Quantum Assisted Calorimeter Simulation

J. Quetzalcoatl Toledo Marín - Research Associate @ TRIUMF :: 10/17/23 :: HEPiX Autumn 2023 Workshop

Acknowledgements

Project Team:

- Wojtek Fedorko @ TRIUMF (PI)
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- Sebastian Gonzalez @ TRIUMF (UG)
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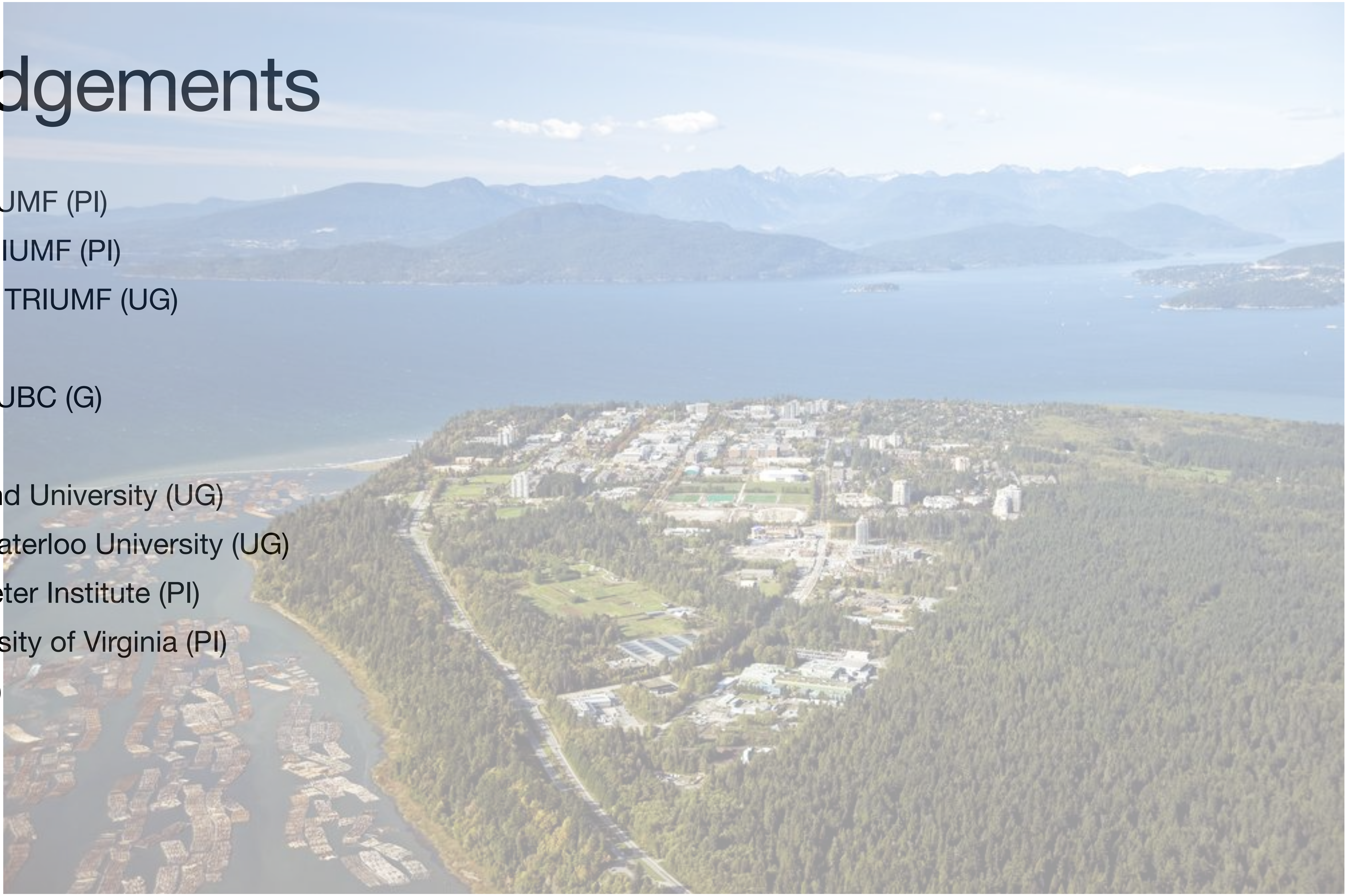
- Abhishek Abhishek @ UBC (G)
- Tiago Vale @ SFU (PD)
- Soren Andersen @ Lund University (UG)
- Sehmimul Hoque @ Waterloo University (UG)
- Roger Melko @ Perimeter Institute (PI)
- Geoffrey Fox @ University of Virginia (PI)
- Eric Paquet @ NRC (R)



Motivation

- Simulation plays a significant role in the design of future experiments but also in the analysis of the current ones.
- One single event fully simulated with Geant4 in an LHC experiment requires about 1000 CPU seconds.
- The calorimeter simulation is by far dominating the total simulation time.
- **AI generator models are being developed in particular for the simulation of calorimeters.**

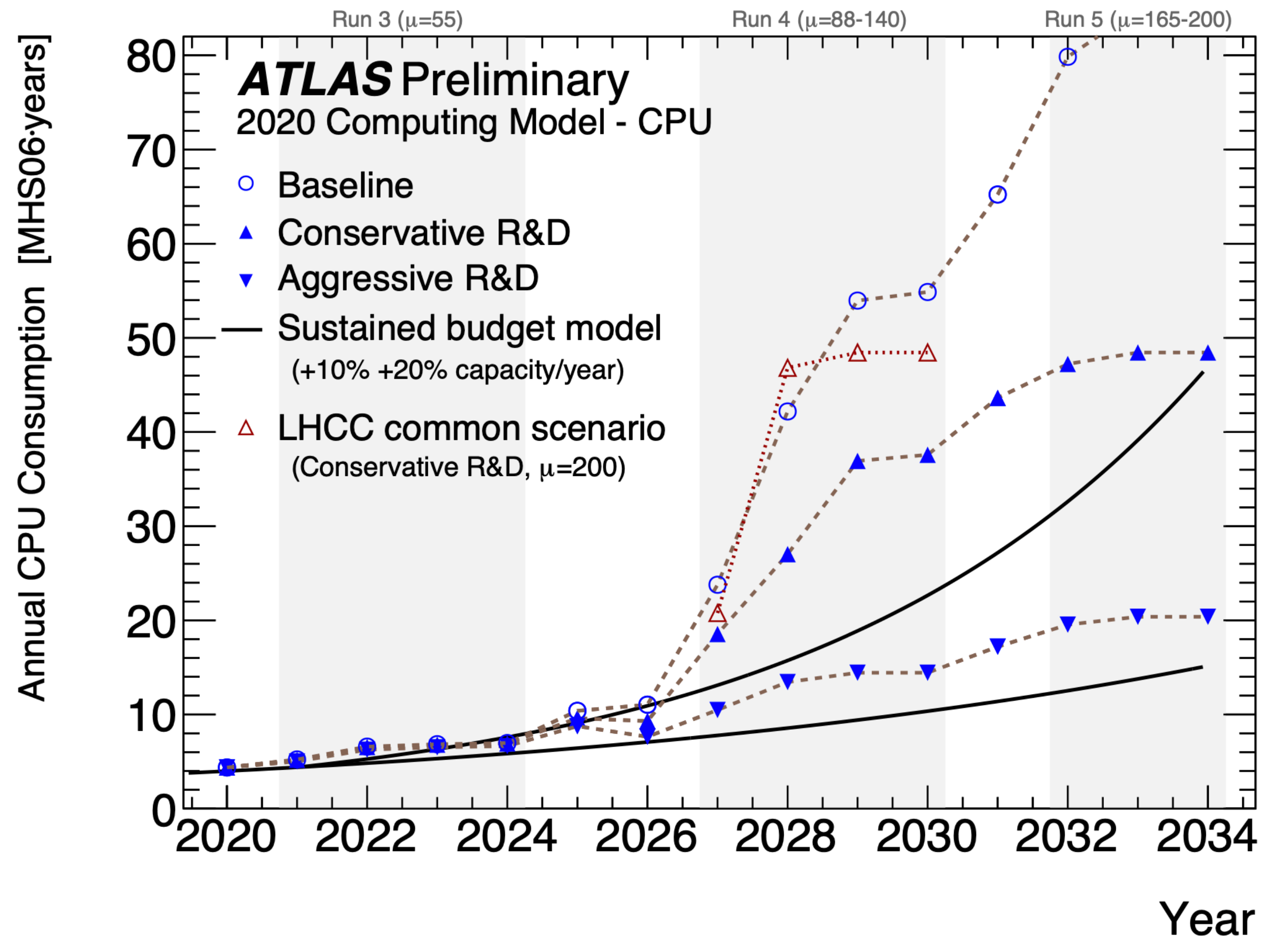


Figure 1. Projected CPU requirements of ATLAS experiment between 2020 and 2034 based on 2020 assessment. Three scenarios are shown, corresponding to an ambitious ("aggressive"), modest ("conservative") and minimal ("baseline") development program. The black lines indicate annual improvements of 10% and 20% in the computational capacity of new hardware for a given cost, assuming a sustained level of annual investment. The blue dots with the brown lines represent the 3 ATLAS scenarios following the present LHC schedule. The red triangles indicate the Conservative R&D scenario under an assumption of the LHC reaching in average 200 primary vertexes per one bunch crossing (μ) in Run4 (2028-2030).

Motivation

- One particle impacting a calorimeter can lead to thousands of secondary particles (called the shower) to be tracked through the detector, while only the total energy deposit per sensitive element (a cell) is useful.
- Can we go directly from the impacting particle parameter to the cell energy deposits?
- Could this speed up the simulation framework?

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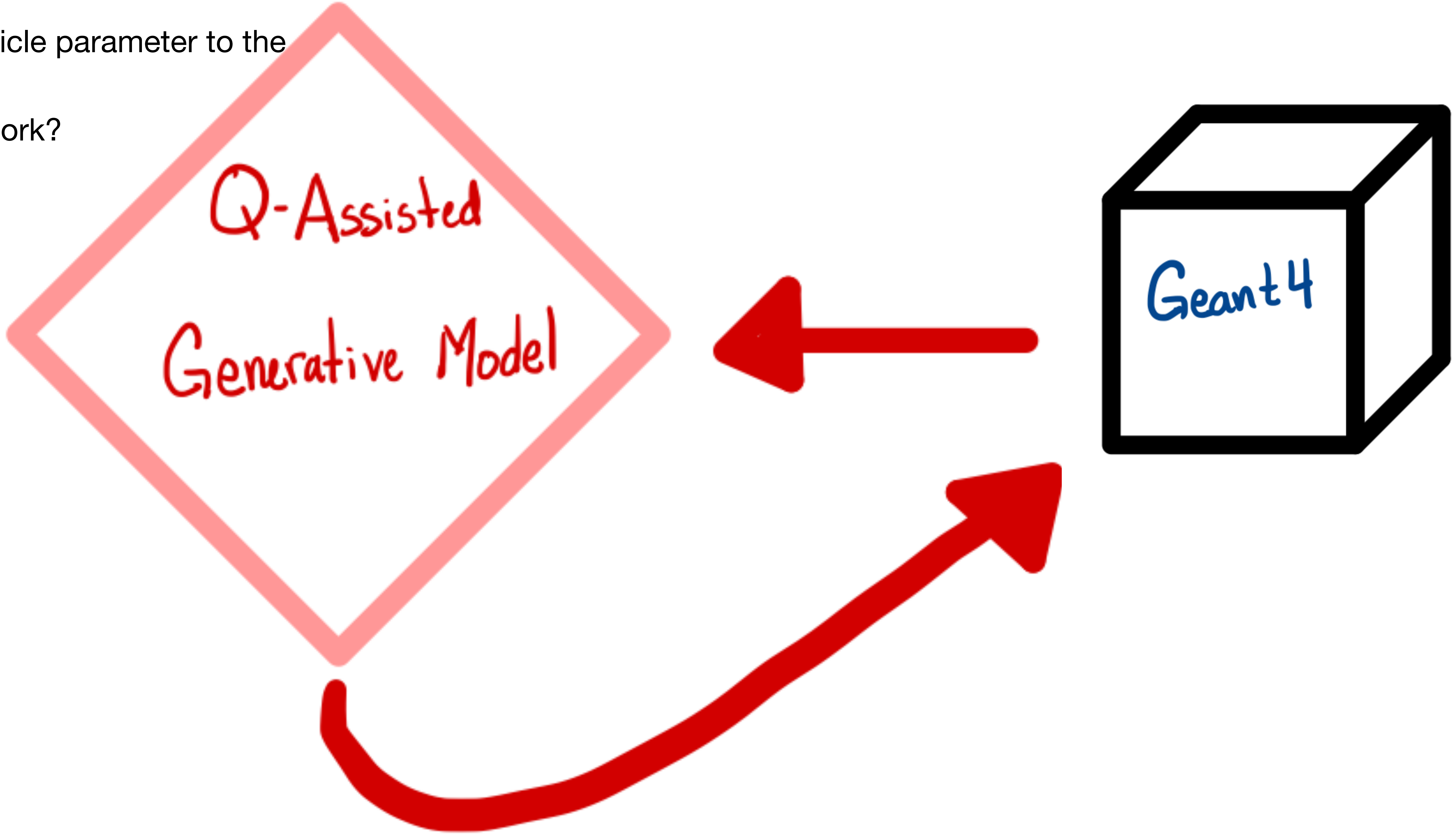

Motivation

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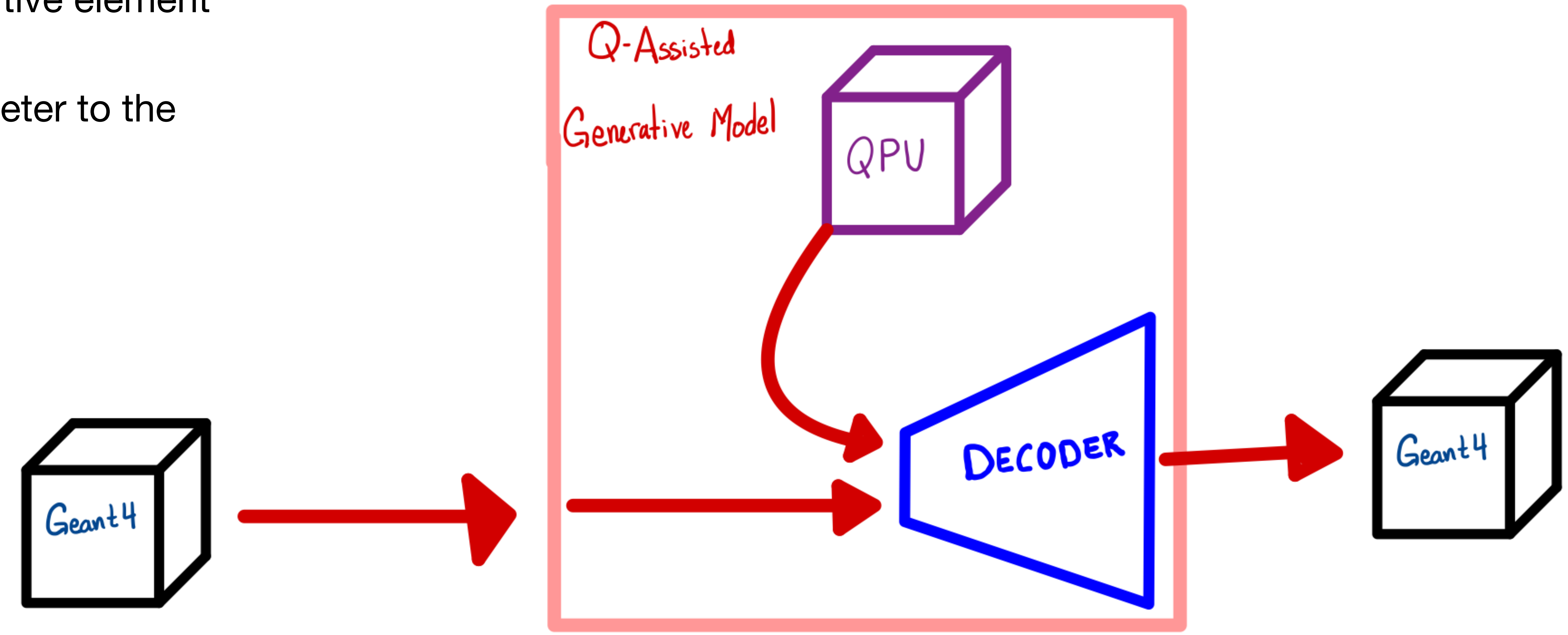


Contents

- Generative Models
    - Variational Autoencoders (VAE)
    - Restricted Boltzmann Machines (RBM)
    - Discrete VAE
- Quantum Annealers (QA)
- Dataset
- Results
- Conclusions

Generative Models

Simplest Example: Box-Muller Method

$$\int_0^1 dU_1 Uni(U_1) \int_0^1 dU_2 Uni(U_2) = \int_{-\infty}^{\infty} dZ_1 \mathcal{N}(Z_1 | 0,1) \int_{-\infty}^{\infty} dZ_2 \mathcal{N}(Z_2 | 0,1) = 1$$

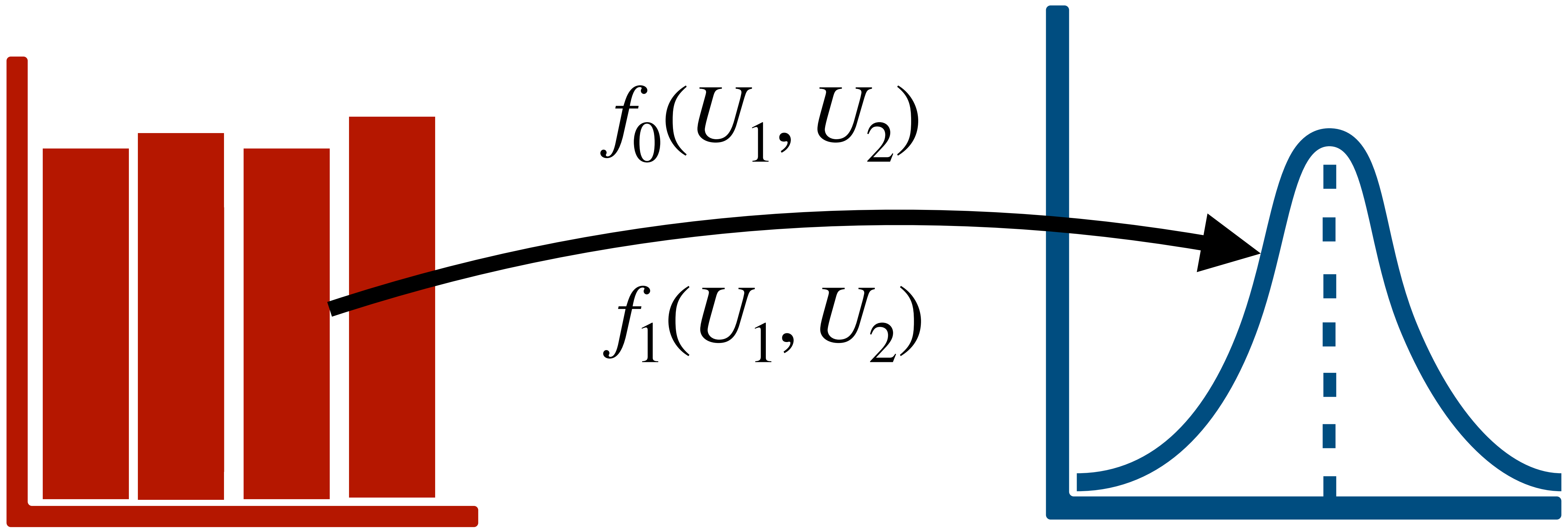
1. Generate two **uniformly** independent, identically distributed random numbers U_1 and U_2.

$$\int_0^{u_1} dU_1 Uni(U_1) \int_0^{u_2} dU_2 Uni(U_2) = \int_a^b \int_c^d dZ_0 dZ_1 \underbrace{\left| \frac{\partial(U_1, U_2)}{\partial(Z_0, Z_1)} \right| Uni(U_1(Z_0, Z_1)) Uni(U_2(Z_0, Z_1))}_{\mathcal{N}(Z_0 | 0,1) \mathcal{N}(Z_1 | 0,1)}$$

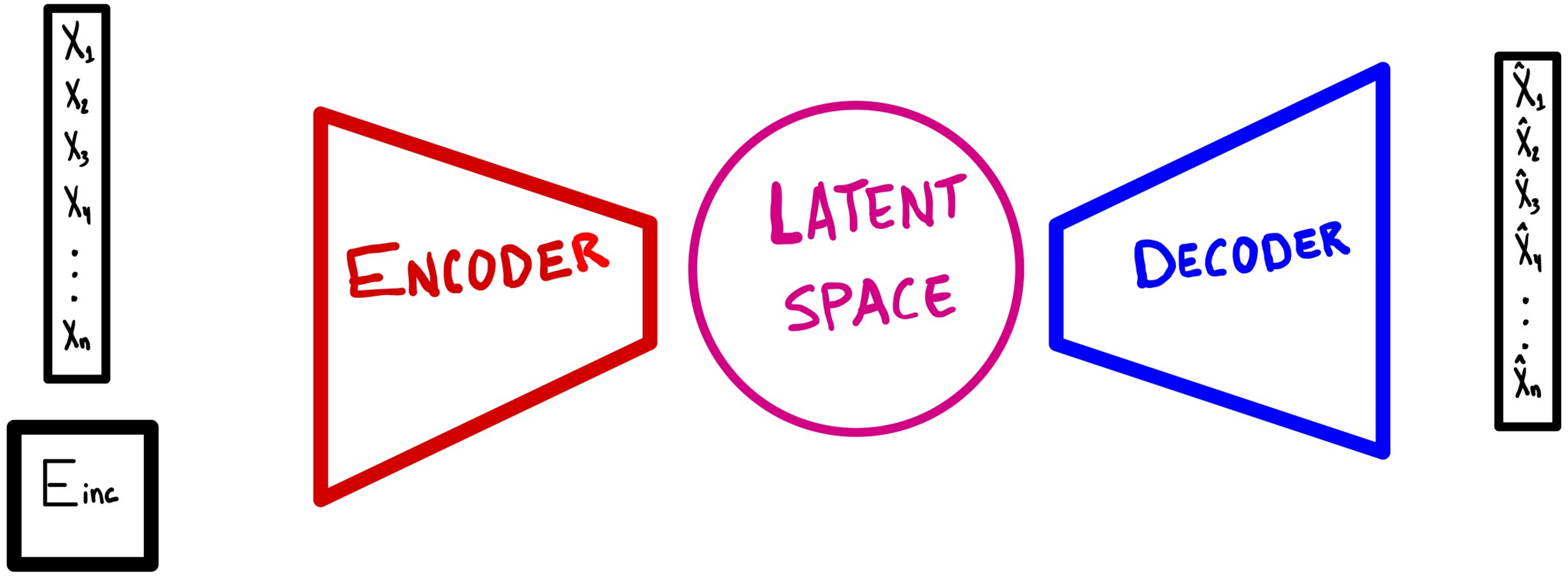
2. Substitute in:

   1. $Z_0 = f_0(U_1, U_2) = \sqrt{-2 \ln U_1} \cos(2\pi U_2)$

   2. $Z_1 = f_1(U_1, U_2) = \sqrt{-2 \ln U_1} \sin(2\pi U_2)$



Variational Autoencoders

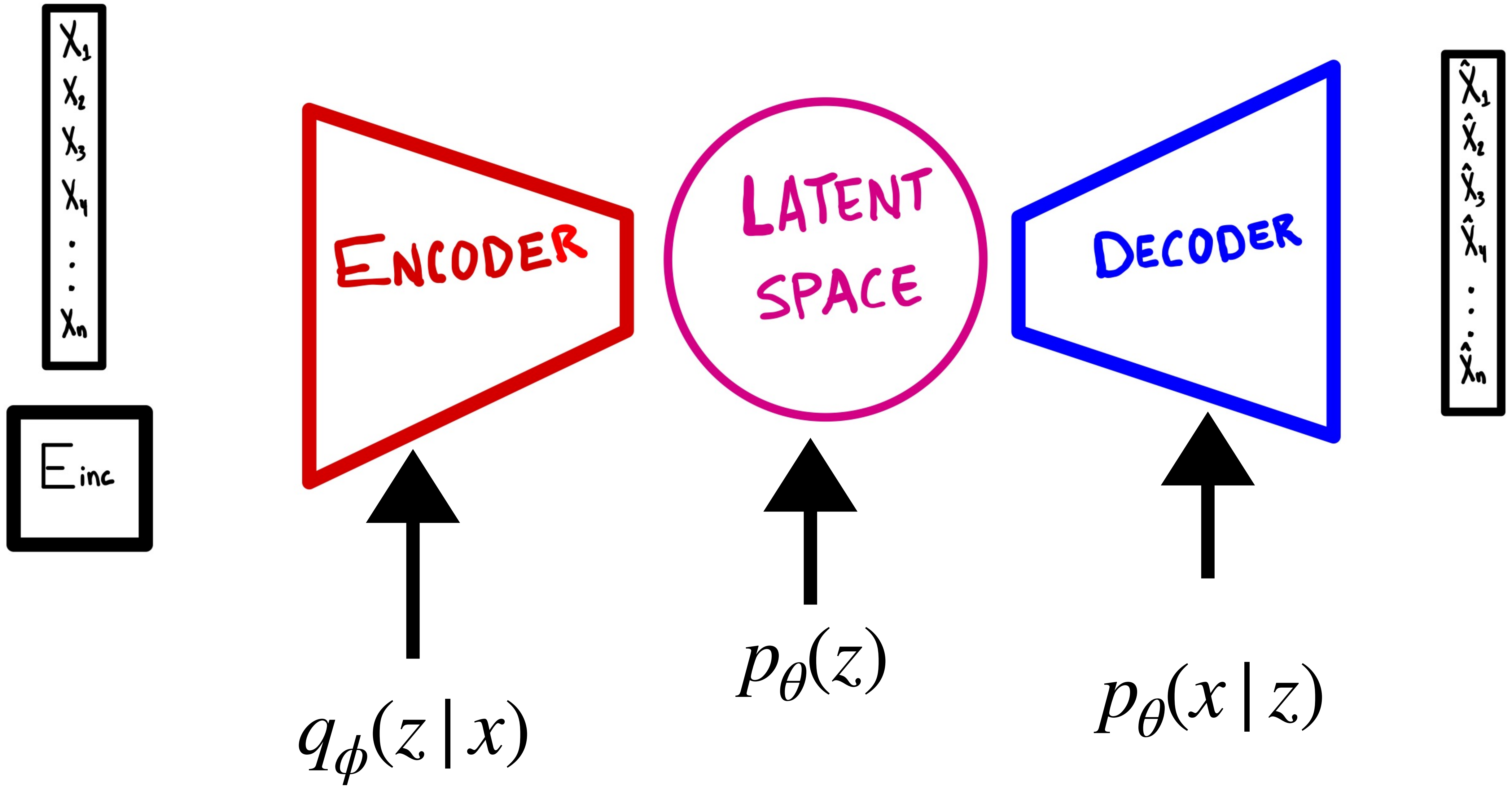


Variational Autoencoders

X: event

Z: Encoded data

Phi and theta are fitting parameters

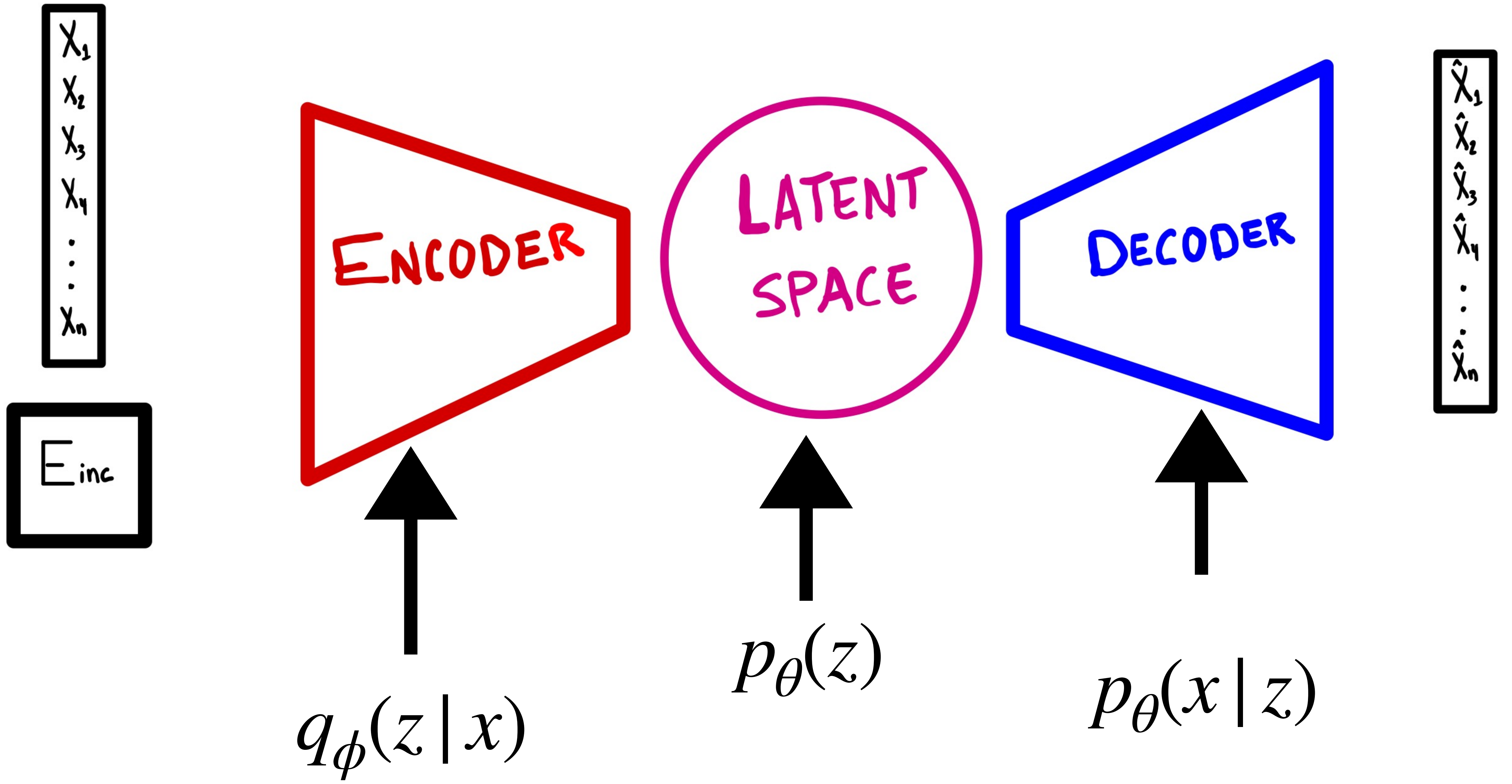


$q_\phi(z|x)$

$p_\theta(z)$

$p_\theta(x|z)$

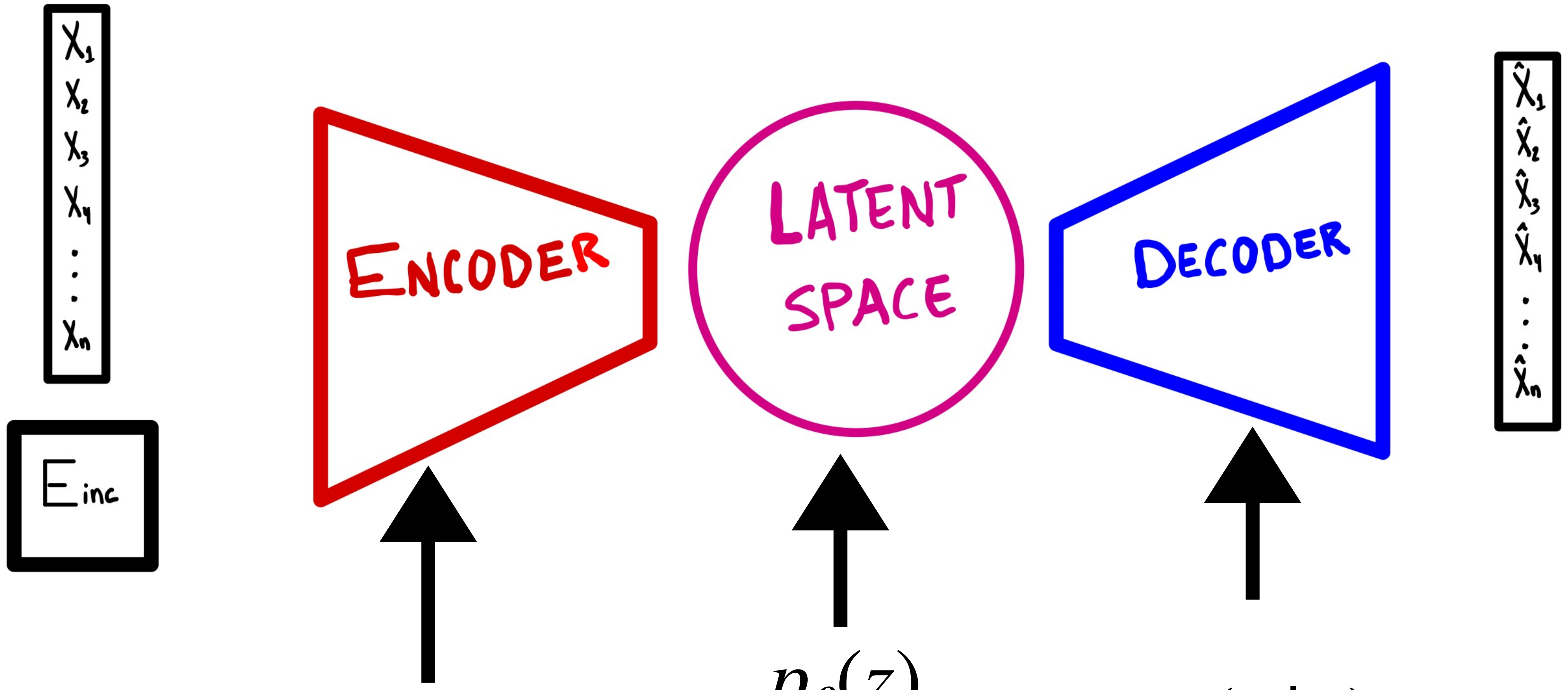
Variational Autoencoders



$q_\phi(z \mid x)$ $p_\theta(z)$ $p_\theta(x \mid z)$

$$\mathscr{L}_{\phi,\theta}(x) = \langle \ln p_\theta(x \mid z) \rangle_{q_\phi(z|x)} - \langle \ln \frac{q_\phi(z \mid x)}{p_\theta(z)} \rangle_{q_\phi(z|x)}$$

Variational Autoencoders

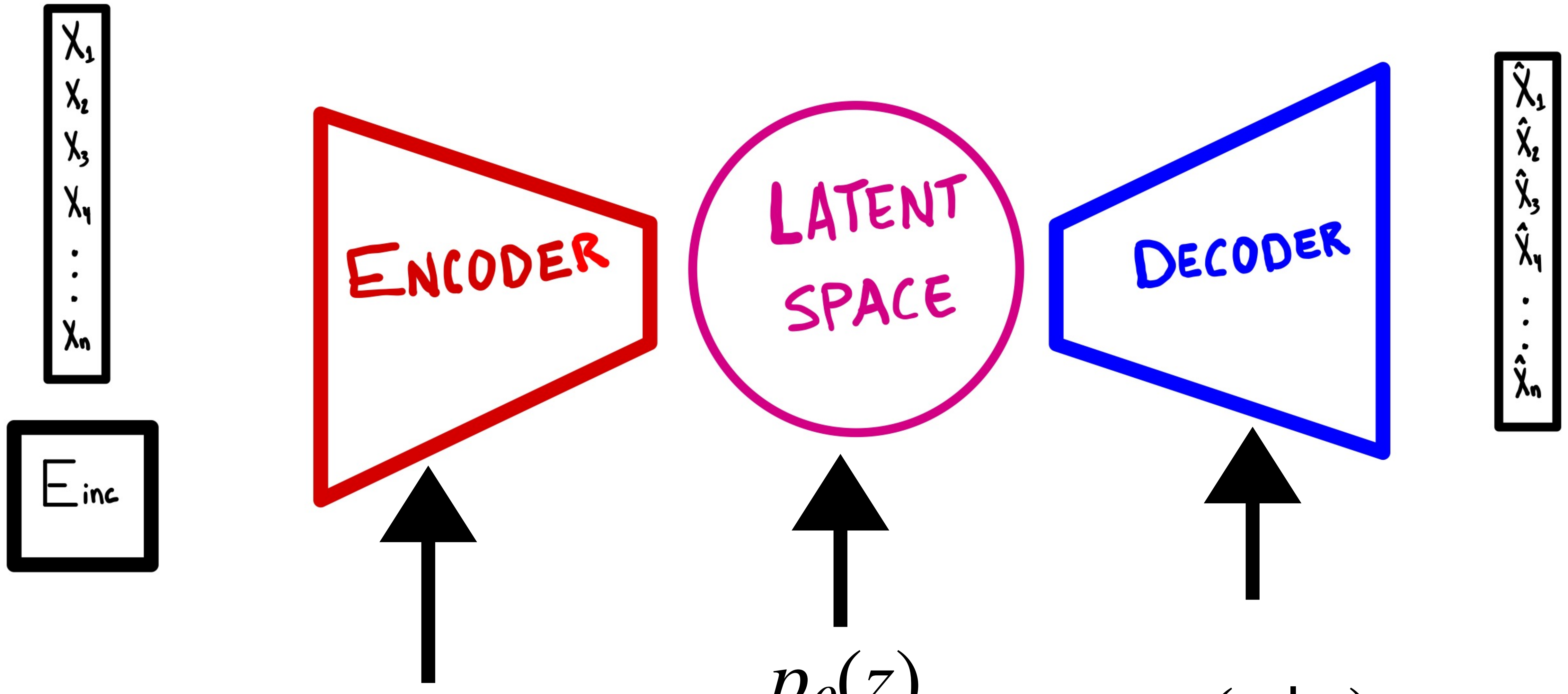


$q_\phi(z \mid x)$ $p_\theta(z)$ $p_\theta(x \mid z)$

$$\mathcal{L}_{\phi,\theta}(x) = \underbrace{\langle \ln p_\theta(x \mid z) \rangle_{q_\phi(z|x)}}_{\text{Reconstruction}} - \underbrace{\left\langle \ln \frac{q_\phi(z \mid x)}{p_\theta(z)} \right\rangle_{q_\phi(z|x)}}_{\text{Regularizer}}$$

Variational Autoencoders

$$\langle f_\phi(z) \rangle_{q_\phi(z|x)} \sim \sum_{z \sim q_\phi(z|x)} f_\phi(z)$$



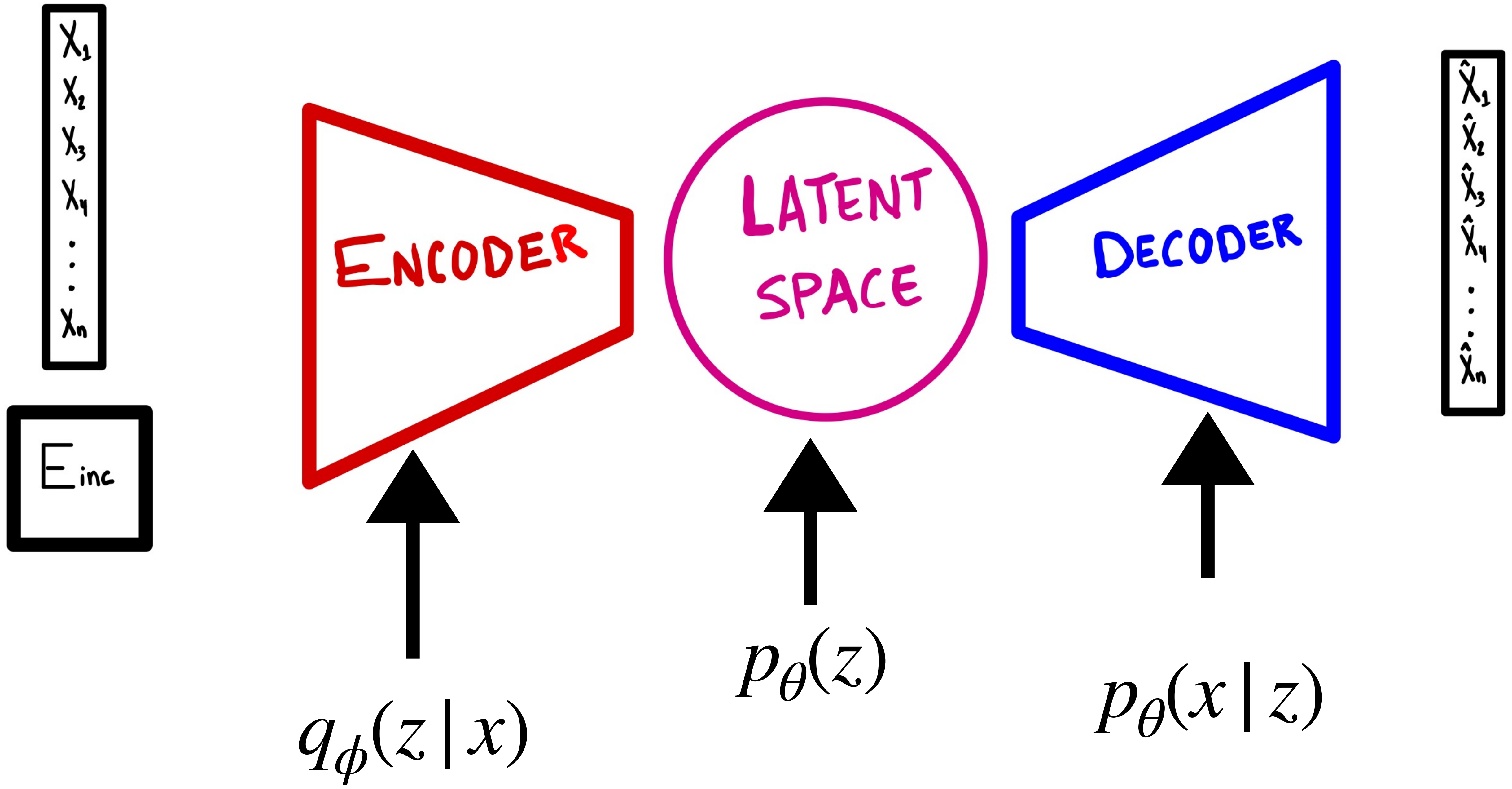
$p_\theta(z)$

$p_\theta(x\,|\,z)$

$q_\phi(z\,|\,x)$

$$\mathcal{L}_{\phi,\theta}(x) = \underbrace{\langle \ln p_\theta(x\,|\,z) \rangle_{q_\phi(z|x)}}_{\text{Reconstruction}} - \underbrace{\left\langle \ln \frac{q_\phi(z\,|\,x)}{p_\theta(z)} \right\rangle_{q_\phi(z|x)}}_{\text{Regularizer}}$$

Variational Autoencoders



X_1 X_2 X_3 X_4 ⋮ X_n
E_{inc}
ENCODER
LATENT SPACE
DECODER
$\hat{X}_1$ $\hat{X}_2$ $\hat{X}_3$ $\hat{X}_4$ ⋮ $\hat{X}_n$
$q_\phi(z\,|\,x)$
$p_\theta(z)$
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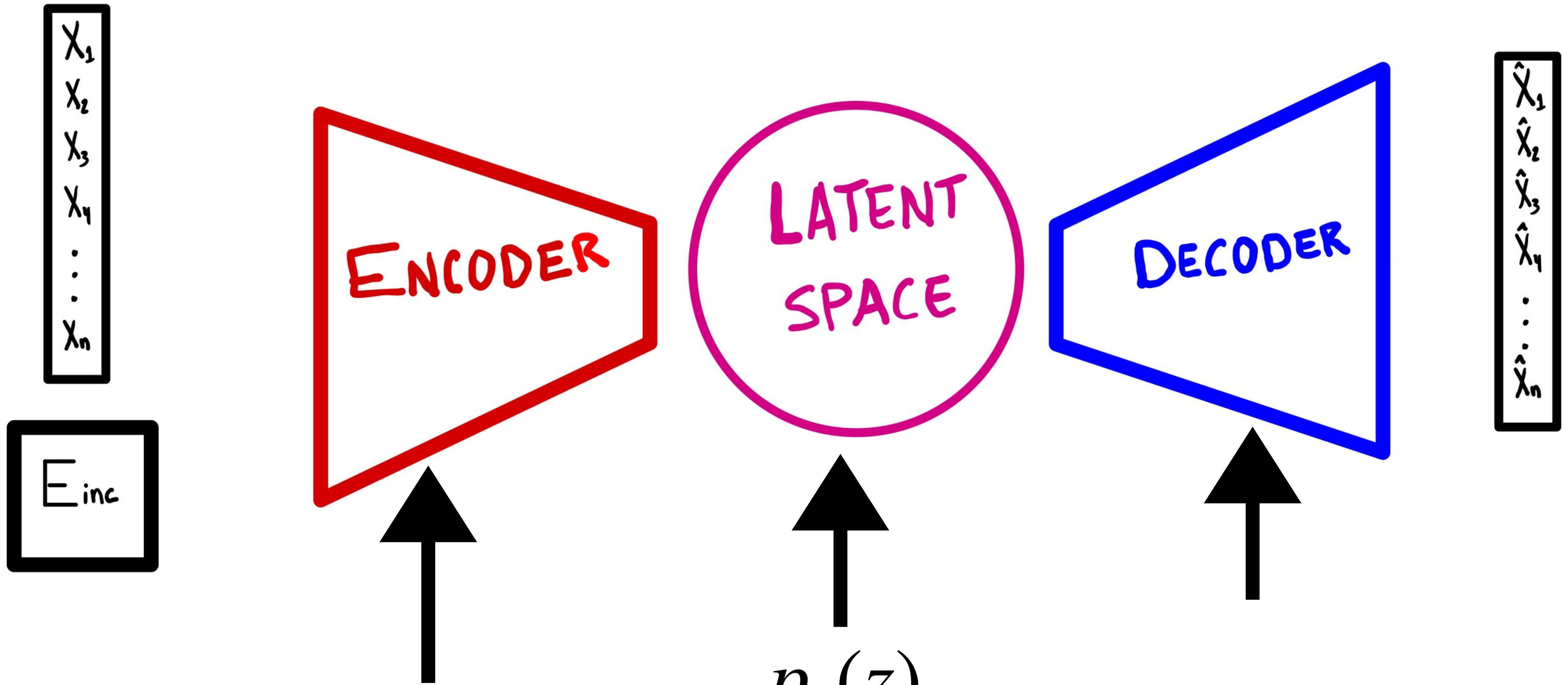
$$\mathscr{L}_{\phi,\theta}(x) = \underbrace{\langle \ln p_\theta(x\,|\,z)\rangle_{q_\phi(z|x)}}_{\text{Reconstruction}} - \underbrace{\langle \ln \frac{q_\phi(z\,|\,x)}{p_\theta(z)}\rangle_{q_\phi(z|x)}}_{\text{Regularizer}}$$

$$\langle f_\phi(z)\rangle_{q_\phi(z|x)} \sim \sum_{z\sim q_\phi(z|x)} f_\phi(z)$$

$$\nabla_\phi \langle f_\phi(z)\rangle_{q_\phi(z|x)} \sim \nabla_\phi \sum_{z\sim q_\phi(z|x)} f_\phi(z)$$

Variational Autoencoders



$q_\phi(z\,|\,x)$ $p_\theta(z)$ $p_\theta(x\,|\,z)$

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$$\nabla_\phi \langle f_\phi(z)\rangle_{q_\phi(z|x)} \sim \nabla_\phi \sum_{z\sim q_\phi(z|x)} f_\phi(z)$$

$$\downarrow$$

$$\nabla_\phi \sum_{\boxed{\epsilon\sim\mathcal{N}(0,1)}} f_\phi(z(\epsilon))$$

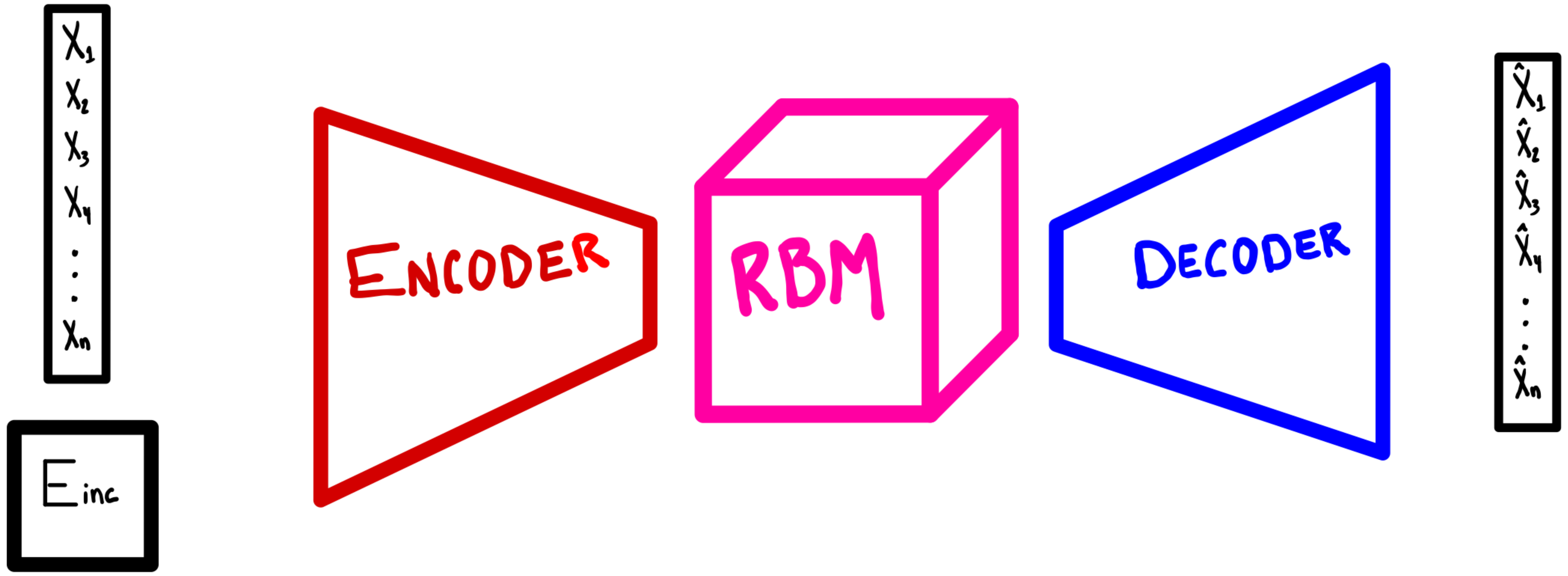
Reparameterization Trick

$$\boxed{z = \mu_\phi(x) + \sigma_\phi(x)\cdot\epsilon}$$

$$\mathcal{N}(\epsilon\,|\,0,1) = |\frac{dz}{d\epsilon}|\,q_\phi(z\,|\,x)$$

Restricted Boltzmann Machine

Why?

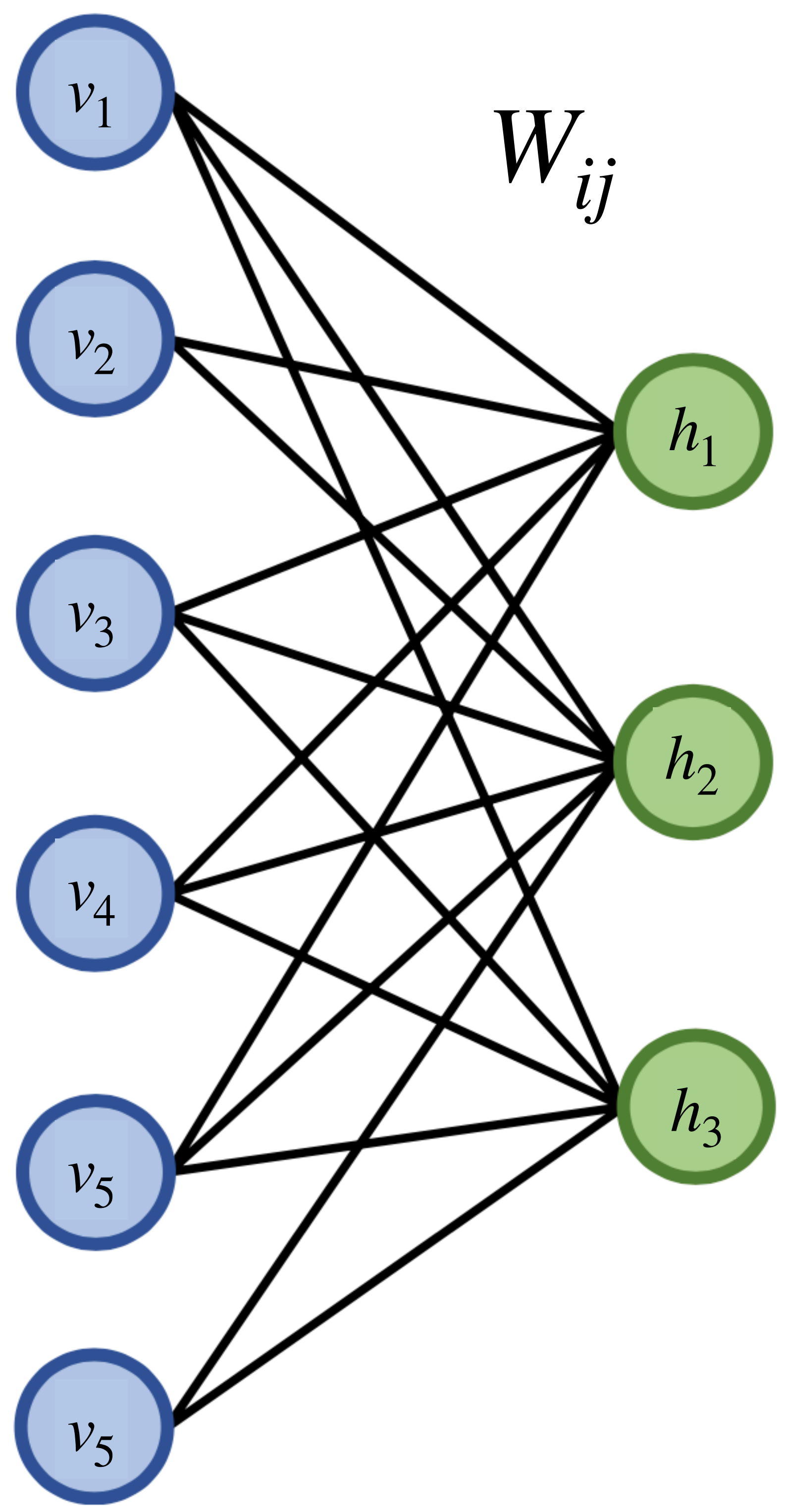


- More expressiveness
- However, this comes at a cost.

Restricted Boltzmann Machine

Basics

$\langle v|$ $|h\rangle$



Suppose a data set $\{v^\alpha\}_{\alpha=1}^{n}$, such that $v_i \in \{0,1\}$.

I) An RBM will fit a Boltzmann distribution, $p(v,h)$, to the data set.

II) The fitting is done by maximizing the log-likelihood, $\ln p(v)$.

III) RBMs are composed by a two-partite graph, where **v** denotes the visible layer and **h** the hidden layer.

$$p(v,h) = \frac{\exp(-E(v,h))}{Z}$$

Boltzmann Dist

$$E(v,h) = -\sum_{i=1}^{n_v} v_i a_i - \sum_{j=1}^{n_h} b_j h_j - \sum_{i,j} v_i W_{ij} h_j$$

Energy

$$Z(W,a,b,\beta=1) = \sum_{v',h'} \exp(-E(v',h'))$$

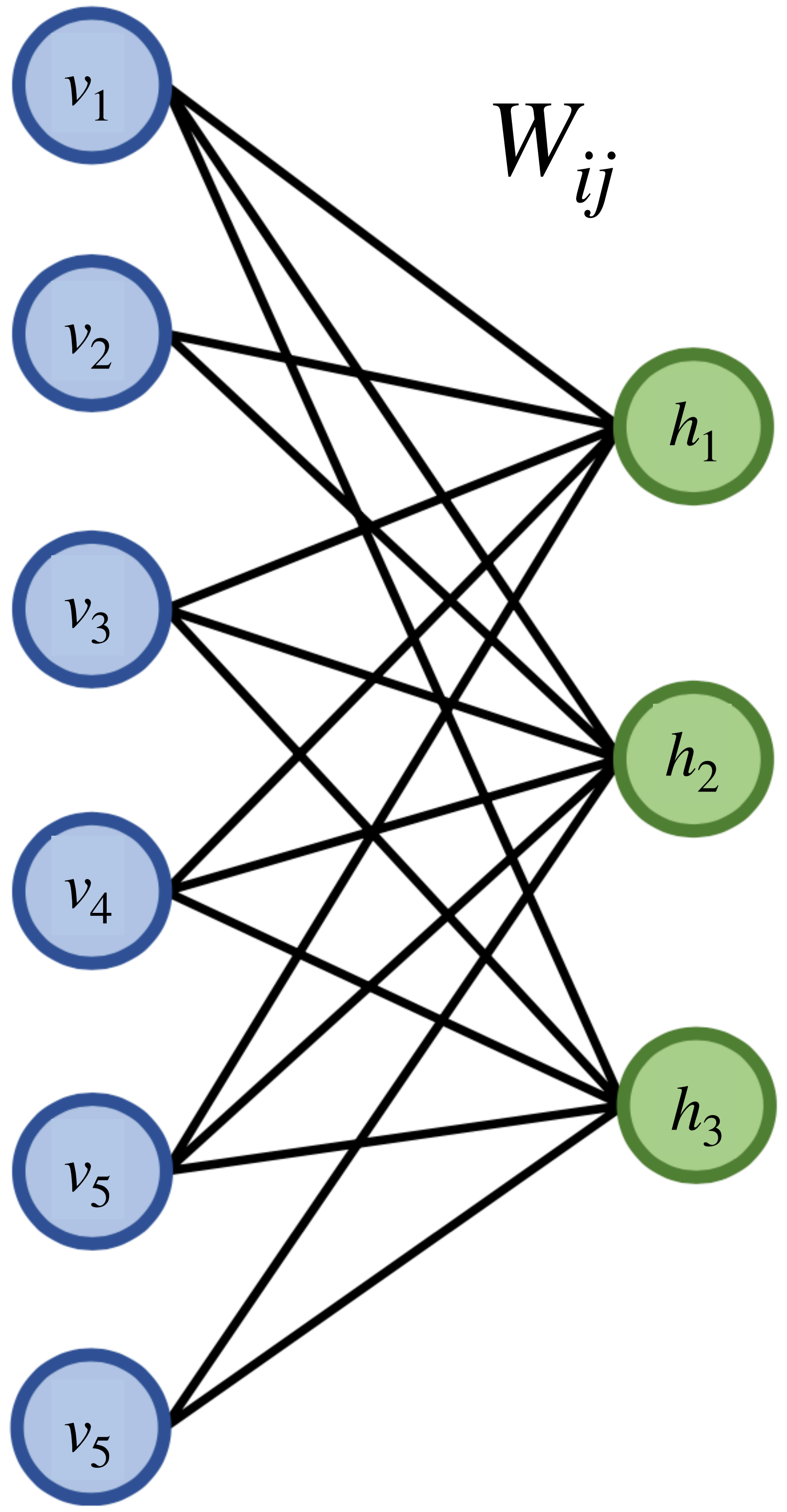
Partition Function

Restricted Boltzmann Machine

Basics

$\langle v |$ $| h \rangle$

$$\frac{\partial \ln p(v)}{\partial W_{ij}} = \langle v_i h_j \rangle_{p(h|v^\alpha)} - \langle v_i h_j \rangle_{p(h',v')}$$



Restricted Boltzmann Machine

Basics

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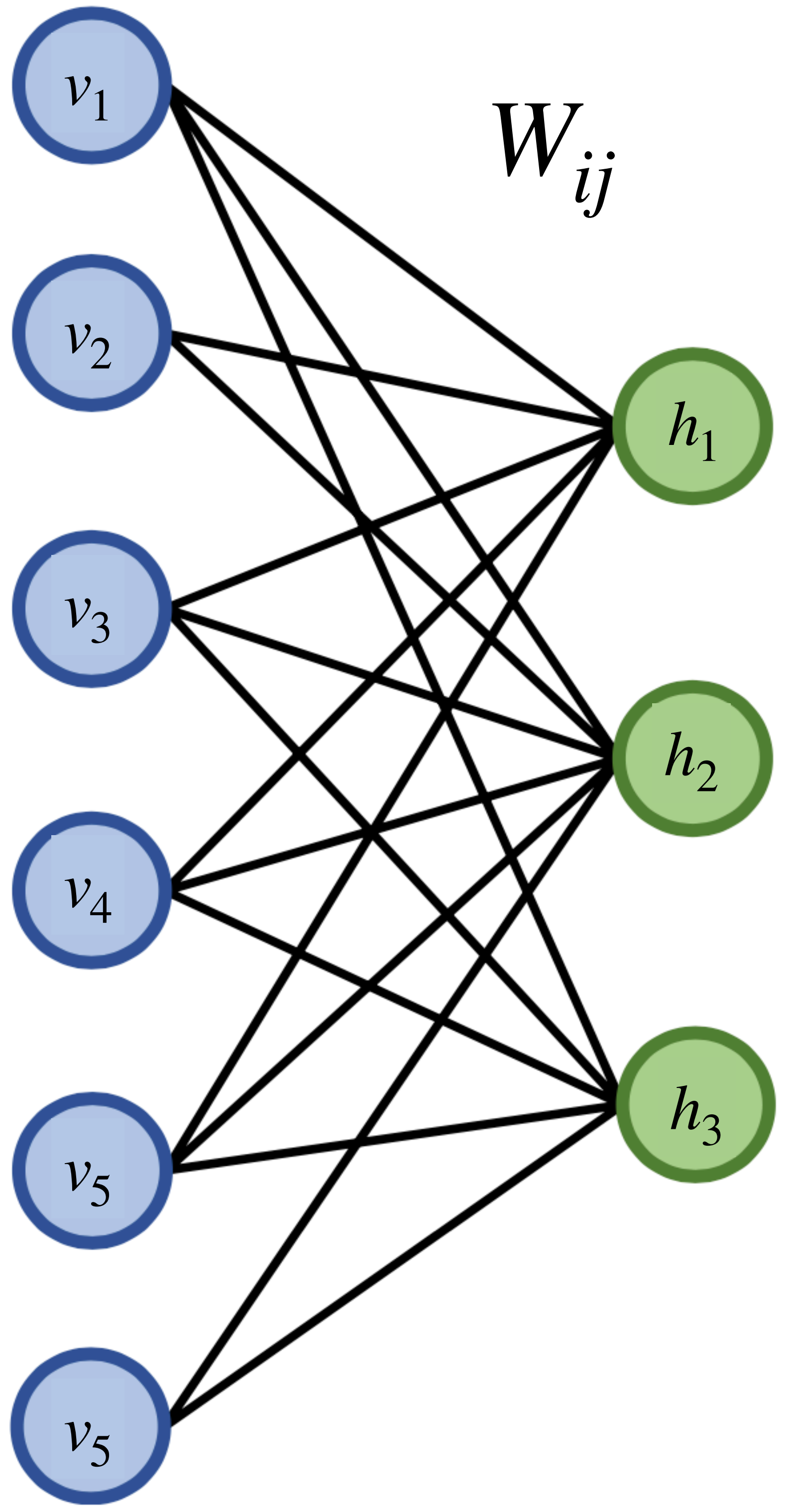

1.Start with random initial vector: $|v\rangle$

2. $|h^{(1)}\rangle \sim B[\sigma(W^t|v^{(0)}\rangle + |b\rangle)]$

3. $|v^{(1)}\rangle \sim B[\sigma(W|h^{(1)}\rangle + |a\rangle)]$

4.Repeat steps 2 and 3 n times.

$$|h^{(n)}\rangle \sim B[\sigma(W^t|v^{(n-1)}\rangle + |b\rangle)]$$
$$|v^{(n)}\rangle \sim B[\sigma(W|h^{(n)}\rangle + |a\rangle)]$$

Restricted Boltzmann Machine

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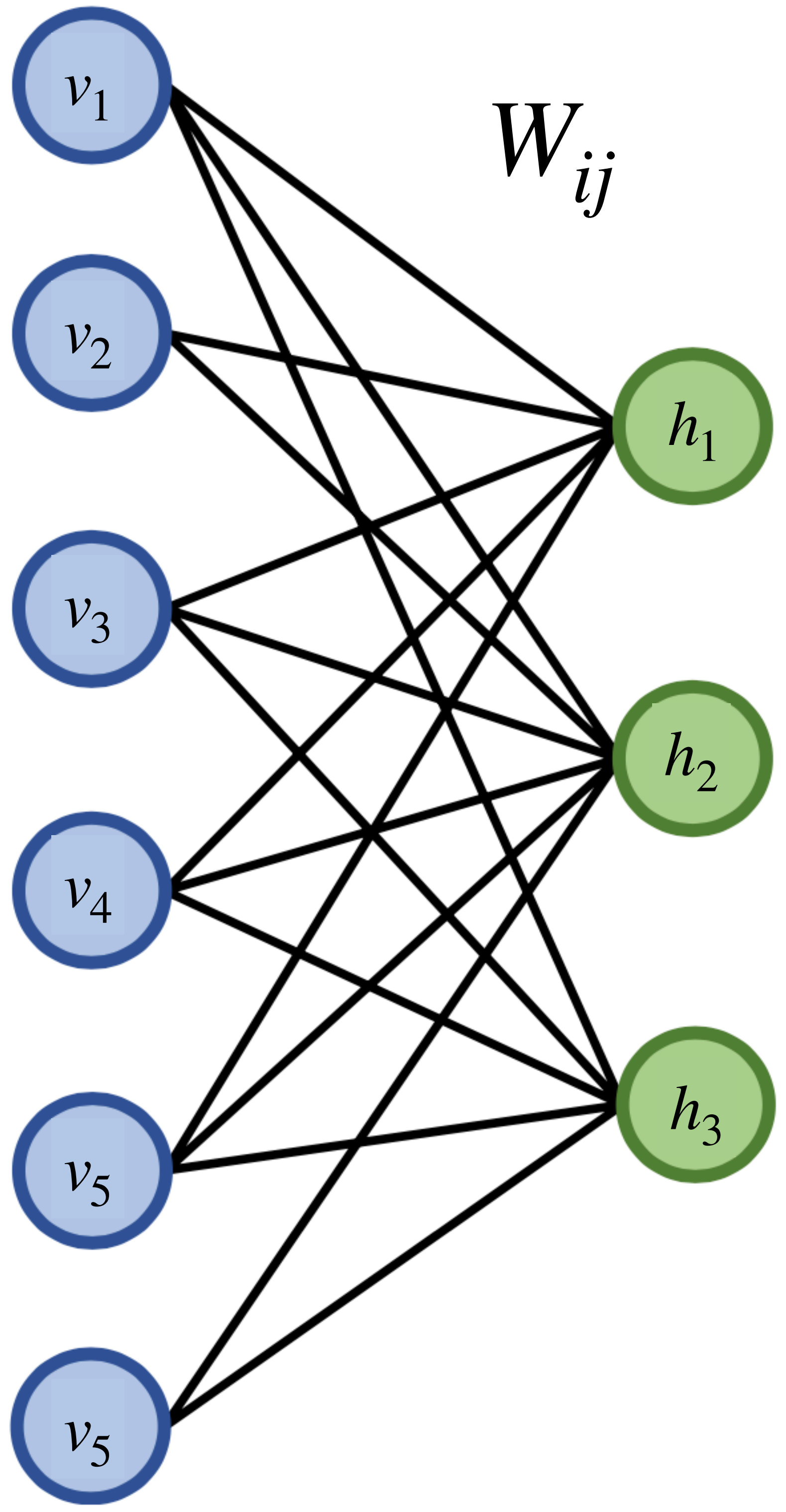

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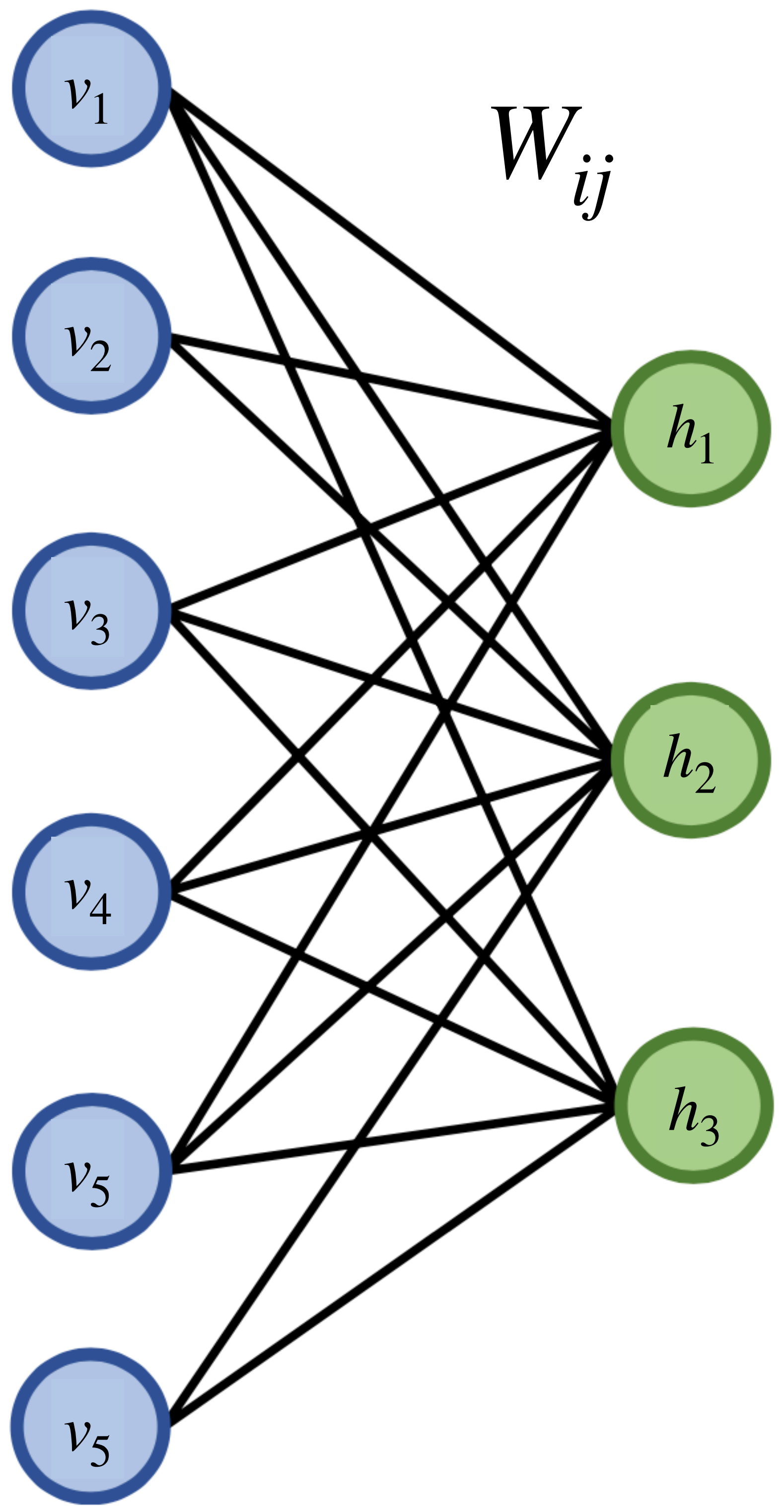
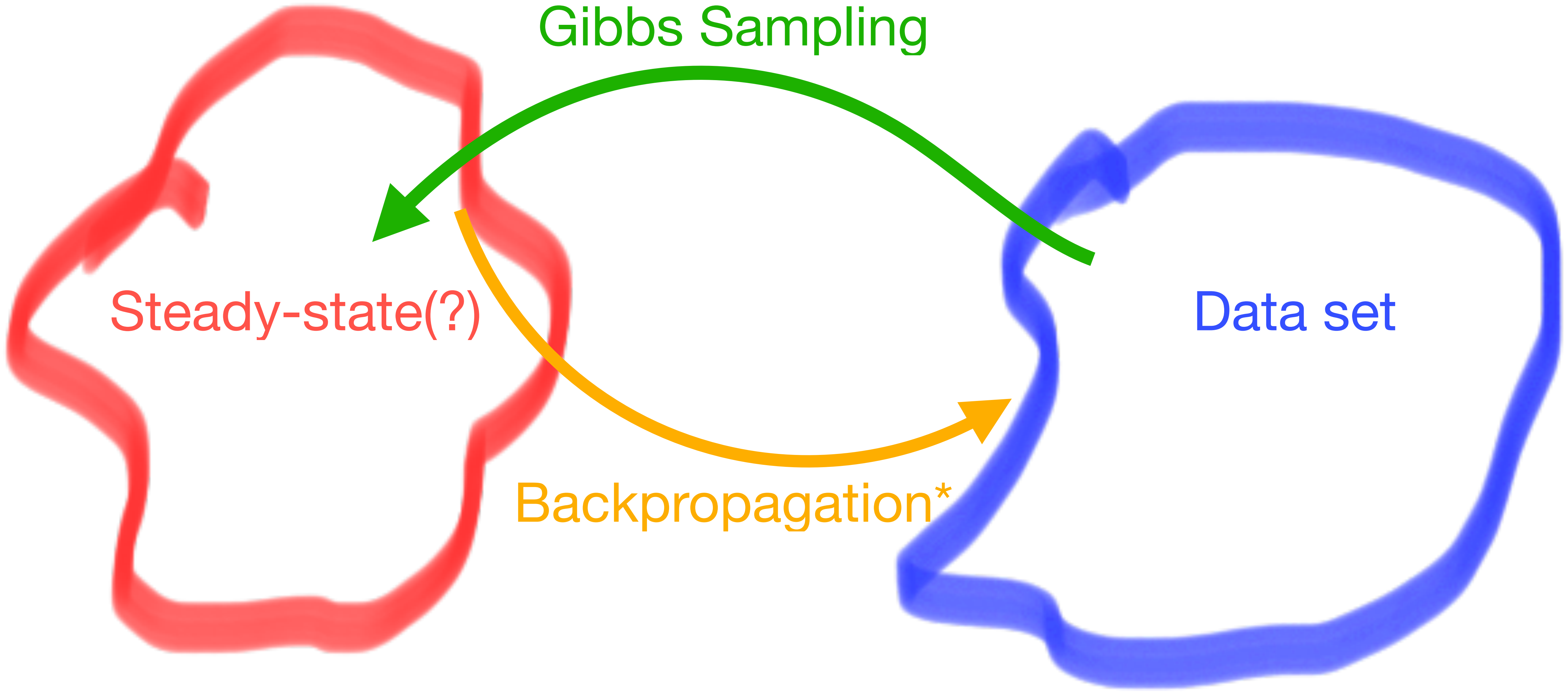
<— Repeat this a number of times equal to batch size.

Restricted Boltzmann Machine

Basics

$\langle v|$ $\quad$ $|h\rangle$





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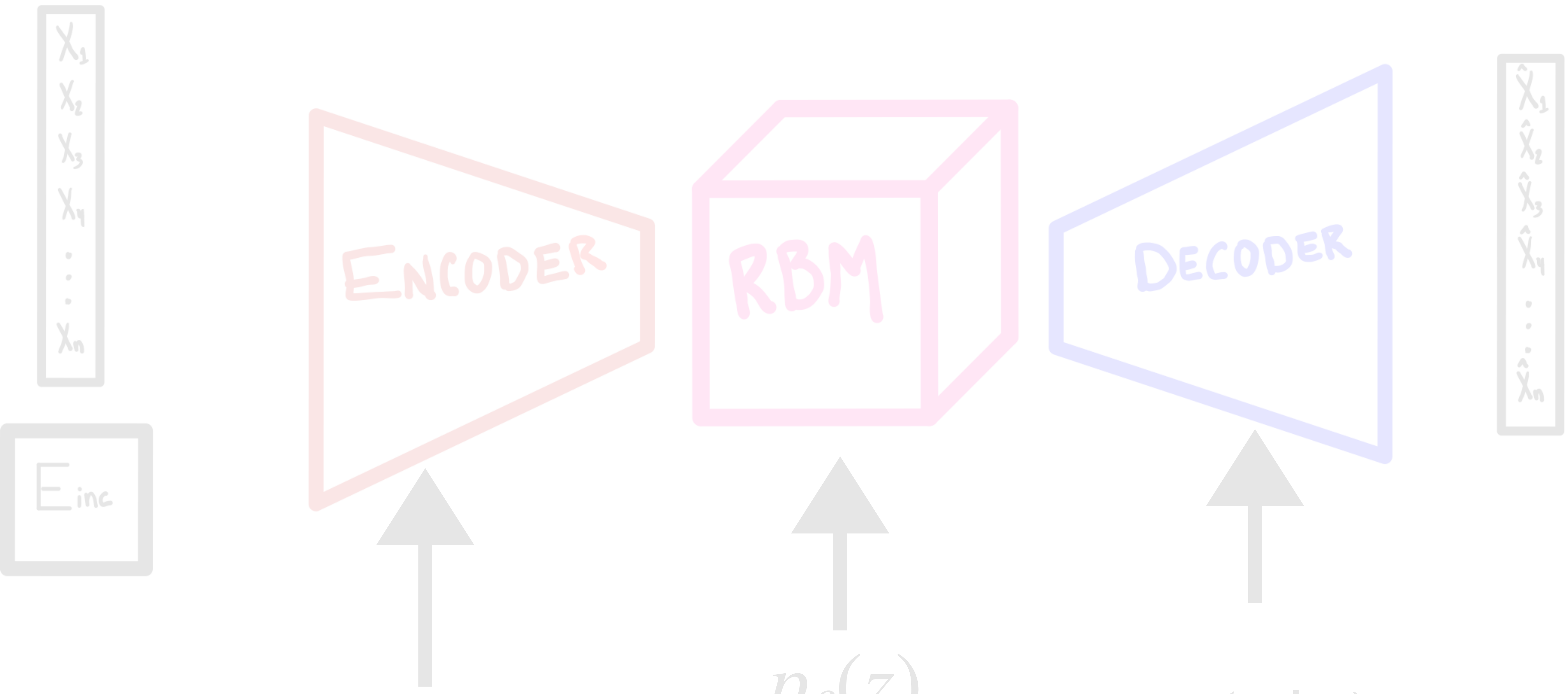
Discrete VAE



$q_\phi(z|x)$ $p_\theta(z)$ $p_\theta(x|z)$

$$\mathcal{L}_{\phi,\theta}(x) = \underbrace{\langle \ln p_\theta(x|z)\rangle_{q_\phi(z|x)}}_{\text{Reconstruction}} - \underbrace{\langle \ln \frac{q_\phi(z|x)}{p_\theta(z)}\rangle_{q_\phi(z|x)}}_{\text{Regularizer}}$$

$$\mathcal{L}_{\phi,\theta}(x) = \ln p_\theta(x) - D_{KL}(q_\phi(z|x)||p_\theta(z|x)) \leq \ln p_\theta(x)$$

$$\langle f_\phi(z)\rangle_{q_\phi(z|x)} \sim \sum_{z\sim q_\phi(z|x)} f_\phi(z)$$

$$\nabla_\phi \langle f_\phi(z)\rangle_{q_\phi(z|x)} \sim \nabla_\phi \sum_{z\sim q_\phi(z|x)} f_\phi(z)$$

↓

$$\nabla_\phi \sum_{\boxed{u\sim Uni(0,1)}} f_\phi(z(u))$$

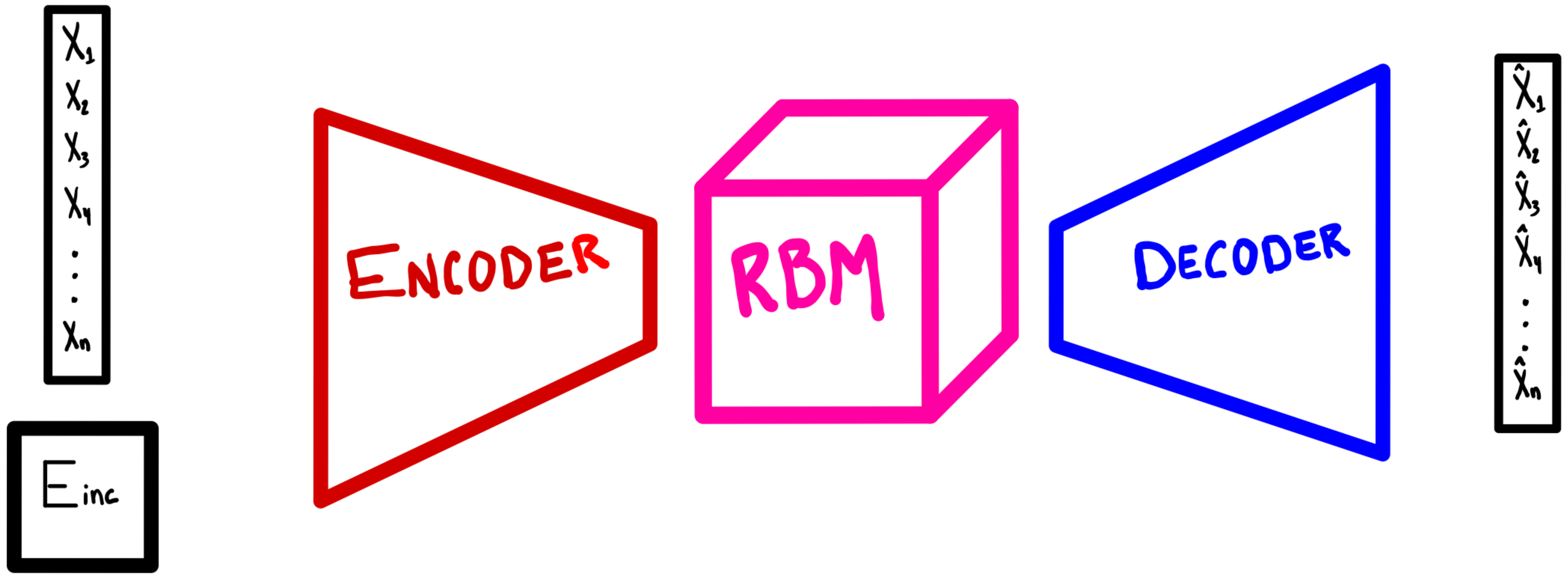
Gumbel Trick

$$\boxed{z = \sigma(\frac{l(\phi,x)+\sigma^{-1}(u)}{\tau})}$$

$$\rho(u) = |\frac{dz}{du}|q_\phi(z|x)$$

Discrete VAE

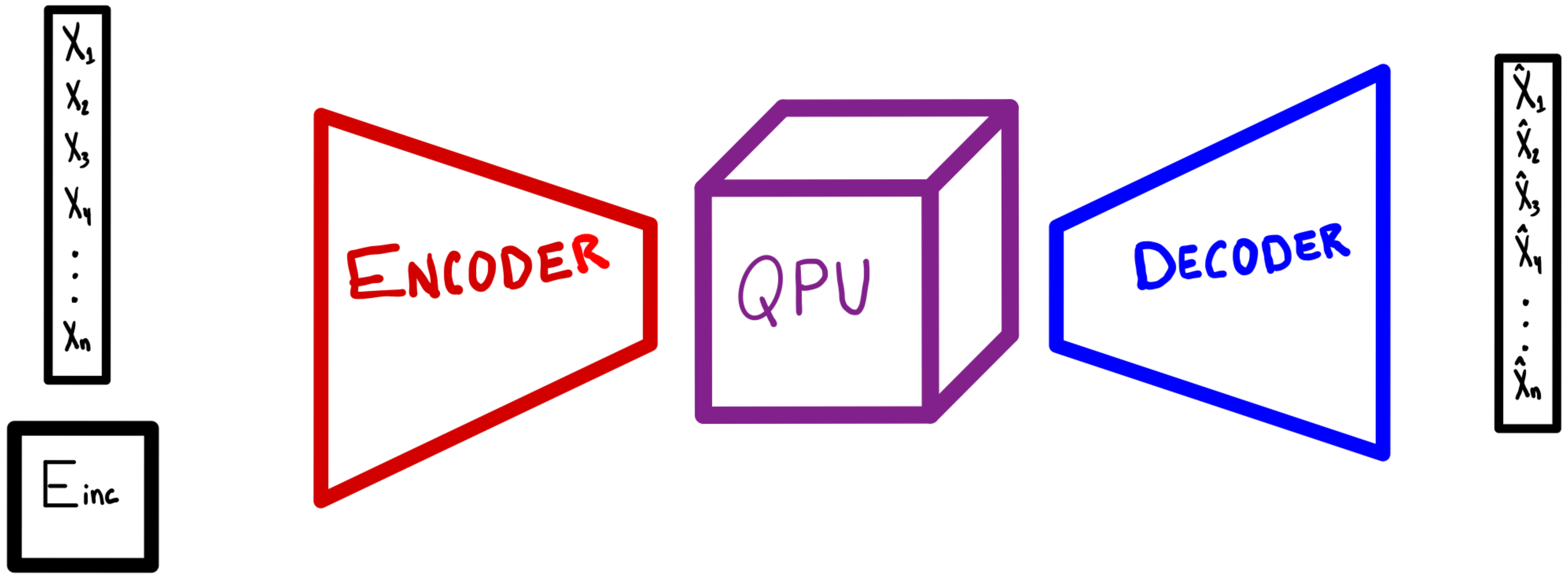
Why use an RBM in latent space?



- More expressiveness
- However, this comes at a cost.

Quantum-Assisted Discrete VAE

Why?



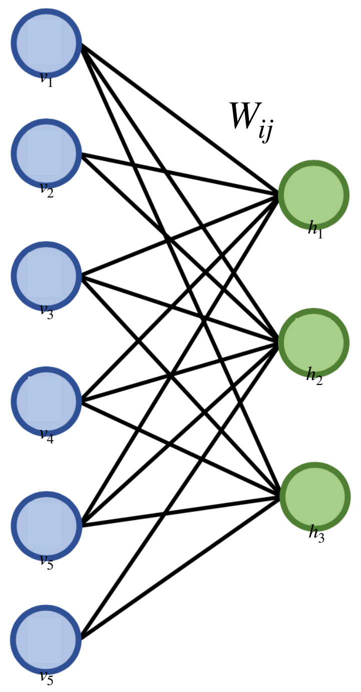
- More expressiveness
- However, this comes at a cost.
- But we might be able to avoid Gibbs sampling…

Quantum Annealer

Topologies

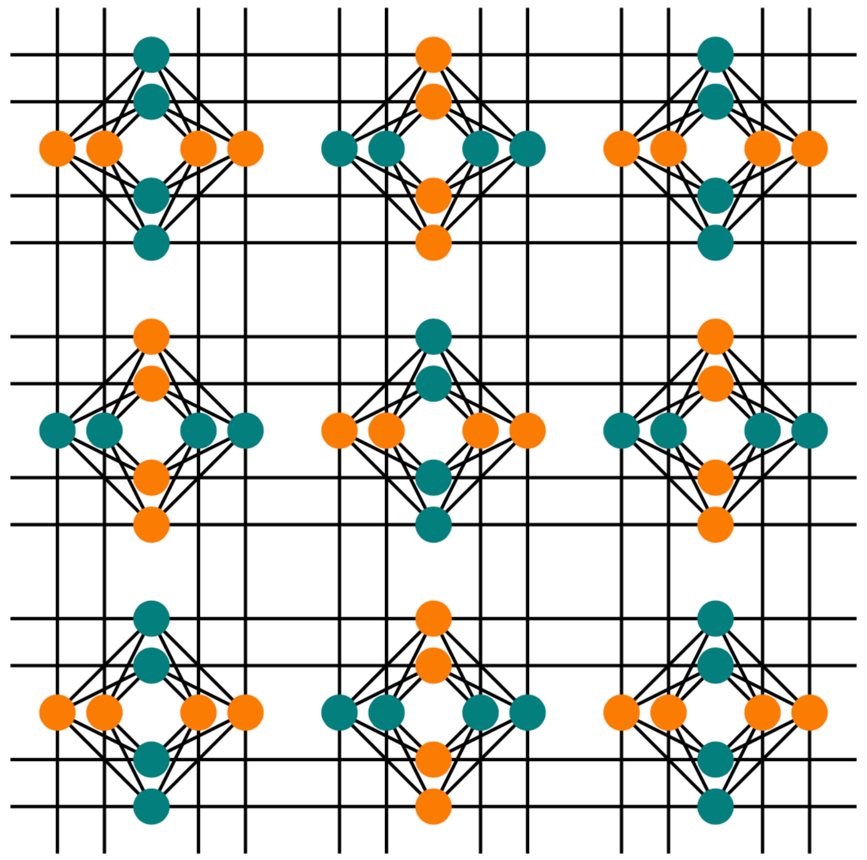
Fully Connected RBM

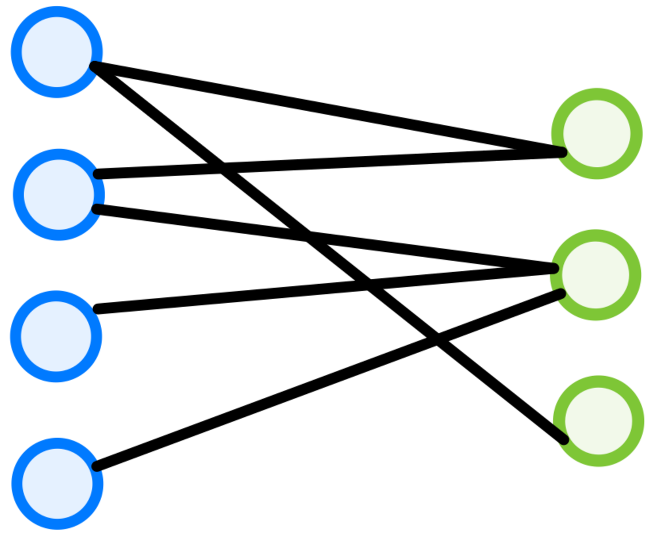
2-partite Graph



Chimera QA

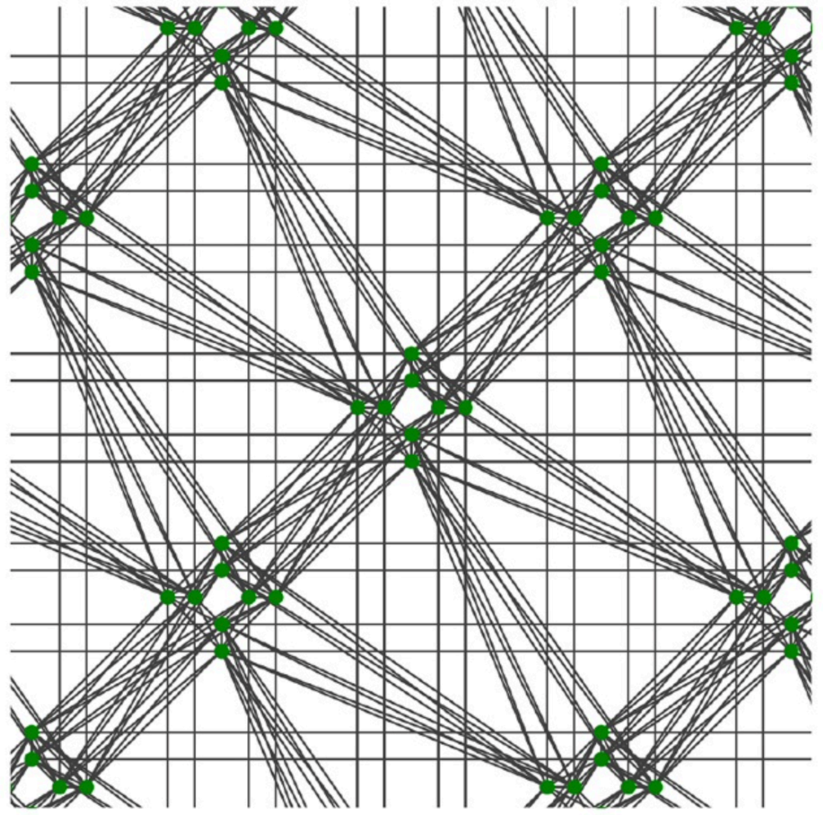
2-partite Graph

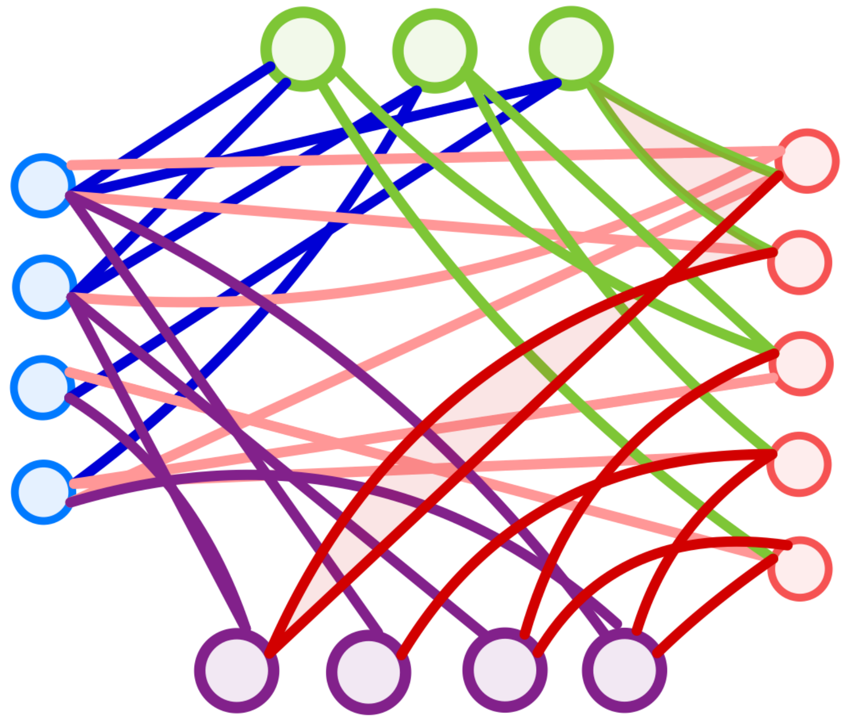




Pegasus QA

4-partite Graph



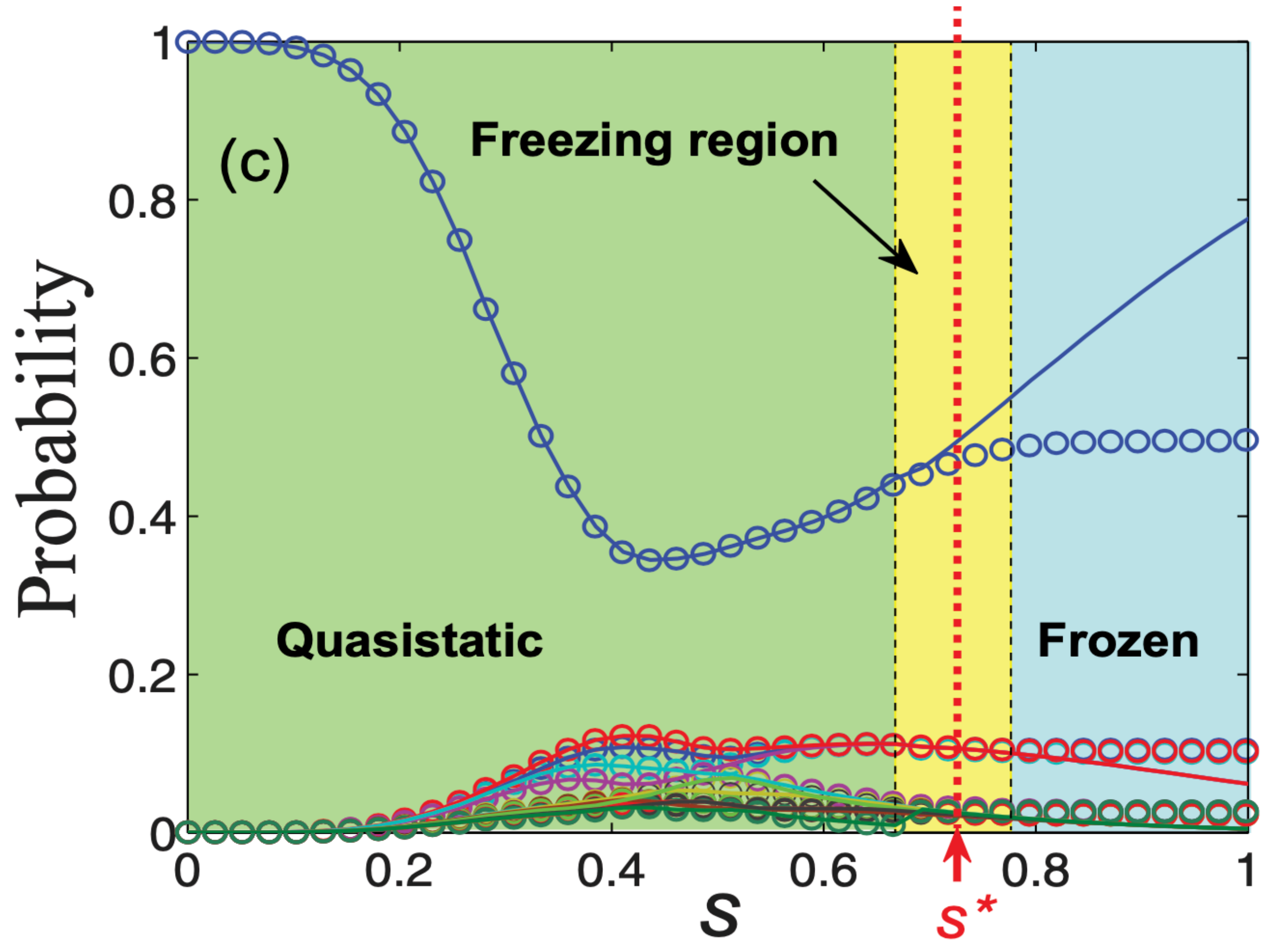


Quantum Annealer

Basics

$$\mathcal{H}_{ising} = \underbrace{-\frac{A(s)}{2}\left(\sum_i \hat{\sigma}_x^{(i)}\right)}_{\substack{\text{Initial Hamiltonian}\\ H_1}} + \underbrace{\frac{B(s)}{2}\left(\sum_i c_i \hat{\sigma}_z^{(i)} + \sum_{i>j} J_{i,j}\hat{\sigma}_z^{(i)}\hat{\sigma}_z^{(j)}\right)}_{\substack{\text{Final Hamiltonian}\\ H_0}}$$

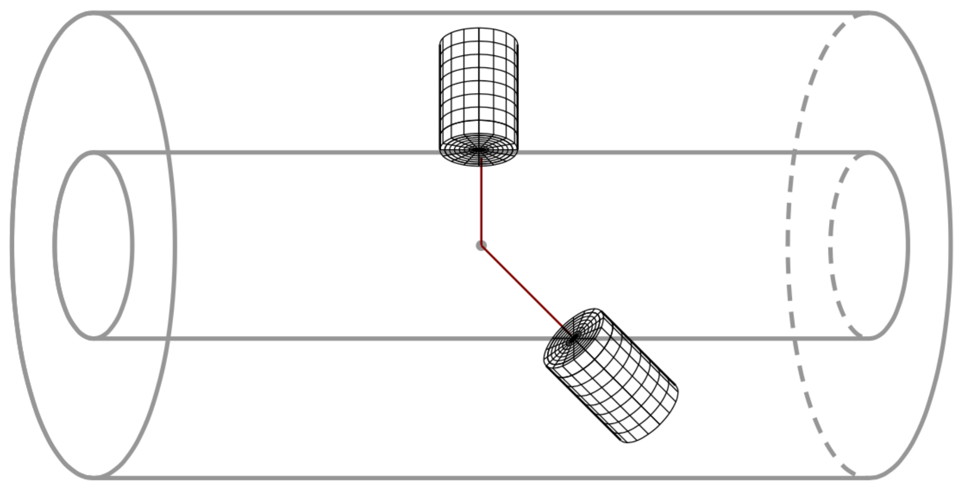
- QA relies on the Adiabatic Approximation.
- The goal is to find the ground state of a Hamiltonian H_0.
- In practice, quantum annealers have a strong interaction with the environment which lead to **thermalization** and **decoherence**.

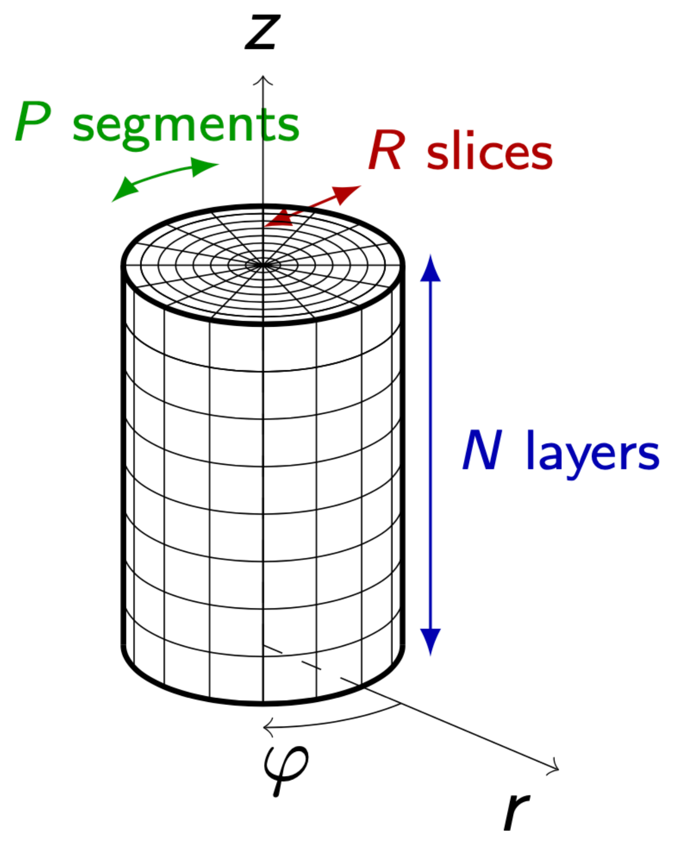


Occupation probabilities during the annealing calculated by using the Redfield formalism (circles) and the Boltzmann distribution (solid lines), assuming T = 40 mK and t_a = 20 μs. All probabilities follow the Boltzmann distribution in the quasistatic region (green) until they start freezing in the freezing region (yellow) and stay constant in the frozen region (blue). All final probabilities are close to the Boltzmann probabilities at the freeze-out point s∗, marked by the vertical (red) dashed line.

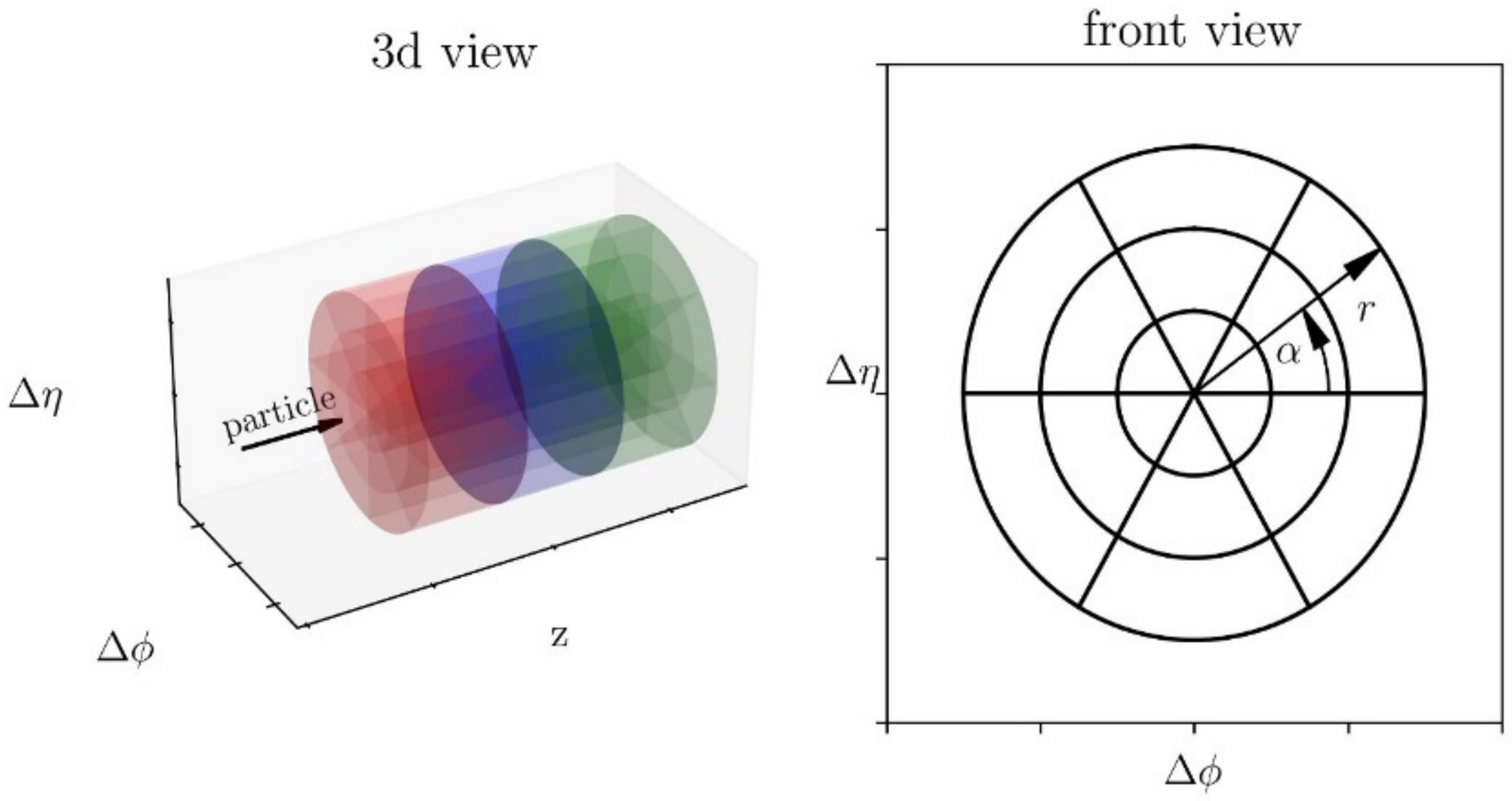
CaloChallange Dataset

Kaggle Challenge Fast Calorimeter Simulation Challenge 2022



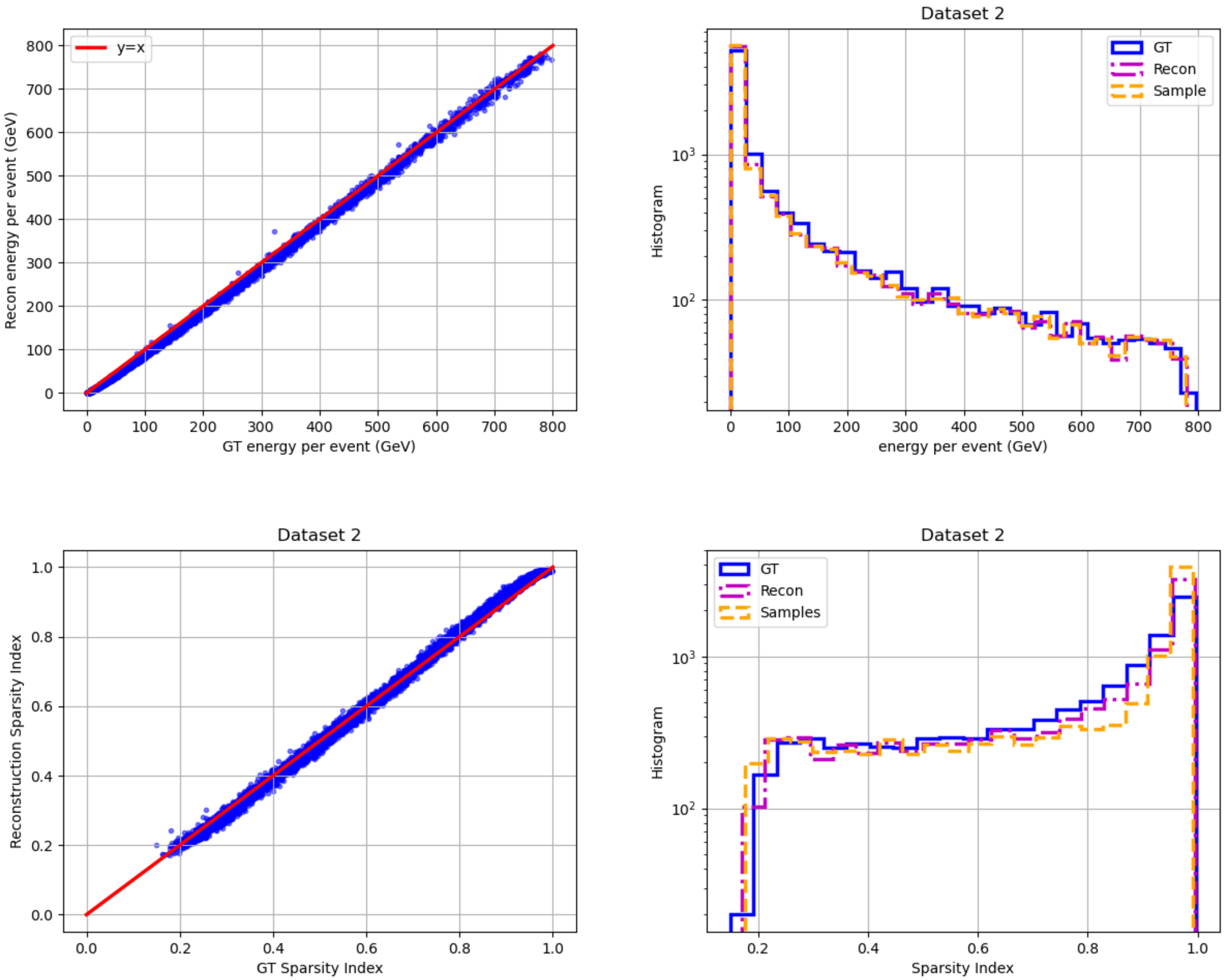


	Dataset
Particle type	Electron showers
Layers	45
Voxels per layer	9 radial * 16 angular
Incident energies	Log-uniform distribution (1GeV-1TeV)
N. of events	100,000



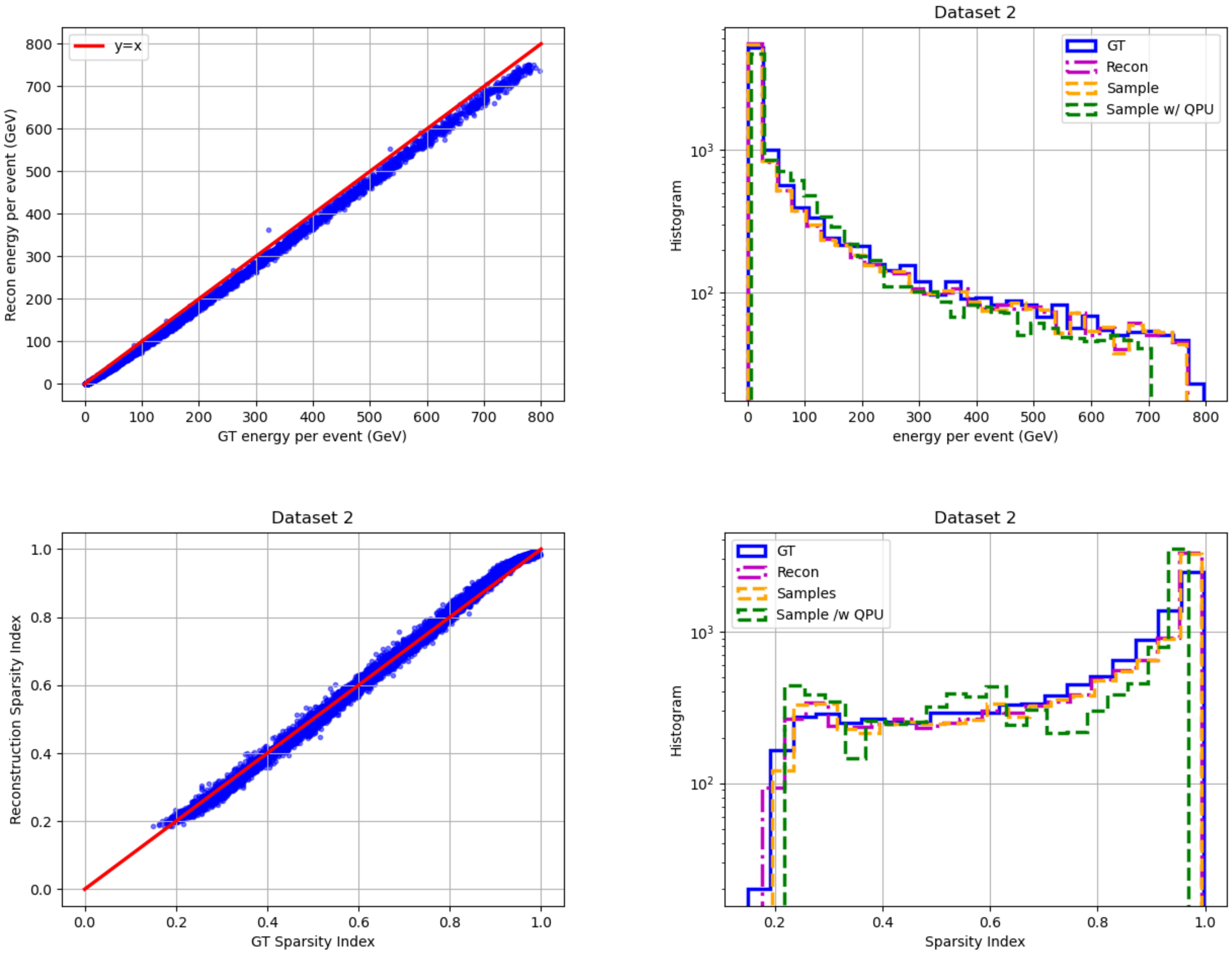
Results

- Chimera Topology
- RBM



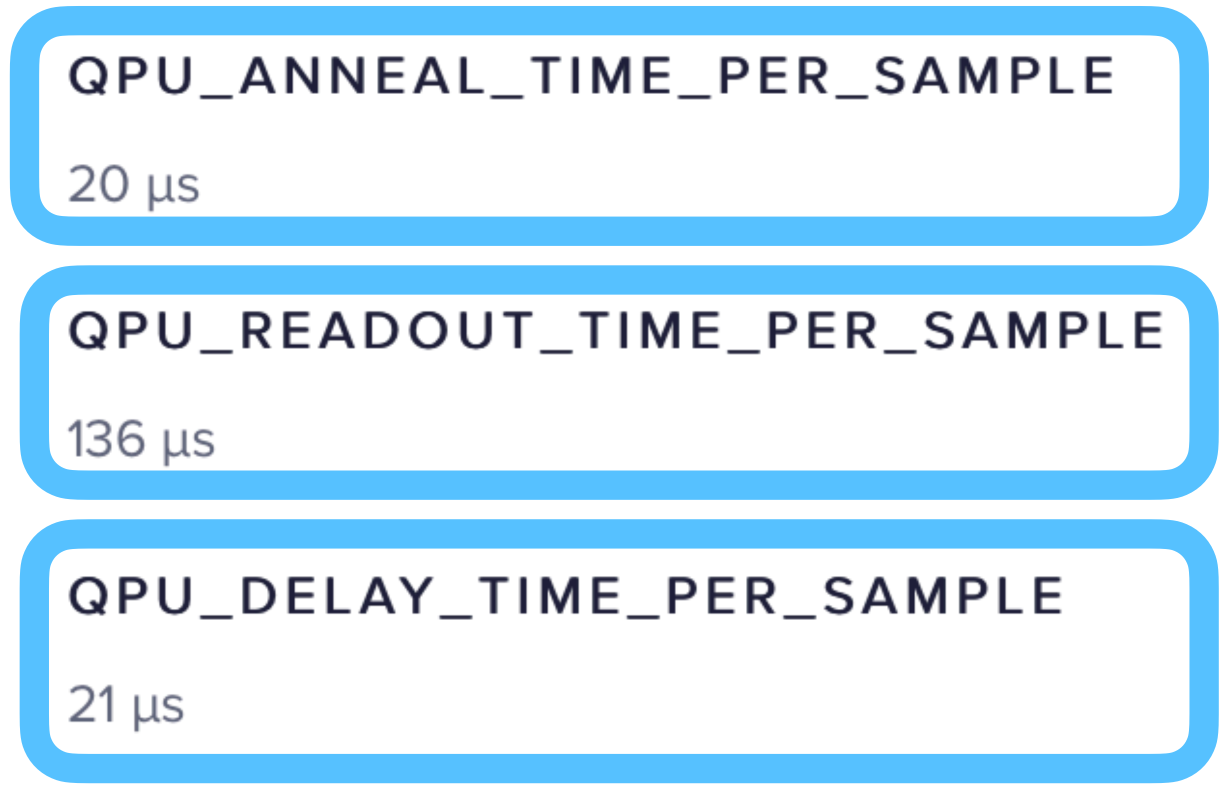
Results

- Pegasus Topology
- QPU & RBM



Results

	Wall time to generate 1024 samples
Geant4	$\sim 1000\ s$
GPU A100	$2.19 \pm 0.14\ s$
QPU	$\sim 0.180\ s$



QPU_ANNEAL_TIME_PER_SAMPLE

20 µs

QPU_READOUT_TIME_PER_SAMPLE

136 µs

QPU_DELAY_TIME_PER_SAMPLE

21 µs

Geant4 time per sample

O(1) s

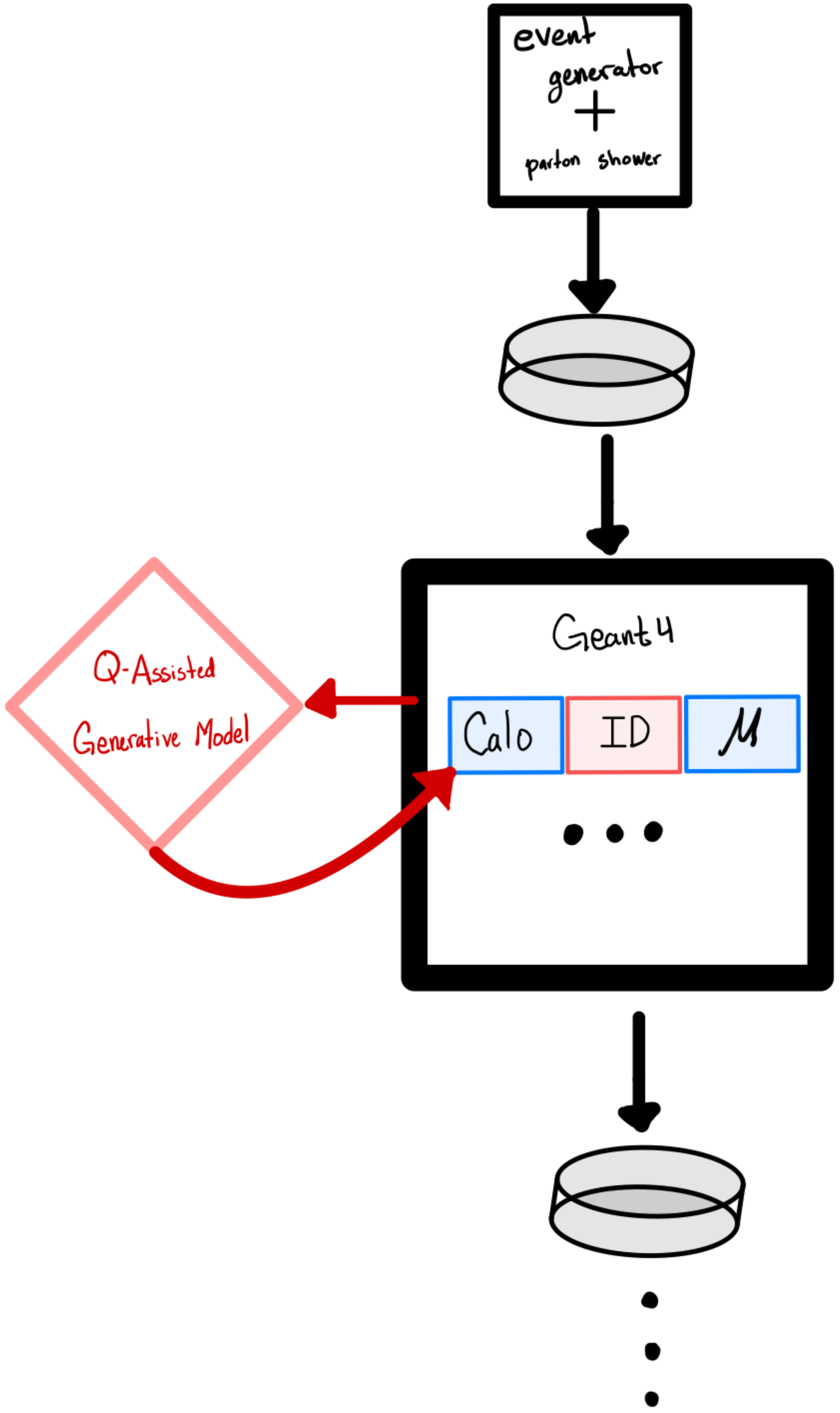
QPU ~12x faster than GPU

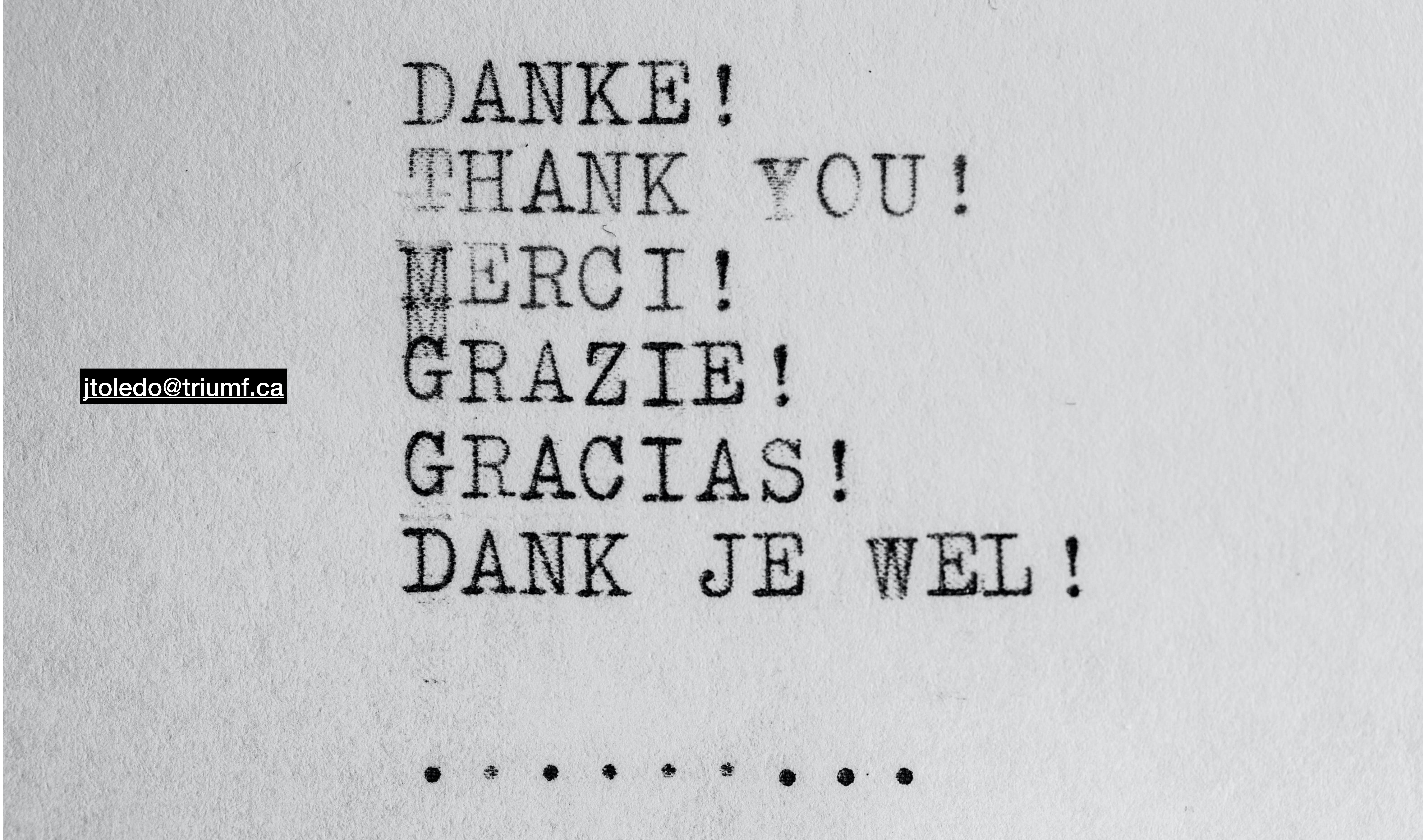
QPU ~10^4x faster than Geant4

Conclusions

First thoughts on infrastructure

- Task specific partial information routing.
  - Particle type
  - Energy of incidence
  - Location
  - Etc.
- Dedicated QPU + GPU resources + networking.
- Event merging back to Geant4 record.
- Batch zipping





DANKE!

THANK YOU!

MERCI!

GRAZIE!

GRACIAS!

DANK JE WEL!

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