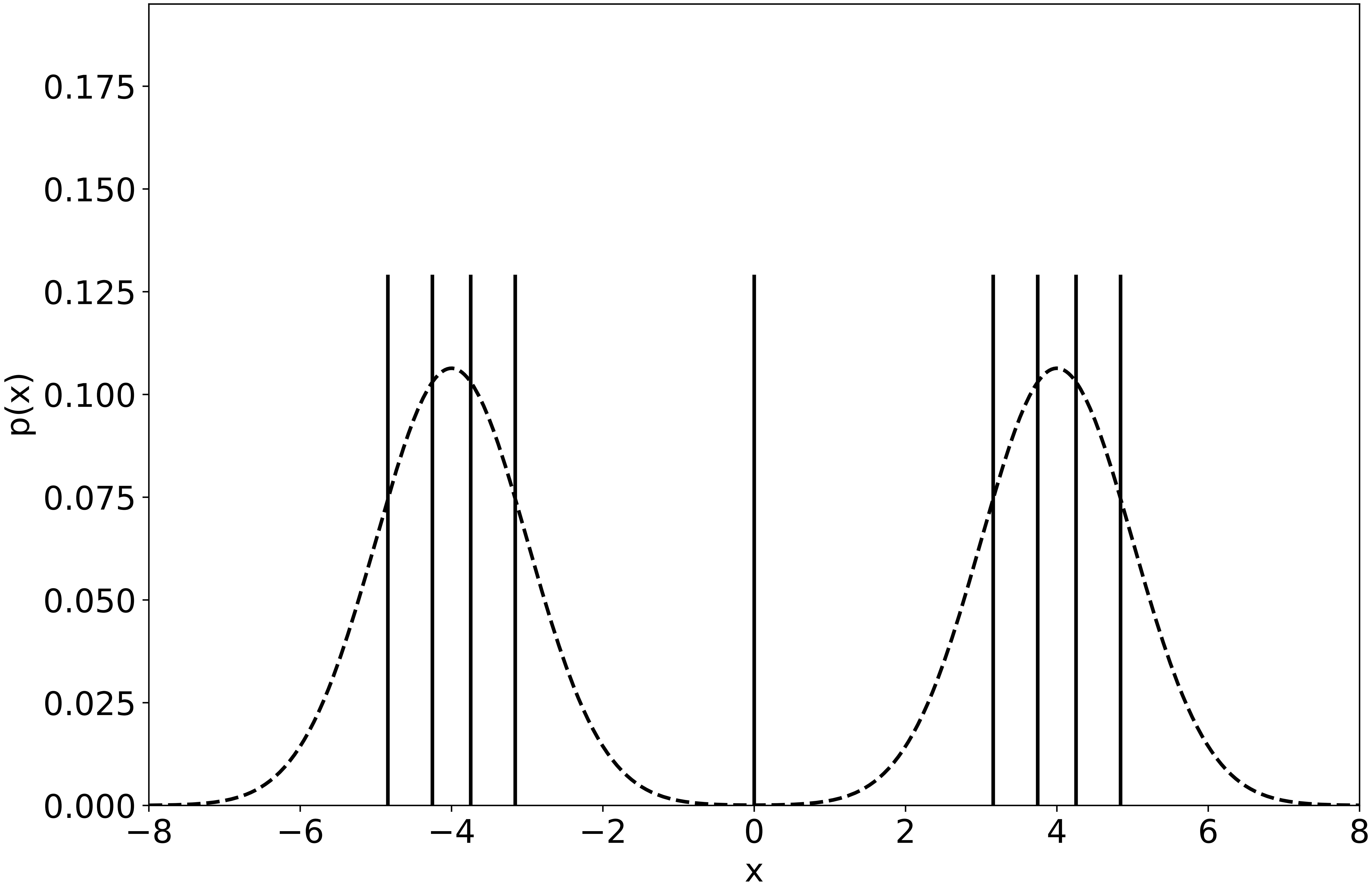
- Draw 100 points from true camel back distribution
- This is designated as the (training) sample
- Calculate fraction of points in each quantile
- Baseline comparison



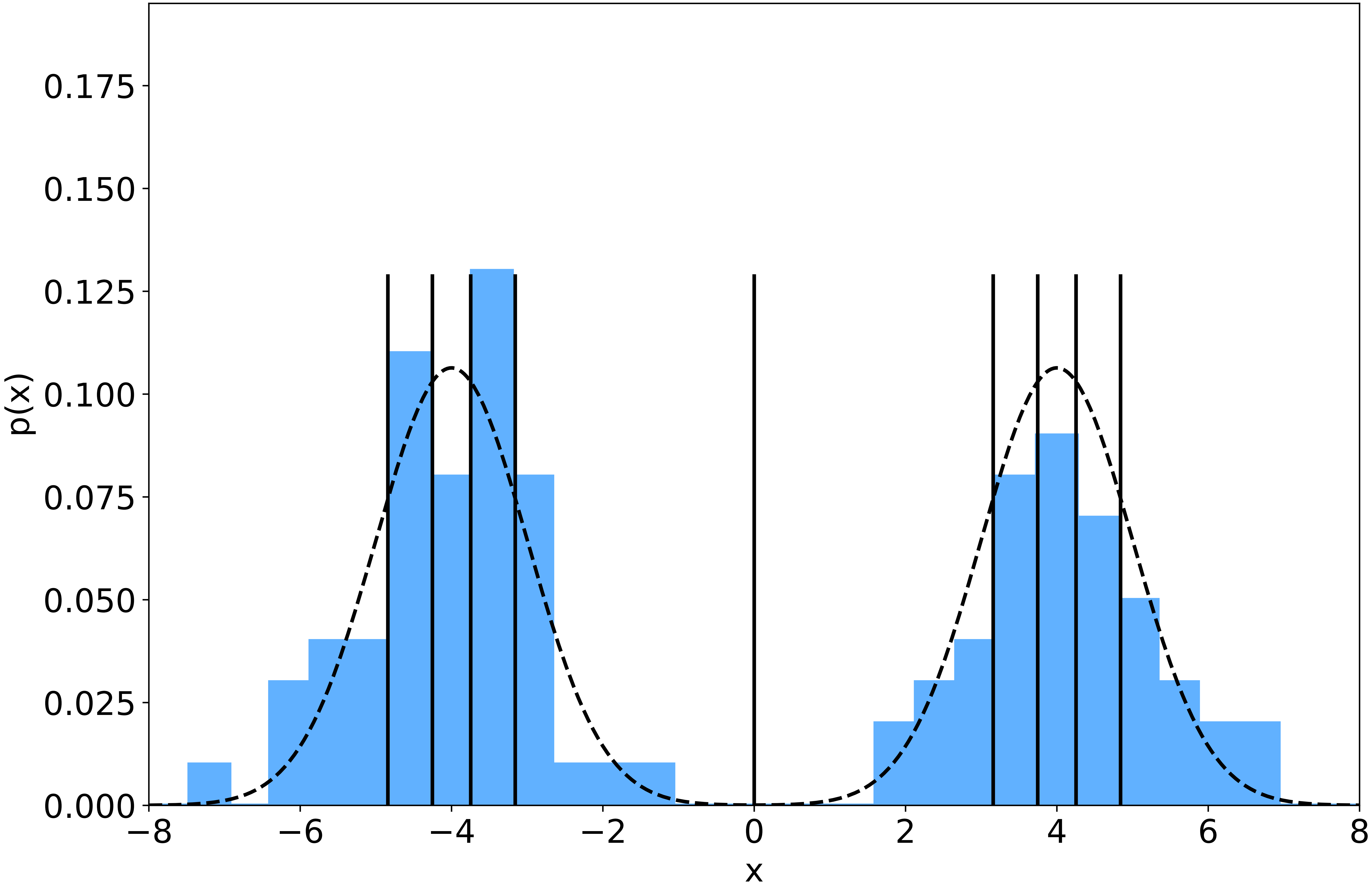
Quantile Measure



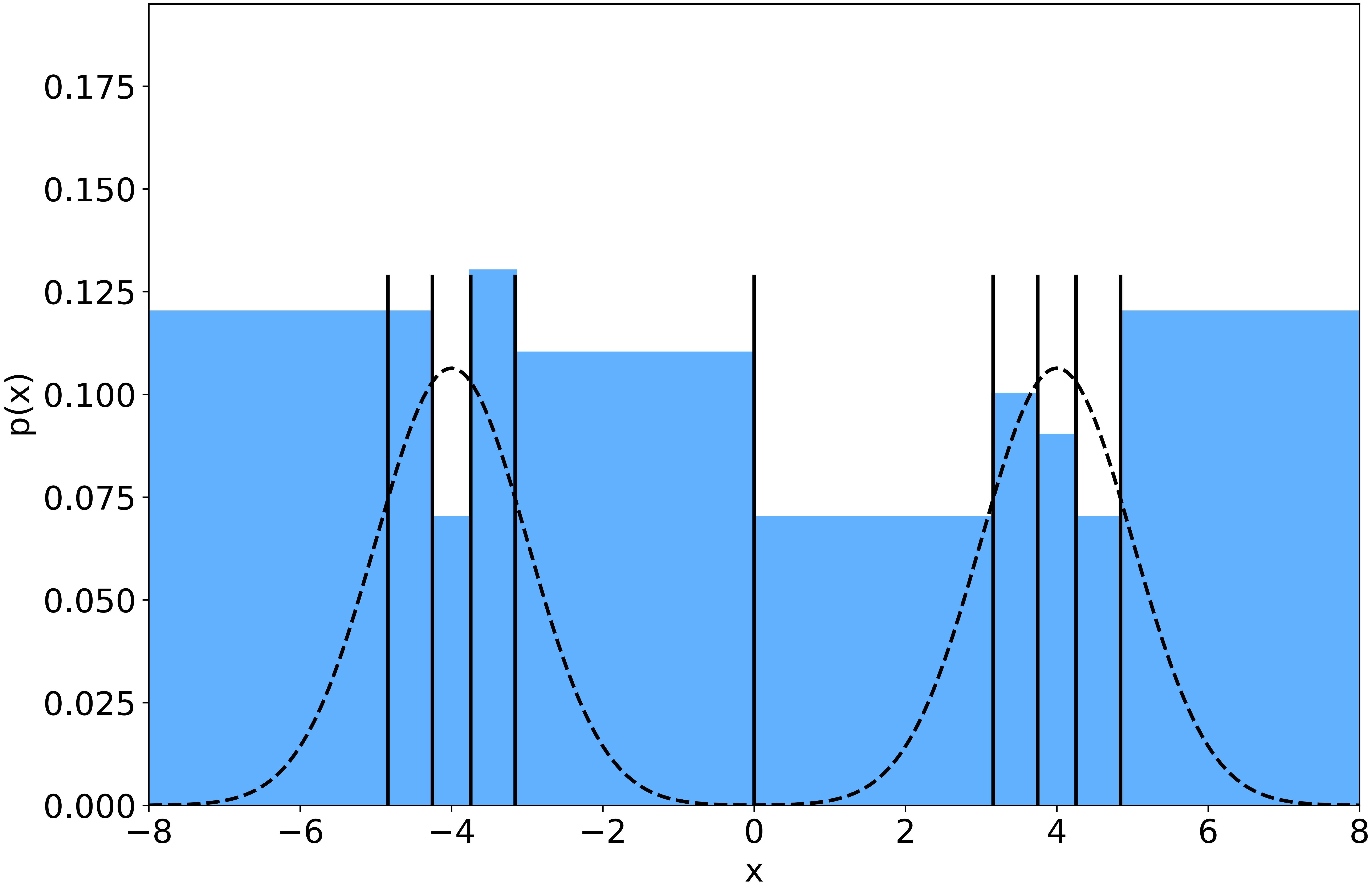
Quantile Measure



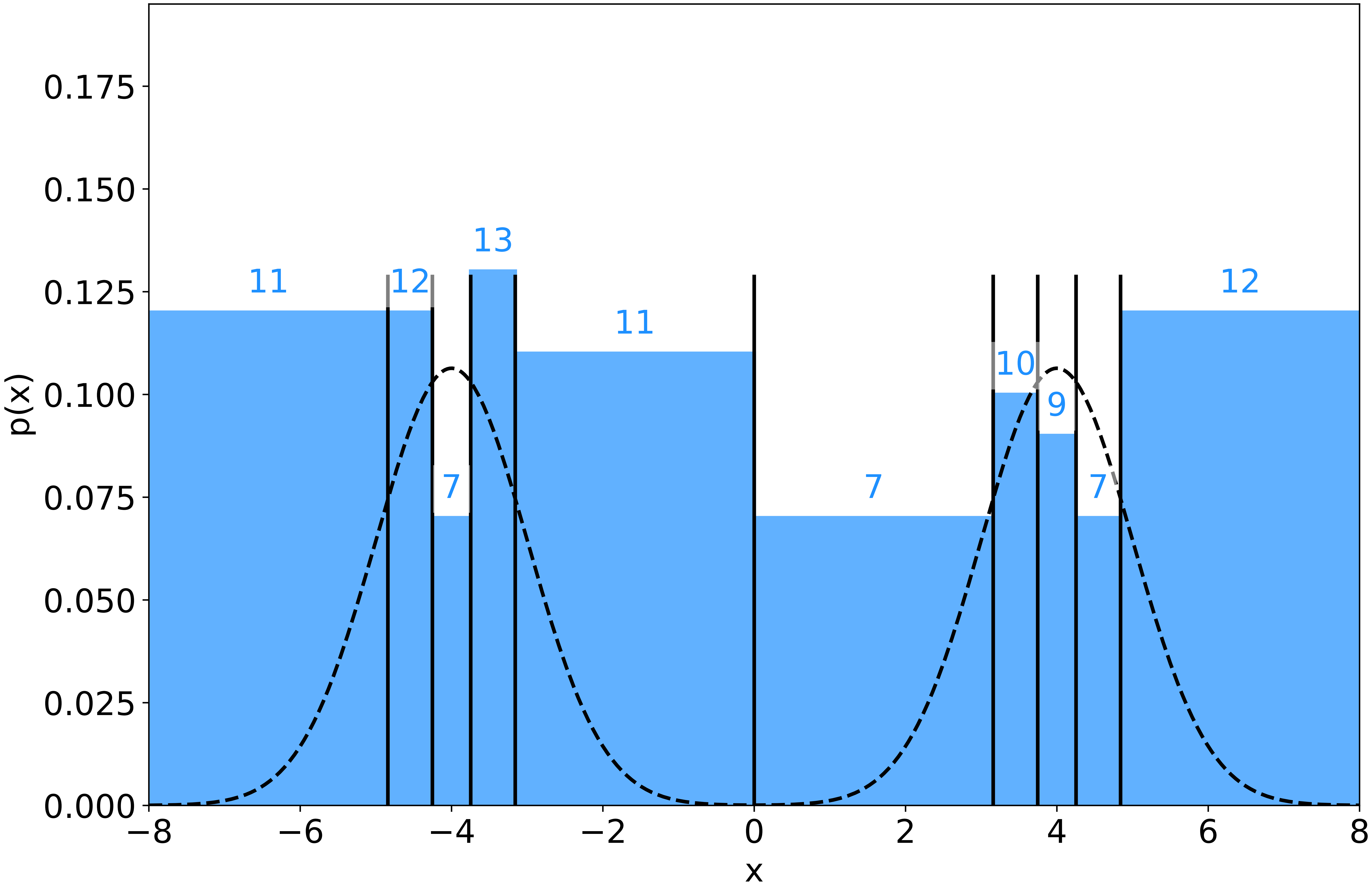
Quantile Measure



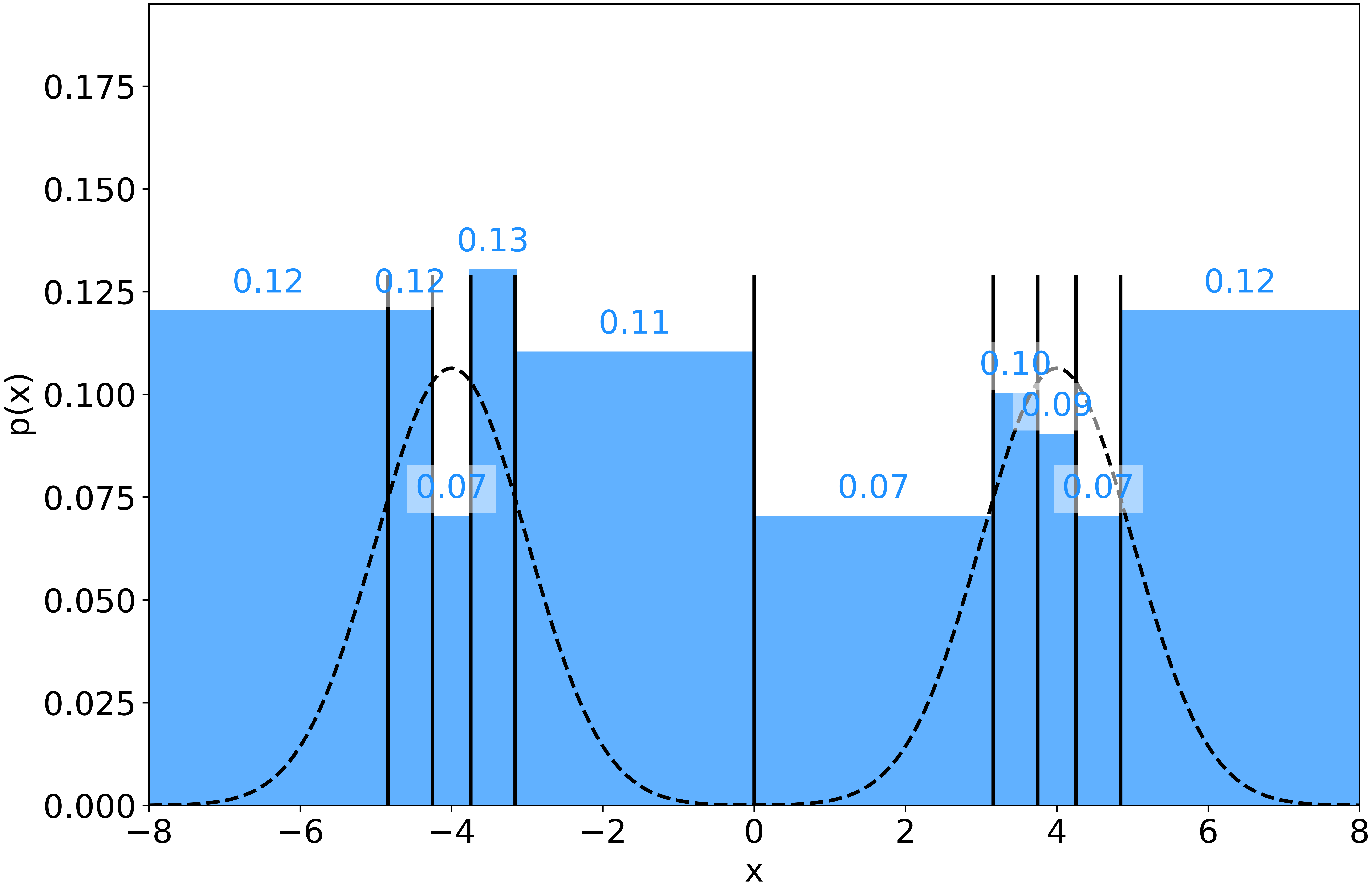
Quantile Measure



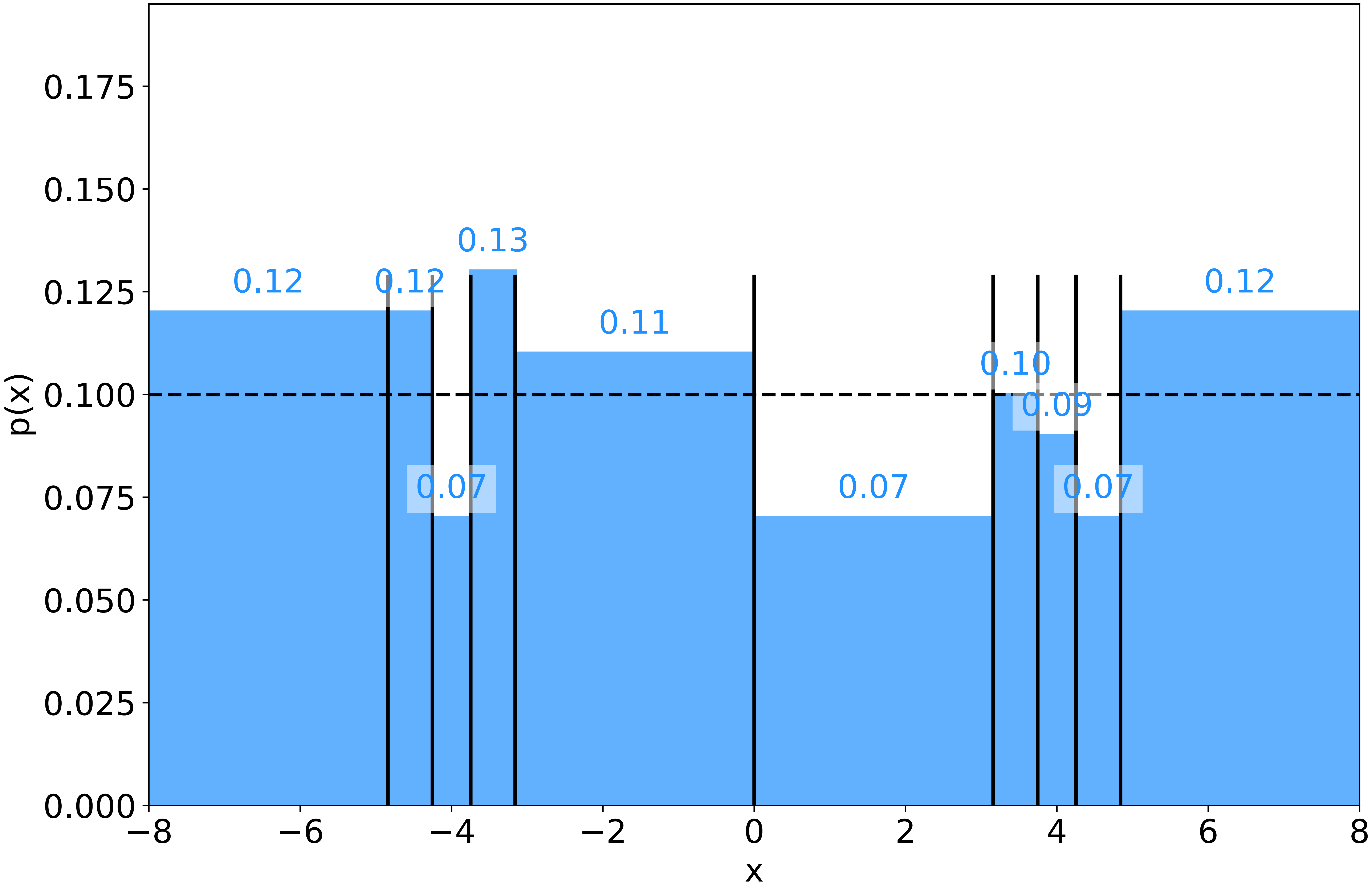
Quantile Measure



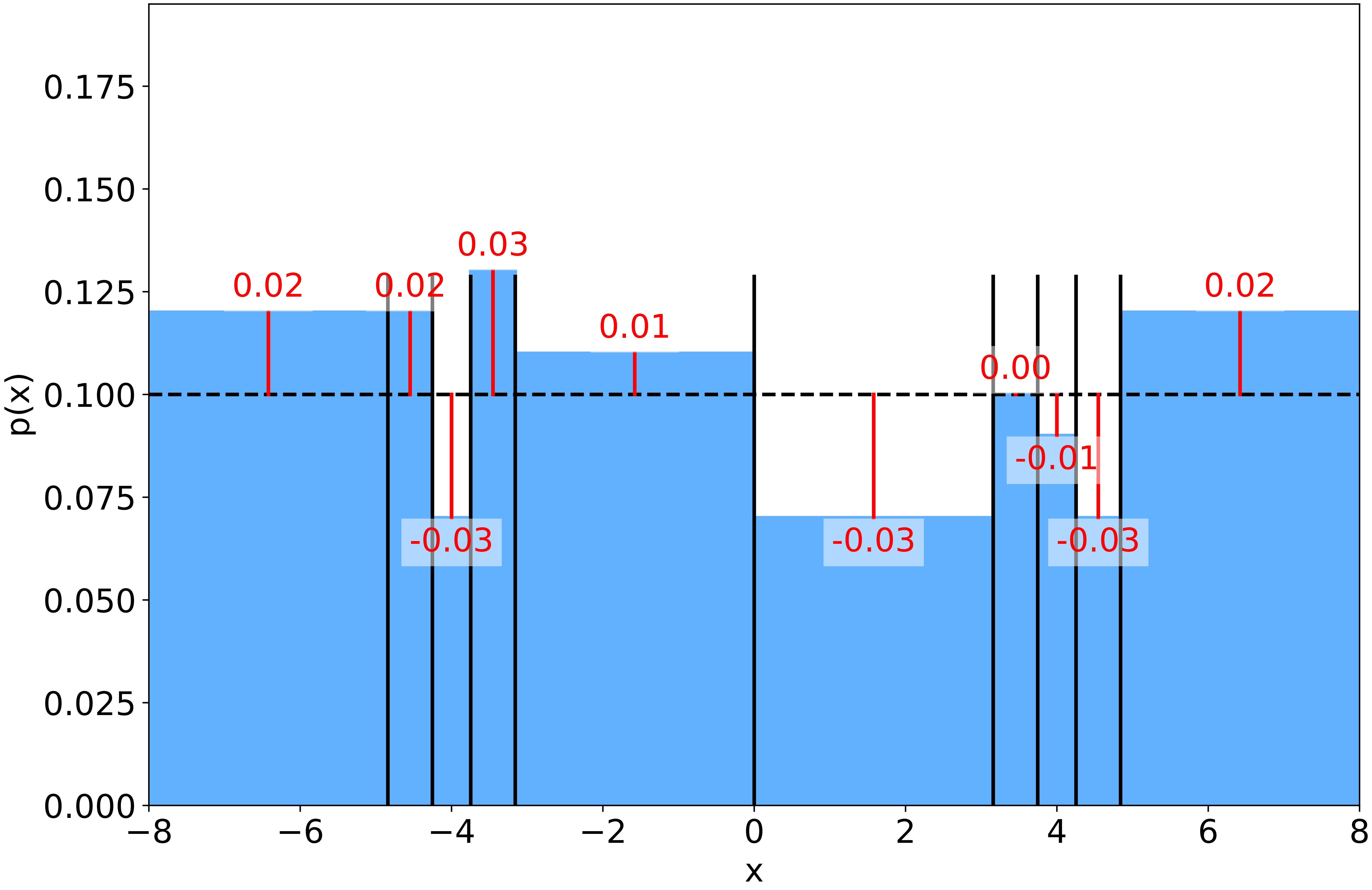
Quantile Measure



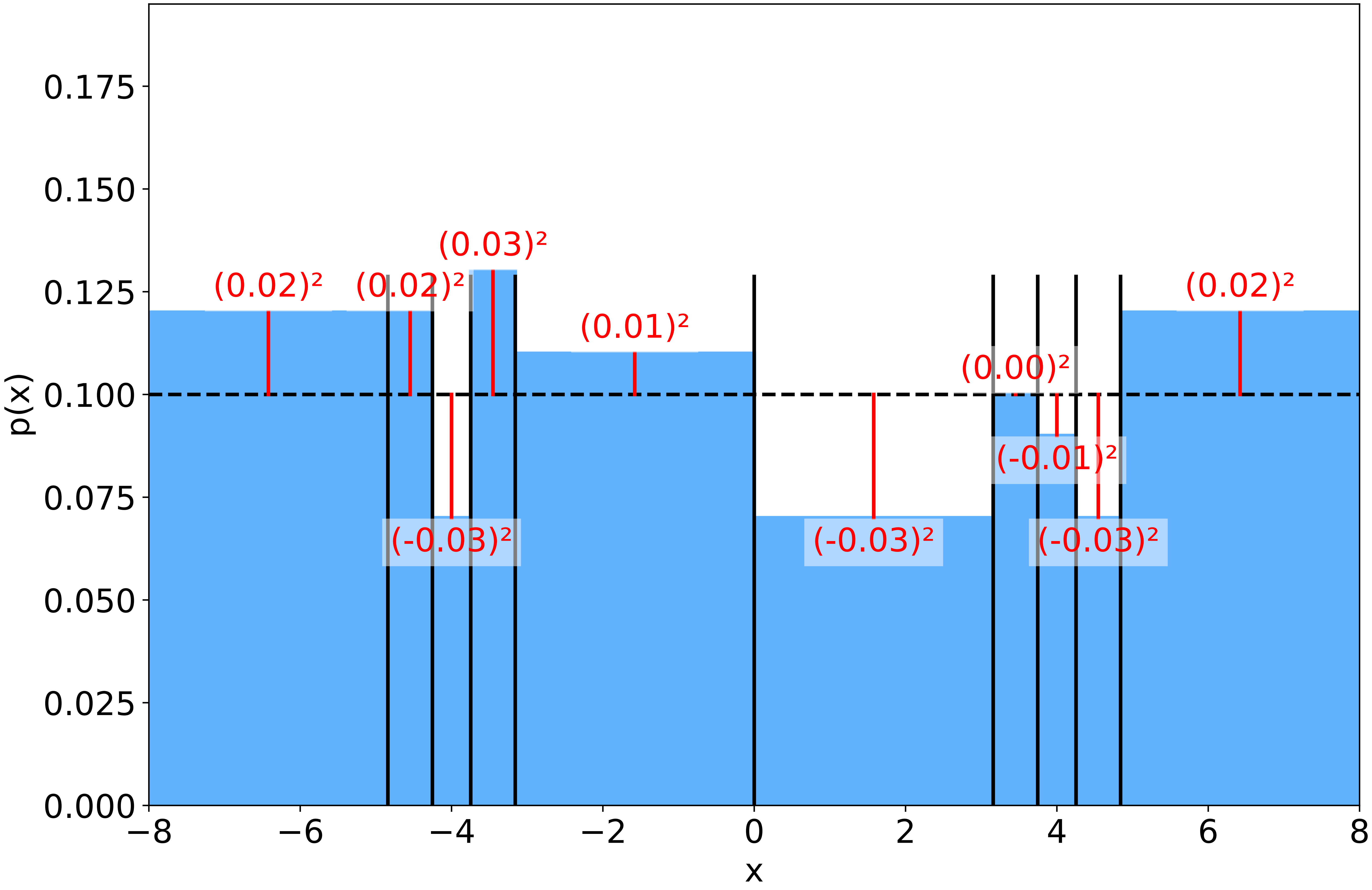
Quantile Measure



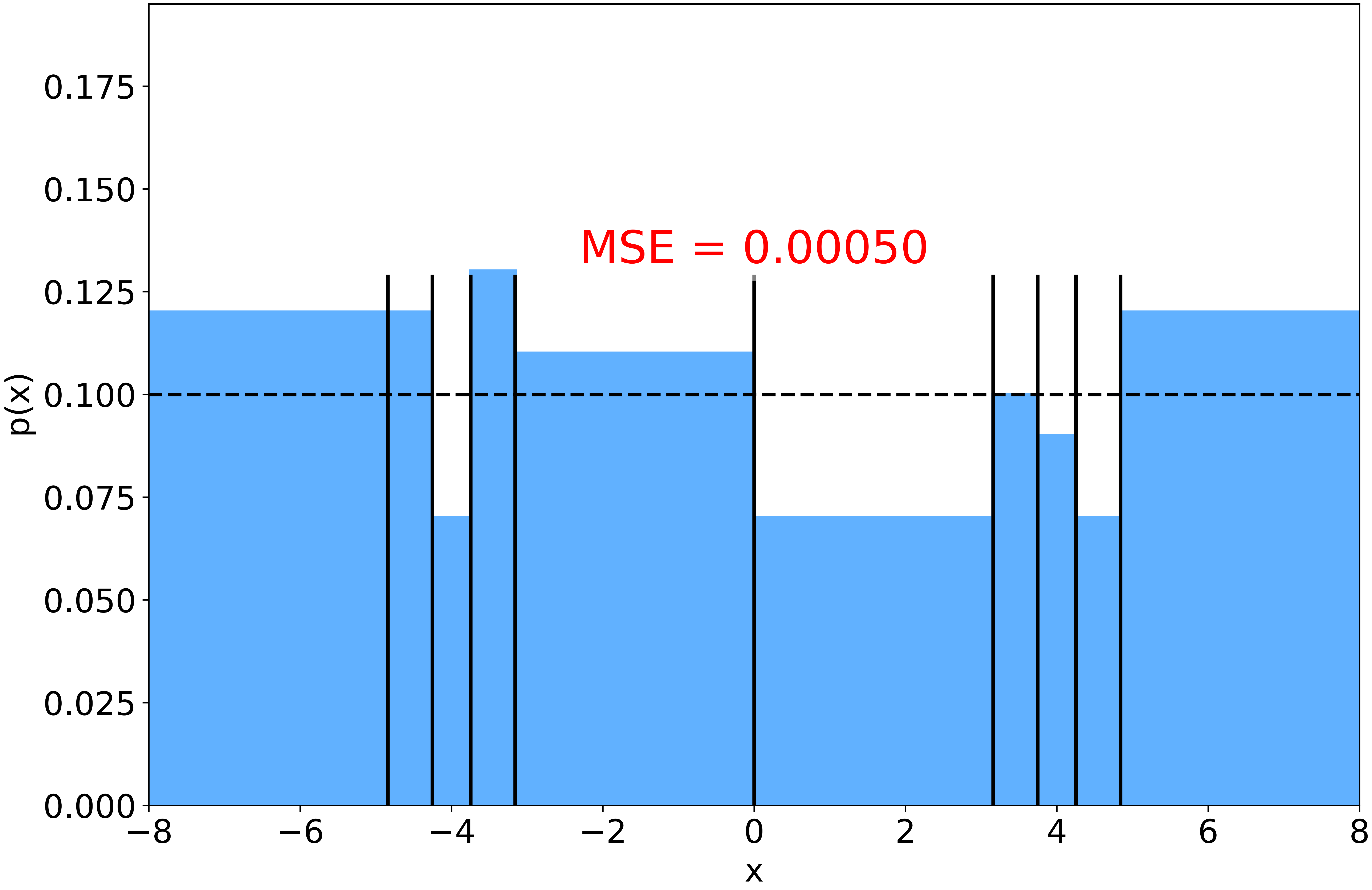
Quantile Measure



Quantile Measure



Quantile Measure

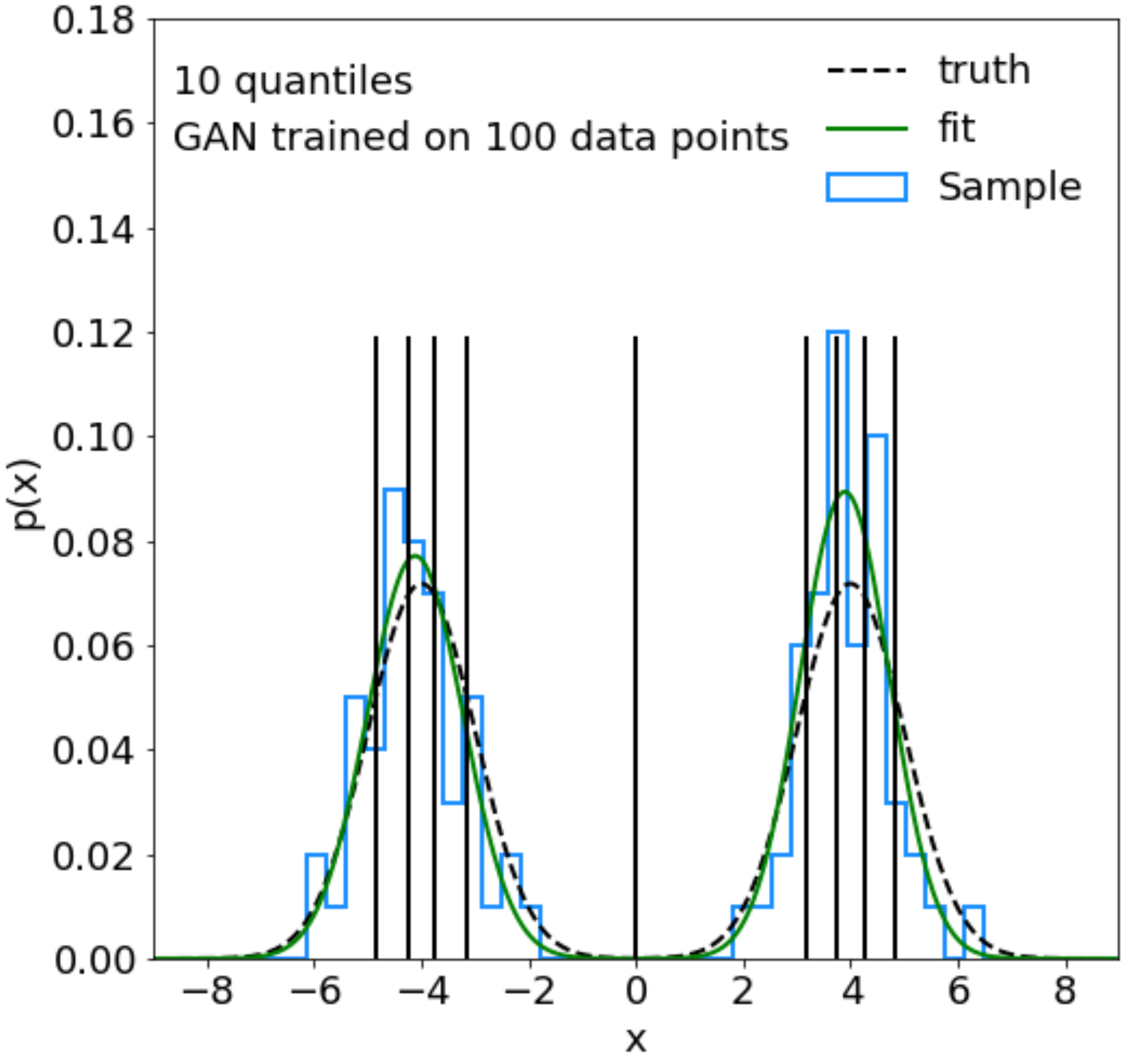


Parameter Fit

- Fit 5 parameter camel back function to training samples

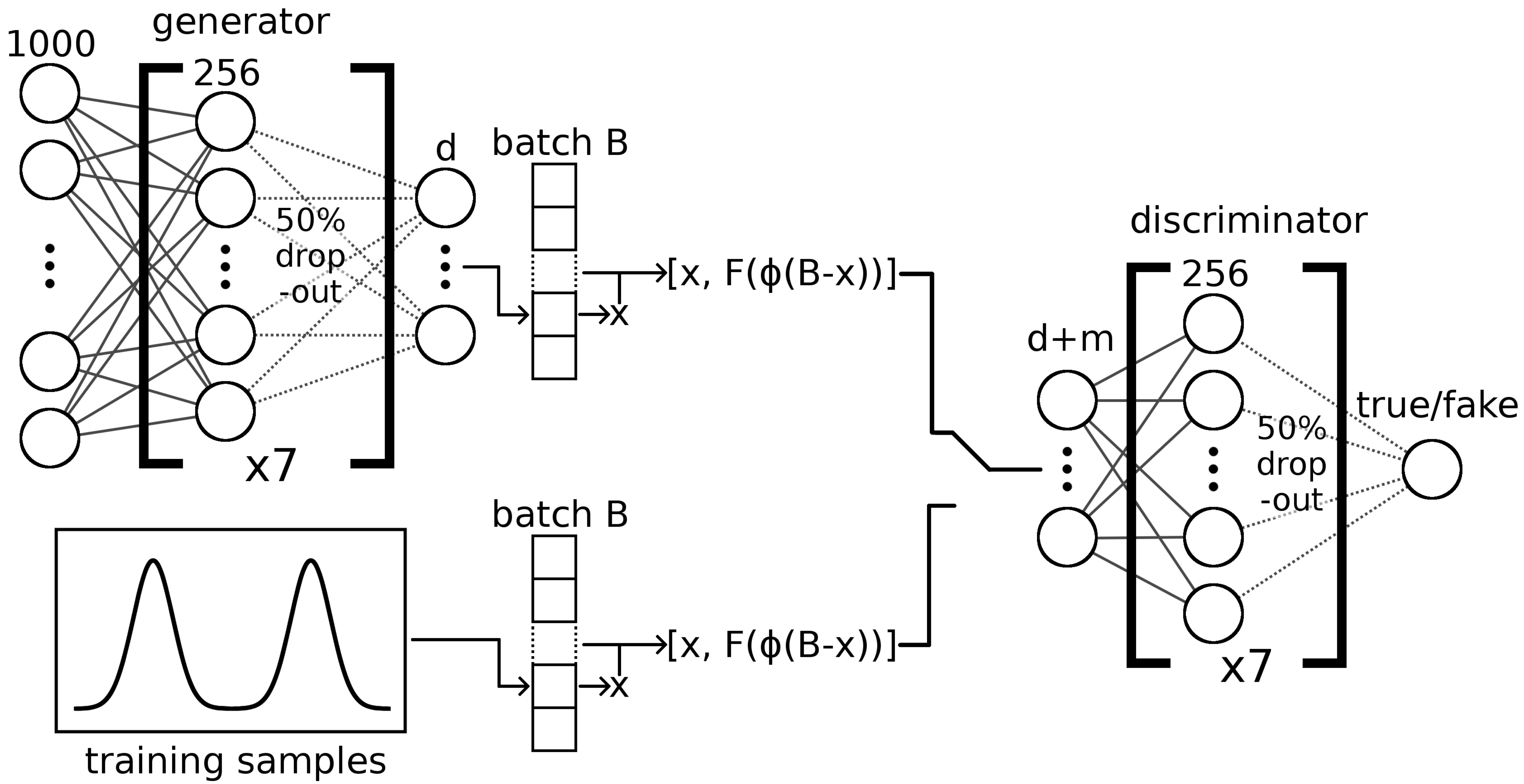
$$p(X) = a\,N_{\mu_1,\sigma_1}(x) \\ +(1-a)N_{\mu_2,\sigma_2}(x)$$

- Analytically calculate integral for each quantile
- Gives upper performance benchmark



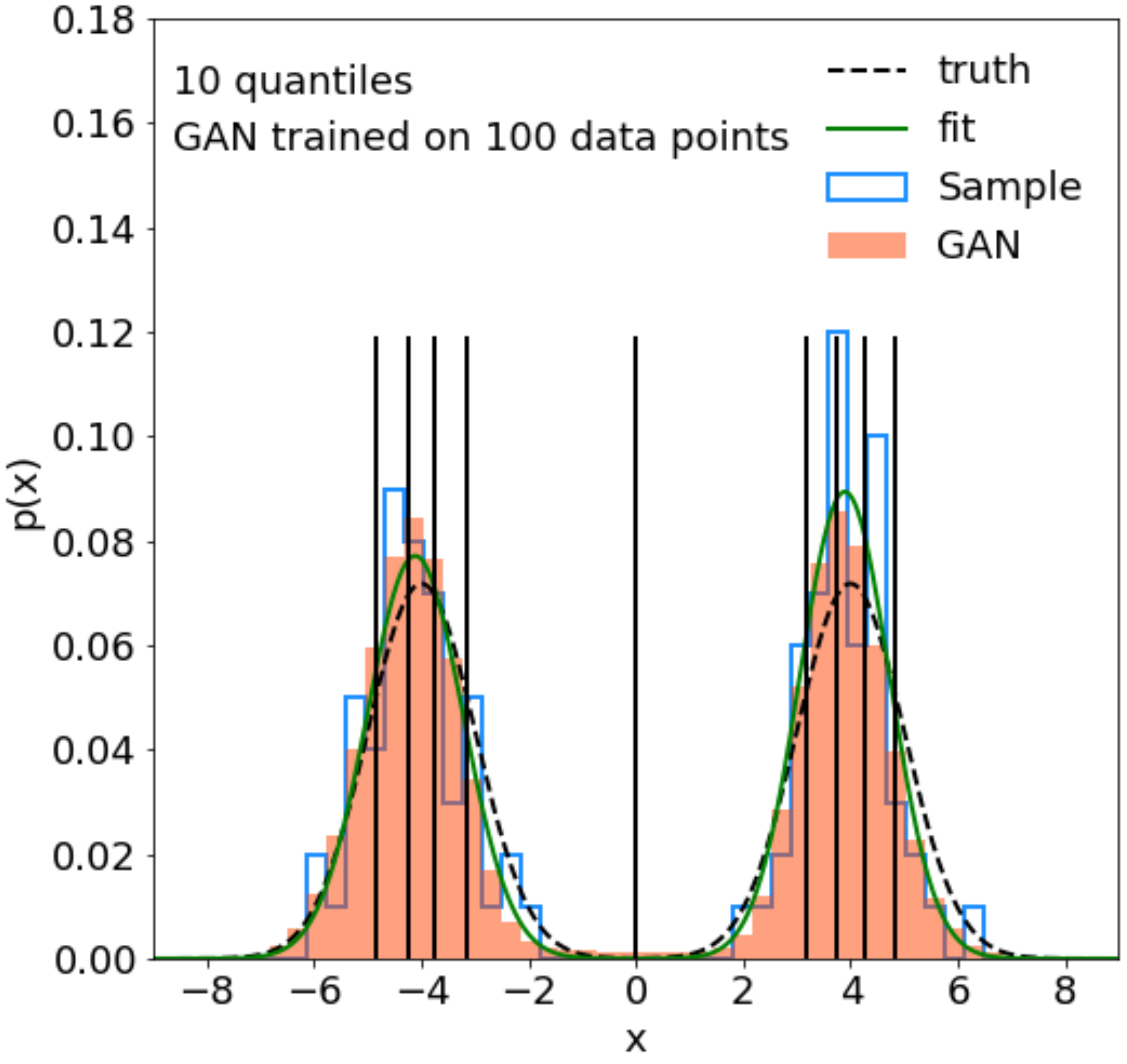
Generative Adversarial Network

- Train GAN on 100 data points from training sample
- Mode-collapse and overfitting problematic
  - Dropout
  - Added training noise
  - Batch-statistics



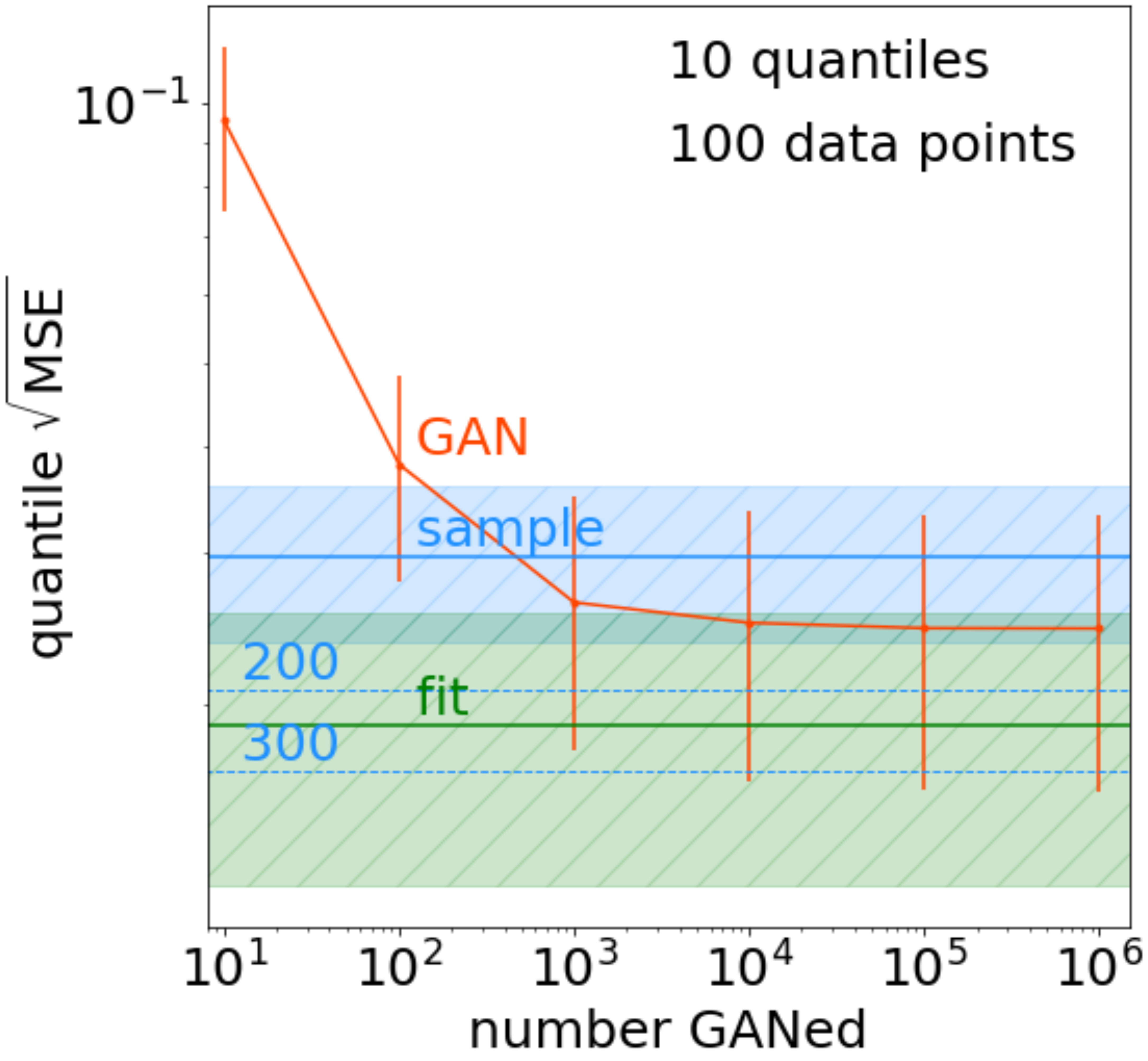
Generative Network

- Generate $O(10^7)$ data points using GAN
- Calculate fraction of points in each quantile
- Compare to train and fit



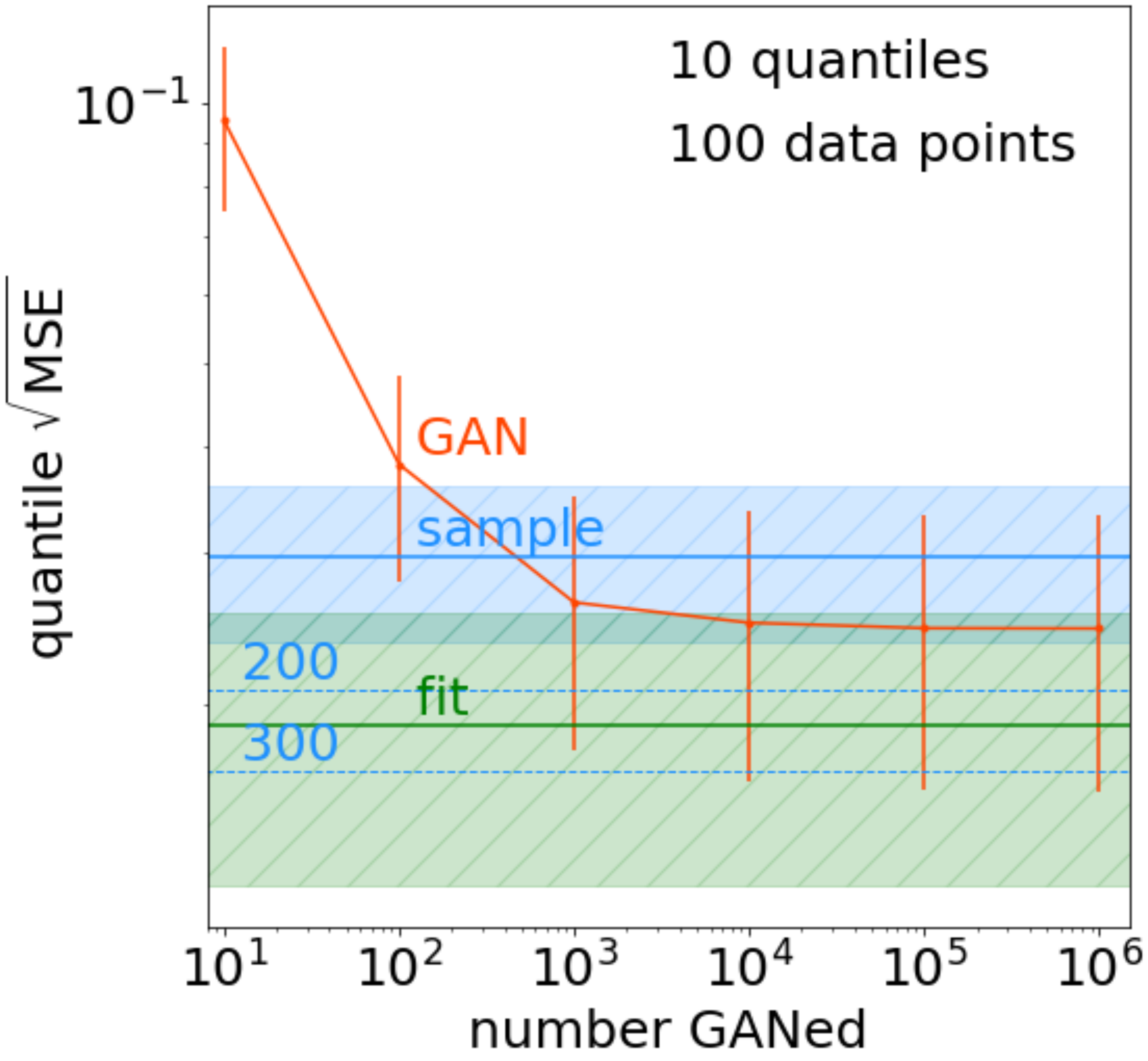
Generative Network

- For 100 training samples, 100 fits and 100 GANs compare MSE
- GAN describes distribution better than training data
- Needs 10,000 GANed points to match 150 true points
- Shifts statistical uncertainty to systematic uncertainty



Generative Network

- How is this possible?
- In terms of information:
  - sample: only data points
  - fit: data + true function
  - GAN: data + smooth, continuous function
- This allows the GAN to interpolate



Intermediate Conclusion

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generative model can speed up simulations