



Turbo-Sim

a generalised generative model with a physical latent space

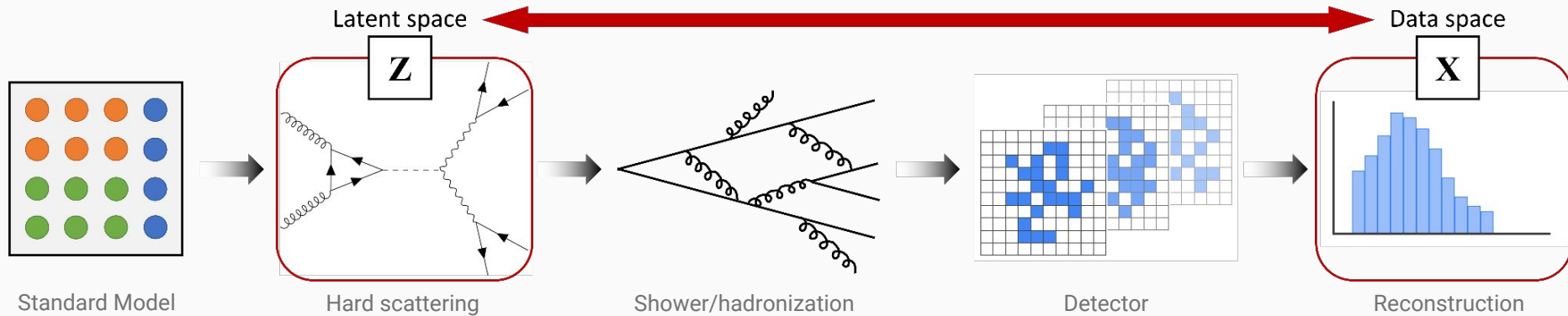
5th Inter-experiment Machine Learning workshop - 12.05.2022

Guillaume Quétant, Mariia Drozdova, Vitaliy Kinakh, Tobias Golling, Slava Voloshynovskiy
[arXiv](#)

Introduction

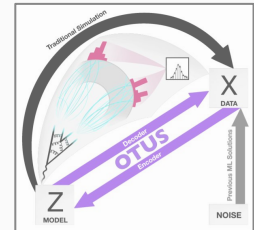
Physical motivation

Transform from theory to observation



- ML network to learn the transformation
- Learn both directions
- Everything is stochastic

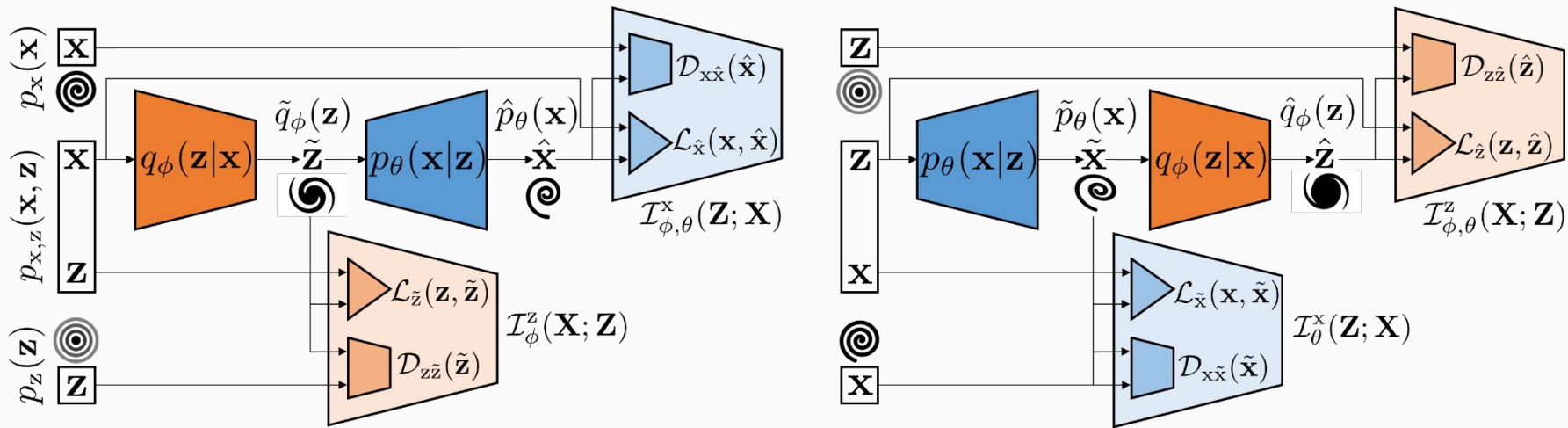
Jessica N. Howard et al.
*Foundations of a Fast, Data-Driven,
Machine-Learned Simulator*. 2021.
arXiv: [2101.08944](https://arxiv.org/abs/2101.08944)



Turbo-Sim

Walkthrough the model

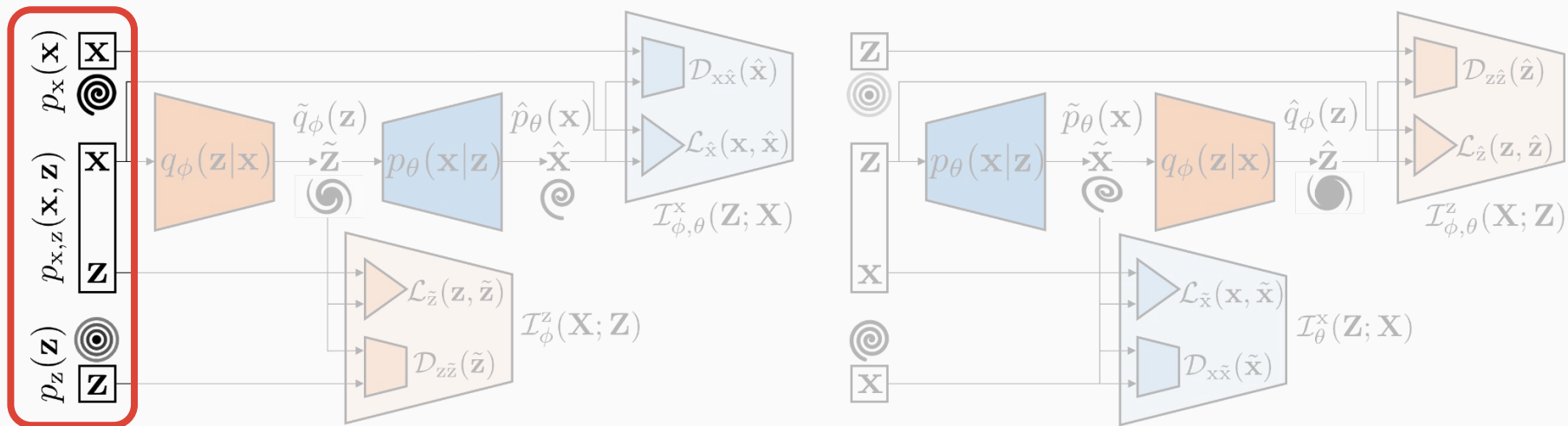
Turbo-Sim: complete framework



Turbo-Sim is a generalised autoencoder: encoder, decoder, eight loss terms and a joint data distribution

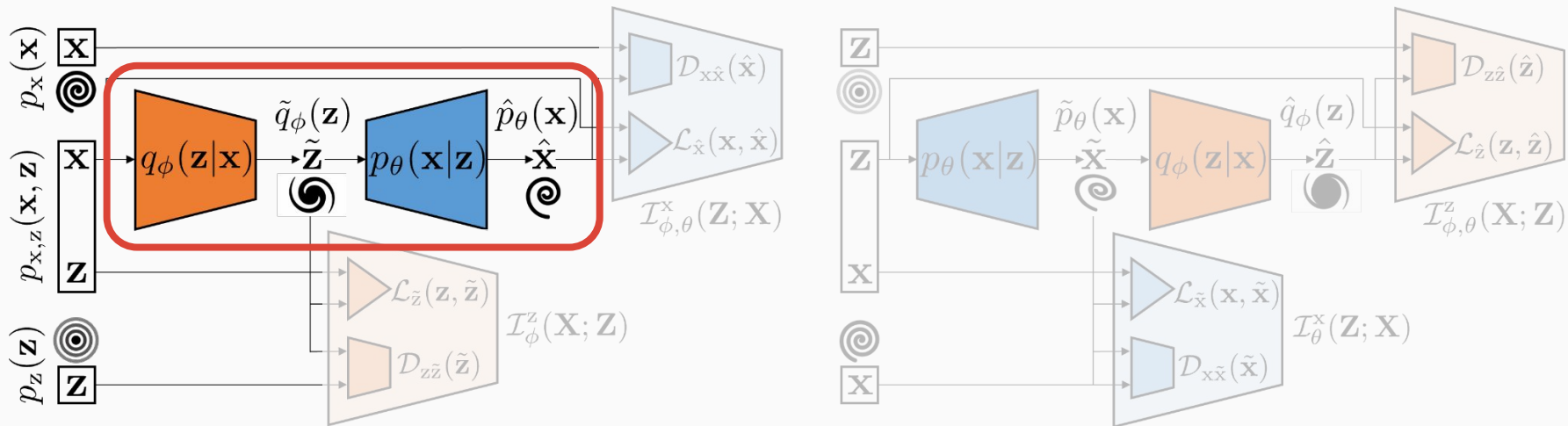
→ Let us dig into it

Turbo-Sim: complete framework



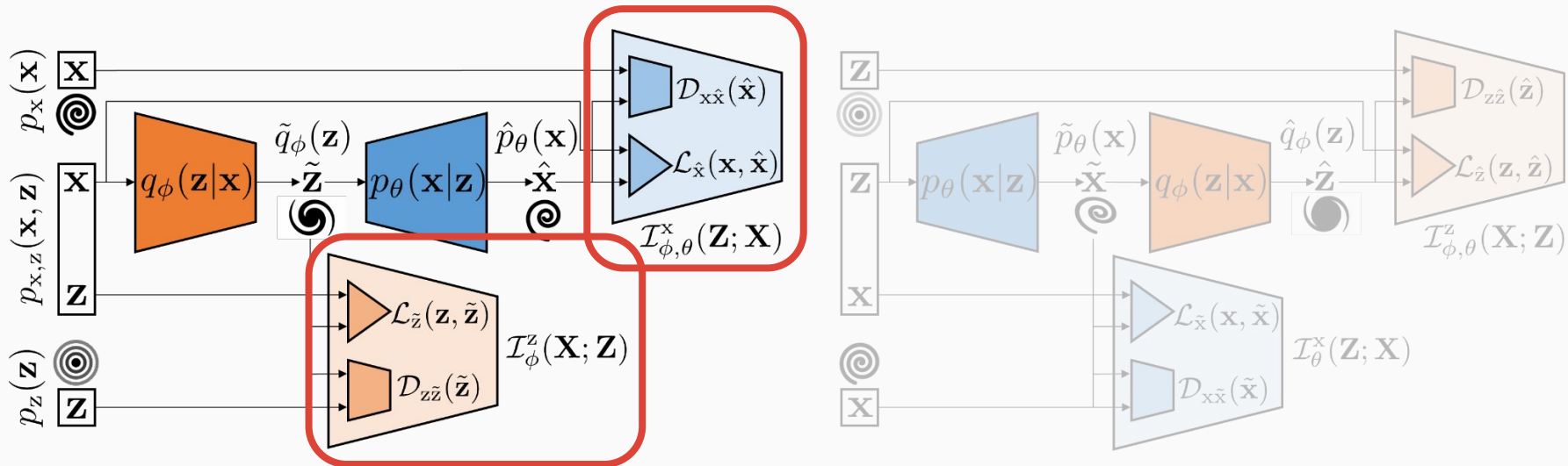
- Data and latent points are **sampled jointly** (they may be independent)
 - **Marginal distributions** are available as well
- In our HEP experiment: **Z = hard scattering space** / **X = reconstruction space**

Turbo-Sim: complete framework



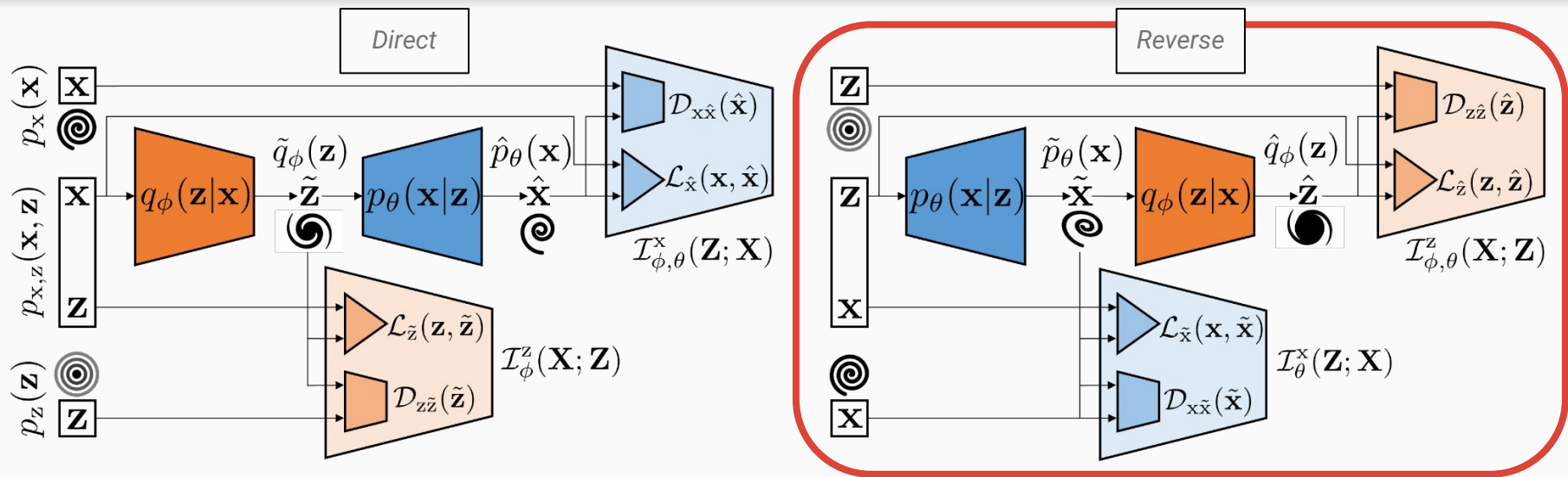
- Autoencoder outputs a latent space and a reconstructed space distributions
- Encoder and decoder should be (stochastic) inverse of each other
- In our HEP experiment: encoder = unfolding / decoder = simulation

Turbo-Sim: complete framework



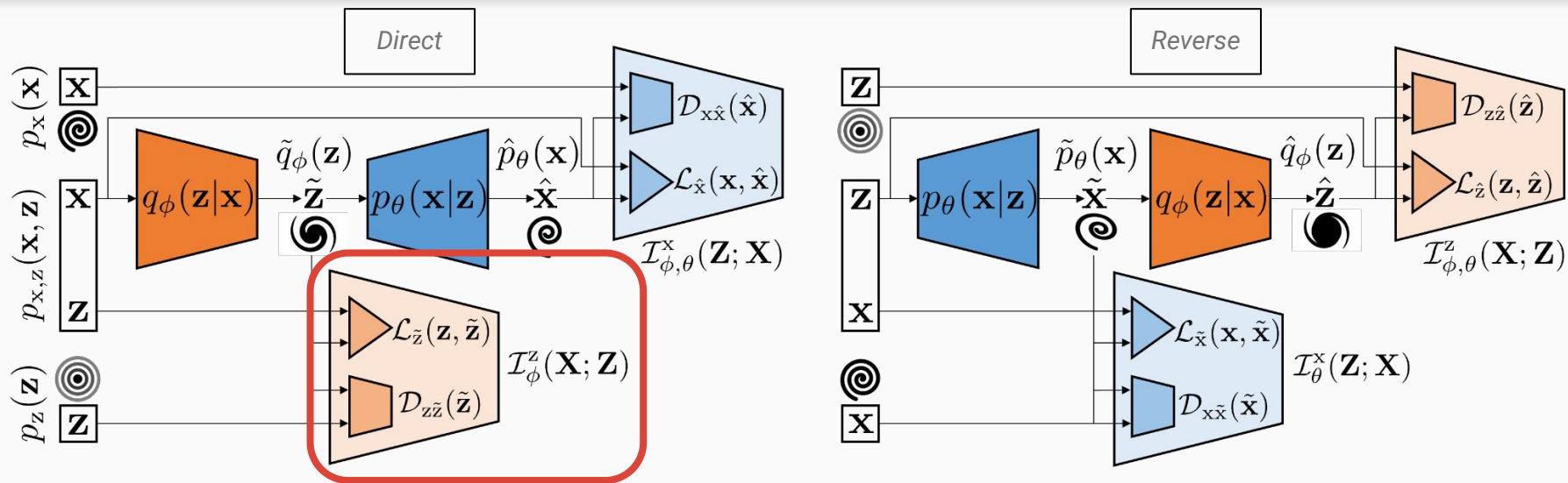
- Supervised and unsupervised losses in both latent and reconstructed spaces
 - Information theory interpretation of several usual models (AAE, GAN)
- In our HEP experiment: $\{\mathbf{z}, \mathbf{x}\}$ pairs for supervised / $\{\mathbf{z}\}, \{\mathbf{x}\}$ marginals for unsupervised

Turbo-Sim: complete framework



- Everything is **symmetrical with $Z \leftrightarrow X$**
- **Four more loss terms** and **two ways of training** (*direct and reverse*)
- In our HEP experiment: should help the network to be **good in unfolding and simulation**

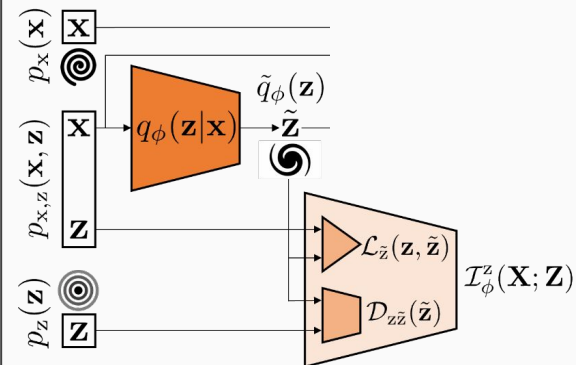
Turbo-Sim: complete framework



→ Let us focus on the derivation of these two terms

Lower bound to the true mutual information

$$\begin{aligned}
 I(\mathbf{X}; \mathbf{Z}) &= \mathbb{E}_{p_{\mathbf{x}, \mathbf{z}}(\mathbf{x}, \mathbf{z})} \left[\log \frac{p_{\mathbf{x}, \mathbf{z}}(\mathbf{x}, \mathbf{z})}{p_{\mathbf{x}}(\mathbf{x})p_{\mathbf{z}}(\mathbf{z})} \right] \\
 &= \mathbb{E}_{p_{\mathbf{x}, \mathbf{z}}(\mathbf{x}, \mathbf{z})} \left[\log \frac{p_{\mathbf{z}|\mathbf{x}}(\mathbf{z}|\mathbf{x})}{p_{\mathbf{z}}(\mathbf{z})} \right] \\
 &= \mathbb{E}_{p_{\mathbf{x}, \mathbf{z}}(\mathbf{x}, \mathbf{z})} \left[\log \frac{p_{\mathbf{z}|\mathbf{x}}(\mathbf{z}|\mathbf{x})}{p_{\mathbf{z}}(\mathbf{z})} \frac{q_{\phi}(\mathbf{z}|\mathbf{x})}{q_{\phi}(\mathbf{z}|\mathbf{x})} \right] \\
 &= \mathbb{E}_{p_{\mathbf{x}, \mathbf{z}}(\mathbf{x}, \mathbf{z})} \left[\log \frac{q_{\phi}(\mathbf{z}|\mathbf{x})}{p_{\mathbf{z}}(\mathbf{z})} \right] + \mathbb{E}_{p_{\mathbf{x}, \mathbf{z}}(\mathbf{x}, \mathbf{z})} \left[\log \frac{p_{\mathbf{z}|\mathbf{x}}(\mathbf{z}|\mathbf{x})}{q_{\phi}(\mathbf{z}|\mathbf{x})} \right] \\
 &= \mathbb{E}_{p_{\mathbf{x}, \mathbf{z}}(\mathbf{x}, \mathbf{z})} \left[\log \frac{q_{\phi}(\mathbf{z}|\mathbf{x})}{p_{\mathbf{z}}(\mathbf{z})} \right] + \mathbb{E}_{p_{\mathbf{x}}(\mathbf{x})} [D_{\text{KL}}(p_{\mathbf{z}|\mathbf{x}}(\mathbf{z}|\mathbf{x}) \| q_{\phi}(\mathbf{z}|\mathbf{x}))] \\
 &\geq \mathbb{E}_{p_{\mathbf{x}, \mathbf{z}}(\mathbf{x}, \mathbf{z})} \left[\log \frac{q_{\phi}(\mathbf{z}|\mathbf{x})}{p_{\mathbf{z}}(\mathbf{z})} \right] \\
 &= \mathbb{E}_{p_{\mathbf{x}, \mathbf{z}}(\mathbf{x}, \mathbf{z})} \left[\log \frac{q_{\phi}(\mathbf{z}|\mathbf{x})}{p_{\mathbf{z}}(\mathbf{z})} \frac{\tilde{q}_{\phi}(\mathbf{z})}{\tilde{q}_{\phi}(\mathbf{z})} \right] = \mathcal{I}_{\phi}^{\mathbf{z}}(\mathbf{X}; \mathbf{Z}),
 \end{aligned}$$

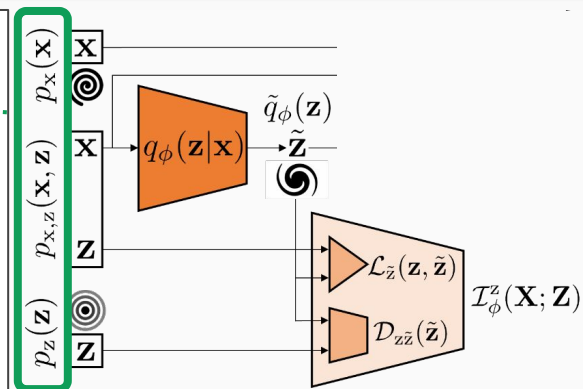


Equality reached for

$$p_{\mathbf{z}|\mathbf{x}}(\mathbf{z}|\mathbf{x}) = q_{\phi}(\mathbf{z}|\mathbf{x})$$

Lower bound to the true mutual information

$$\begin{aligned}
 I(\mathbf{X}; \mathbf{Z}) &= \mathbb{E}_{p_{\mathbf{x}, \mathbf{z}}(\mathbf{x}, \mathbf{z})} \left[\log \frac{p_{\mathbf{x}, \mathbf{z}}(\mathbf{x}, \mathbf{z})}{p_{\mathbf{x}}(\mathbf{x}) p_{\mathbf{z}}(\mathbf{z})} \right] \\
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 &= \mathbb{E}_{p_{\mathbf{x}, \mathbf{z}}(\mathbf{x}, \mathbf{z})} \left[\log \frac{p_{\mathbf{z}|\mathbf{x}}(\mathbf{z}|\mathbf{x})}{p_{\mathbf{z}}(\mathbf{z})} \frac{q_{\phi}(\mathbf{z}|\mathbf{x})}{q_{\phi}(\mathbf{z}|\mathbf{x})} \right] \\
 &= \mathbb{E}_{p_{\mathbf{x}, \mathbf{z}}(\mathbf{x}, \mathbf{z})} \left[\log \frac{q_{\phi}(\mathbf{z}|\mathbf{x})}{p_{\mathbf{z}}(\mathbf{z})} \right] + \mathbb{E}_{p_{\mathbf{x}, \mathbf{z}}(\mathbf{x}, \mathbf{z})} \left[\log \frac{p_{\mathbf{z}|\mathbf{x}}(\mathbf{z}|\mathbf{x})}{q_{\phi}(\mathbf{z}|\mathbf{x})} \right] \\
 &= \mathbb{E}_{p_{\mathbf{x}, \mathbf{z}}(\mathbf{x}, \mathbf{z})} \left[\log \frac{q_{\phi}(\mathbf{z}|\mathbf{x})}{p_{\mathbf{z}}(\mathbf{z})} \right] + \mathbb{E}_{p_{\mathbf{x}}(\mathbf{x})} [D_{\text{KL}}(p_{\mathbf{z}|\mathbf{x}}(\mathbf{z}|\mathbf{x}) \| q_{\phi}(\mathbf{z}|\mathbf{x}))] \\
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 &= \mathbb{E}_{p_{\mathbf{x}, \mathbf{z}}(\mathbf{x}, \mathbf{z})} \left[\log \frac{q_{\phi}(\mathbf{z}|\mathbf{x})}{p_{\mathbf{z}}(\mathbf{z})} \frac{\tilde{q}_{\phi}(\mathbf{z})}{\tilde{q}_{\phi}(\mathbf{z})} \right] = \mathcal{I}_{\phi}^{\mathbf{z}}(\mathbf{X}; \mathbf{Z}),
 \end{aligned}$$

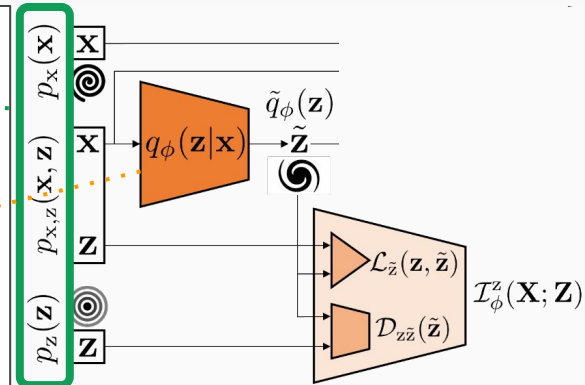


Equality reached for

$$p_{\mathbf{z}|\mathbf{x}}(\mathbf{z}|\mathbf{x}) = q_{\phi}(\mathbf{z}|\mathbf{x})$$

Lower bound to the true mutual information

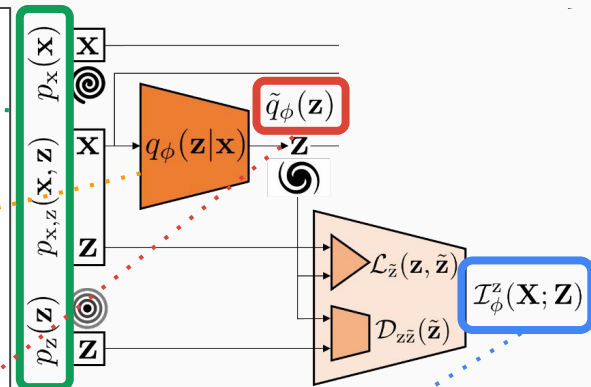
$$\begin{aligned}
 I(\mathbf{X}; \mathbf{Z}) &= \mathbb{E}_{p_{\mathbf{x}, \mathbf{z}}(\mathbf{x}, \mathbf{z})} \left[\log \frac{p_{\mathbf{x}, \mathbf{z}}(\mathbf{X}, \mathbf{Z})}{p_{\mathbf{x}}(\mathbf{X}) p_{\mathbf{z}}(\mathbf{Z})} \right] \\
 &= \mathbb{E}_{p_{\mathbf{x}, \mathbf{z}}(\mathbf{x}, \mathbf{z})} \left[\log \frac{p_{\mathbf{z}|\mathbf{x}}(\mathbf{Z}|\mathbf{X})}{p_{\mathbf{z}}(\mathbf{Z})} \right] \\
 &= \mathbb{E}_{p_{\mathbf{x}, \mathbf{z}}(\mathbf{x}, \mathbf{z})} \left[\log \frac{p_{\mathbf{z}|\mathbf{x}}(\mathbf{Z}|\mathbf{X})}{p_{\mathbf{z}}(\mathbf{Z})} \frac{q_{\phi}(\mathbf{Z}|\mathbf{X})}{q_{\phi}(\mathbf{Z}|\mathbf{X})} \right] \\
 &= \mathbb{E}_{p_{\mathbf{x}, \mathbf{z}}(\mathbf{x}, \mathbf{z})} \left[\log \frac{q_{\phi}(\mathbf{Z}|\mathbf{X})}{p_{\mathbf{z}}(\mathbf{Z})} \right] + \mathbb{E}_{p_{\mathbf{x}, \mathbf{z}}(\mathbf{x}, \mathbf{z})} \left[\log \frac{p_{\mathbf{z}|\mathbf{x}}(\mathbf{Z}|\mathbf{X})}{q_{\phi}(\mathbf{Z}|\mathbf{X})} \right] \\
 &= \mathbb{E}_{p_{\mathbf{x}, \mathbf{z}}(\mathbf{x}, \mathbf{z})} \left[\log \frac{q_{\phi}(\mathbf{Z}|\mathbf{X})}{p_{\mathbf{z}}(\mathbf{Z})} \right] + \mathbb{E}_{p_{\mathbf{x}}(\mathbf{x})} [D_{\text{KL}}(p_{\mathbf{z}|\mathbf{x}}(\mathbf{Z}|\mathbf{X}) \| q_{\phi}(\mathbf{Z}|\mathbf{X}))] \\
 &\geq \mathbb{E}_{p_{\mathbf{x}, \mathbf{z}}(\mathbf{x}, \mathbf{z})} \left[\log \frac{q_{\phi}(\mathbf{Z}|\mathbf{X})}{p_{\mathbf{z}}(\mathbf{Z})} \right] \\
 &= \mathbb{E}_{p_{\mathbf{x}, \mathbf{z}}(\mathbf{x}, \mathbf{z})} \left[\log \frac{q_{\phi}(\mathbf{Z}|\mathbf{X})}{p_{\mathbf{z}}(\mathbf{Z})} \frac{\tilde{q}_{\phi}(\mathbf{Z})}{\tilde{q}_{\phi}(\mathbf{Z})} \right] = \mathcal{I}_{\phi}^{\mathbf{z}}(\mathbf{X}; \mathbf{Z}),
 \end{aligned}$$



Equality reached for
 $p_{\mathbf{z}|\mathbf{x}}(\mathbf{z}|\mathbf{x}) = q_{\phi}(\mathbf{z}|\mathbf{x})$

Lower bound to the true mutual information

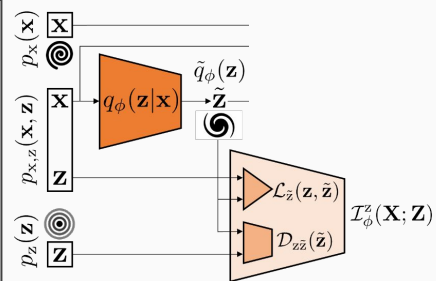
$$\begin{aligned}
 I(\mathbf{X}; \mathbf{Z}) &= \mathbb{E}_{p_{\mathbf{x}, \mathbf{z}}(\mathbf{x}, \mathbf{z})} \left[\log \frac{p_{\mathbf{x}, \mathbf{z}}(\mathbf{x}, \mathbf{z})}{p_{\mathbf{x}}(\mathbf{x}) p_{\mathbf{z}}(\mathbf{z})} \right] \\
 &= \mathbb{E}_{p_{\mathbf{x}, \mathbf{z}}(\mathbf{x}, \mathbf{z})} \left[\log \frac{p_{\mathbf{z}|\mathbf{x}}(\mathbf{z}|\mathbf{x})}{p_{\mathbf{z}}(\mathbf{z})} \right] \\
 &= \mathbb{E}_{p_{\mathbf{x}, \mathbf{z}}(\mathbf{x}, \mathbf{z})} \left[\log \frac{p_{\mathbf{z}|\mathbf{x}}(\mathbf{z}|\mathbf{x})}{p_{\mathbf{z}}(\mathbf{z})} \frac{q_{\phi}(\mathbf{z}|\mathbf{x})}{q_{\phi}(\mathbf{z}|\mathbf{x})} \right] \\
 &= \mathbb{E}_{p_{\mathbf{x}, \mathbf{z}}(\mathbf{x}, \mathbf{z})} \left[\log \frac{q_{\phi}(\mathbf{z}|\mathbf{x})}{p_{\mathbf{z}}(\mathbf{z})} \right] + \mathbb{E}_{p_{\mathbf{x}, \mathbf{z}}(\mathbf{x}, \mathbf{z})} \left[\log \frac{p_{\mathbf{z}|\mathbf{x}}(\mathbf{z}|\mathbf{x})}{q_{\phi}(\mathbf{z}|\mathbf{x})} \right] \\
 &= \mathbb{E}_{p_{\mathbf{x}, \mathbf{z}}(\mathbf{x}, \mathbf{z})} \left[\log \frac{q_{\phi}(\mathbf{z}|\mathbf{x})}{p_{\mathbf{z}}(\mathbf{z})} \right] + \mathbb{E}_{p_{\mathbf{x}}(\mathbf{x})} [D_{\text{KL}}(p_{\mathbf{z}|\mathbf{x}}(\mathbf{z}|\mathbf{x}) \| q_{\phi}(\mathbf{z}|\mathbf{x}))] \\
 &\geq \mathbb{E}_{p_{\mathbf{x}, \mathbf{z}}(\mathbf{x}, \mathbf{z})} \left[\log \frac{q_{\phi}(\mathbf{z}|\mathbf{x})}{p_{\mathbf{z}}(\mathbf{z})} \right] \\
 &= \mathbb{E}_{p_{\mathbf{x}, \mathbf{z}}(\mathbf{x}, \mathbf{z})} \left[\log \frac{q_{\phi}(\mathbf{z}|\mathbf{x})}{p_{\mathbf{z}}(\mathbf{z})} \frac{\tilde{q}_{\phi}(\mathbf{z})}{\tilde{q}_{\phi}(\mathbf{z})} \right] = \mathcal{I}_{\phi}^{\mathbf{z}}(\mathbf{X}; \mathbf{Z}),
 \end{aligned}$$



Equality reached for
 $p_{\mathbf{z}|\mathbf{x}}(\mathbf{z}|\mathbf{x}) = q_{\phi}(\mathbf{z}|\mathbf{x})$

Lower bound to the approximate mutual information

$$\begin{aligned}\mathcal{I}_\phi^z(\mathbf{X}; \mathbf{Z}) &= \mathbb{E}_{p_{\mathbf{x},z}(\mathbf{x},z)} \left[\log \frac{q_\phi(\mathbf{z}|\mathbf{x})}{p_z(\mathbf{z})} \frac{\tilde{q}_\phi(\mathbf{z})}{\tilde{q}_\phi(\mathbf{z})} \right] \\ &= \mathbb{E}_{p_{\mathbf{x},z}(\mathbf{x},z)} [\log q_\phi(\mathbf{z}|\mathbf{x})] - \mathbb{E}_{p_{\mathbf{x},z}(\mathbf{x},z)} \left[\log \frac{p_z(\mathbf{z})}{\tilde{q}_\phi(\mathbf{z})} \right] - \mathbb{E}_{p_{\mathbf{x},z}(\mathbf{x},z)} [\log \tilde{q}_\phi(\mathbf{z})] \\ &= \mathbb{E}_{p_{\mathbf{x}}(\mathbf{x})} \mathbb{E}_{p_{z|\mathbf{x}}(\mathbf{z}|\mathbf{x})} [\log q_\phi(\mathbf{z}|\mathbf{x})] - \mathbb{E}_{p_z(\mathbf{z})} \left[\log \frac{p_z(\mathbf{z})}{\tilde{q}_\phi(\mathbf{z})} \right] - \mathbb{E}_{p_z(\mathbf{z})} [\log \tilde{q}_\phi(\mathbf{z})] \\ &= \mathbb{E}_{p_{\mathbf{x}}(\mathbf{x})} \mathbb{E}_{p_{z|\mathbf{x}}(\mathbf{z}|\mathbf{x})} [\log q_\phi(\mathbf{z}|\mathbf{x})] - D_{\text{KL}}(p_z(\mathbf{z}) \parallel \tilde{q}_\phi(\mathbf{z})) + H(p_z(\mathbf{z}); \tilde{q}_\phi(\mathbf{z})) \\ &\geq \mathbb{E}_{p_{\mathbf{x}}(\mathbf{x})} \mathbb{E}_{p_{z|\mathbf{x}}(\mathbf{z}|\mathbf{x})} [\log q_\phi(\mathbf{z}|\mathbf{x})] - D_{\text{KL}}(p_z(\mathbf{z}) \parallel \tilde{q}_\phi(\mathbf{z})) \\ &\simeq \mathbb{E}_{p_{\mathbf{x}}(\mathbf{x})} \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})} [\log q_\phi(\mathbf{z}|\mathbf{x})] - D_{\text{KL}}(p_z(\mathbf{z}) \parallel \tilde{q}_\phi(\mathbf{z})),\end{aligned}$$

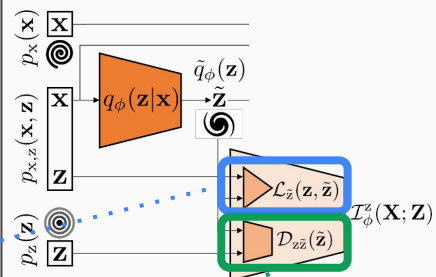


Equality *not* reached for (but the maximum value is)

$$p_{z|\mathbf{x}}(\mathbf{z}|\mathbf{x}) = q_\phi(\mathbf{z}|\mathbf{x})$$

Lower bound to the approximate mutual information

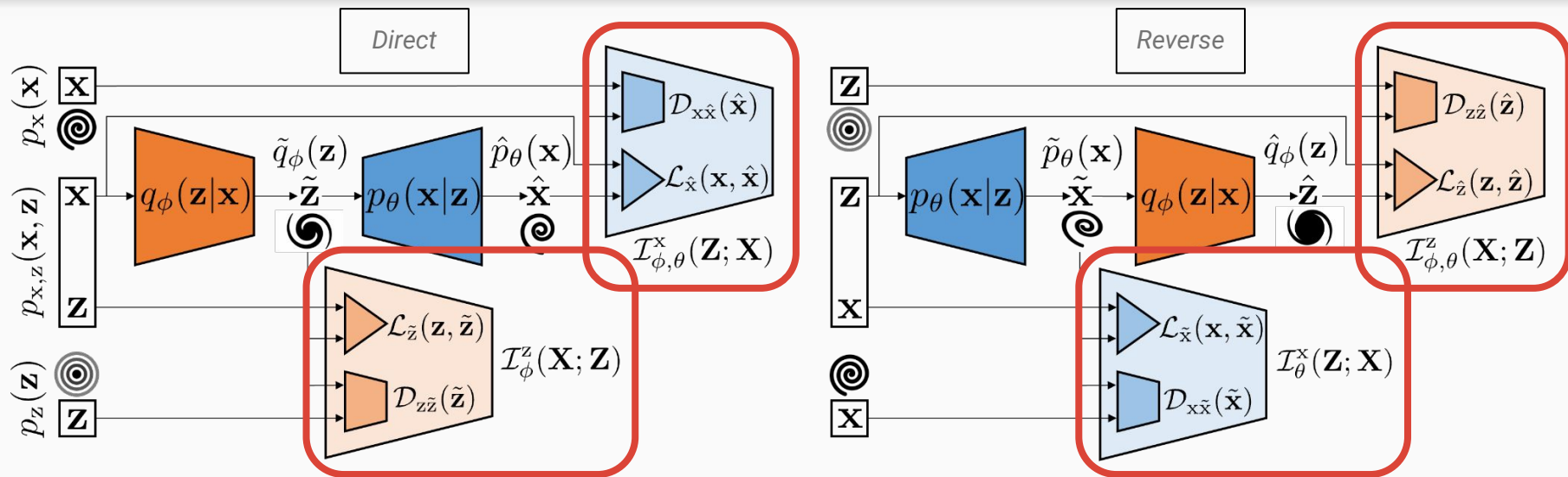
$$\begin{aligned}
 \mathcal{I}_\phi^z(\mathbf{X}; \mathbf{Z}) &= \mathbb{E}_{p_{\mathbf{x}, \mathbf{z}}(\mathbf{x}, \mathbf{z})} \left[\log \frac{q_\phi(\mathbf{z}|\mathbf{x})}{p_z(\mathbf{z})} \frac{\tilde{q}_\phi(\mathbf{z})}{\tilde{q}_\phi(\mathbf{z})} \right] \\
 &= \mathbb{E}_{p_{\mathbf{x}, \mathbf{z}}(\mathbf{x}, \mathbf{z})} [\log q_\phi(\mathbf{z}|\mathbf{x})] - \mathbb{E}_{p_{\mathbf{x}, \mathbf{z}}(\mathbf{x}, \mathbf{z})} \left[\log \frac{p_z(\mathbf{z})}{\tilde{q}_\phi(\mathbf{z})} \right] - \mathbb{E}_{p_{\mathbf{x}, \mathbf{z}}(\mathbf{x}, \mathbf{z})} [\log \tilde{q}_\phi(\mathbf{z})] \\
 &= \mathbb{E}_{p_{\mathbf{x}}(\mathbf{x})} \mathbb{E}_{p_{z|\mathbf{x}}(\mathbf{z}|\mathbf{x})} [\log q_\phi(\mathbf{z}|\mathbf{x})] - \mathbb{E}_{p_z(\mathbf{z})} \left[\log \frac{p_z(\mathbf{z})}{\tilde{q}_\phi(\mathbf{z})} \right] - \mathbb{E}_{p_z(\mathbf{z})} [\log \tilde{q}_\phi(\mathbf{z})] \\
 &= \mathbb{E}_{p_{\mathbf{x}}(\mathbf{x})} \mathbb{E}_{p_{z|\mathbf{x}}(\mathbf{z}|\mathbf{x})} [\log q_\phi(\mathbf{z}|\mathbf{x})] - D_{\text{KL}}(p_z(\mathbf{z}) \parallel \tilde{q}_\phi(\mathbf{z})) + H(p_z(\mathbf{z}); \tilde{q}_\phi(\mathbf{z})) \\
 &\geq \mathbb{E}_{p_{\mathbf{x}}(\mathbf{x})} \mathbb{E}_{p_{z|\mathbf{x}}(\mathbf{z}|\mathbf{x})} [\log q_\phi(\mathbf{z}|\mathbf{x})] - D_{\text{KL}}(p_z(\mathbf{z}) \parallel \tilde{q}_\phi(\mathbf{z})) \\
 &\simeq \mathbb{E}_{p_{\mathbf{x}}(\mathbf{x})} \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})} [\log q_\phi(\mathbf{z}|\mathbf{x})] - D_{\text{KL}}(p_z(\mathbf{z}) \parallel \tilde{q}_\phi(\mathbf{z})),
 \end{aligned}$$



Equality *not* reached for (but the maximum value is)

$$p_{z|\mathbf{x}}(\mathbf{z}|\mathbf{x}) = q_\phi(\mathbf{z}|\mathbf{x})$$

Turbo-Sim: complete framework



→ Similar decompositions lead to the six other terms

Turbo-Sim: losses

Turbo-Sim vs Bounded Information Bottleneck AE:

$$\bar{\mathcal{L}}^{\text{Direct}}(\phi, \theta) = -\mathcal{I}_{\phi}^{\mathbf{z}}(\mathbf{X}; \mathbf{Z}) - \alpha \mathcal{I}_{\phi, \theta}^{\mathbf{x}}(\mathbf{Z}; \mathbf{X})$$

$$\mathcal{L}_{\text{BIB-AE}}(\theta, \phi) = I_{\phi}(\mathbf{X}; \mathbf{Z}) - \beta I_{\theta, \phi}^{\text{UL}}(\mathbf{Z}; \mathbf{X})$$

(1912.00830)

Mutual information between input and latent space

- Turbo-Sim: maximised (*loss is minimised*)
- BIB-AE: minimised

Turbo-Sim: losses

Turbo-Sim vs Bounded Information Bottleneck AE:

$$\bar{\mathcal{L}}^{\text{Direct}}(\phi, \theta) = -\mathcal{I}_{\phi}^{\mathbf{Z}}(\mathbf{X}; \mathbf{Z}) - \alpha \mathcal{I}_{\phi, \theta}^{\mathbf{X}}(\mathbf{Z}; \mathbf{X})$$

$$\mathcal{L}_{\text{BIB-AE}}(\theta, \phi) = I_{\phi}(\mathbf{X}; \mathbf{Z}) - \beta I_{\theta, \phi}^{\text{U}_L}(\mathbf{Z}; \mathbf{X})$$

(1912.00830)

Mutual information between input and latent space

- Turbo-Sim: **maximised** (*loss is minimised*)
- BIB-AE: minimised

Turbo-Sim: losses

Direct and reverse losses:

$$\bar{\mathcal{L}}^{\text{Direct}}(\phi, \theta) = \mathcal{L}_{\tilde{\mathbf{z}}}(\mathbf{z}, \tilde{\mathbf{z}}) + \mathcal{D}_{\mathbf{z}\tilde{\mathbf{z}}}(\tilde{\mathbf{z}}) + \alpha \mathcal{L}_{\hat{\mathbf{x}}}(\mathbf{x}, \hat{\mathbf{x}}) + \alpha \mathcal{D}_{\mathbf{x}\hat{\mathbf{x}}}(\hat{\mathbf{x}})$$

$$\bar{\mathcal{L}}^{\text{Reverse}}(\phi, \theta) = \mathcal{L}_{\tilde{\mathbf{x}}}(\mathbf{x}, \tilde{\mathbf{x}}) + \mathcal{D}_{\mathbf{x}\tilde{\mathbf{x}}}(\tilde{\mathbf{x}}) + \beta \mathcal{L}_{\hat{\mathbf{z}}}(\mathbf{z}, \hat{\mathbf{z}}) + \beta \mathcal{D}_{\mathbf{z}\hat{\mathbf{z}}}(\hat{\mathbf{z}})$$

Total loss:

$$\bar{\mathcal{L}}^{\text{Turbo}}(\phi, \theta) = \bar{\mathcal{L}}^{\text{Direct}}(\phi, \theta) + \gamma \bar{\mathcal{L}}^{\text{Reverse}}(\phi, \theta)$$

Turbo-Sim: losses

Direct and reverse losses:

Adversarial AutoEncoder (AAE)

$$\bar{\mathcal{L}}^{\text{Direct}}(\phi, \theta) = \mathcal{L}_{\tilde{\mathbf{z}}}(\mathbf{z}, \tilde{\mathbf{z}}) + \mathcal{D}_{\mathbf{z}\tilde{\mathbf{z}}}(\tilde{\mathbf{z}}) + \alpha \mathcal{L}_{\hat{\mathbf{x}}}(\mathbf{x}, \hat{\mathbf{x}}) + \alpha \mathcal{D}_{\mathbf{x}\hat{\mathbf{x}}}(\hat{\mathbf{x}})$$

$$\bar{\mathcal{L}}^{\text{Reverse}}(\phi, \theta) = \mathcal{L}_{\tilde{\mathbf{x}}}(\mathbf{x}, \tilde{\mathbf{x}}) + \mathcal{D}_{\mathbf{x}\tilde{\mathbf{x}}}(\tilde{\mathbf{x}}) + \beta \mathcal{L}_{\hat{\mathbf{z}}}(\mathbf{z}, \hat{\mathbf{z}}) + \beta \mathcal{D}_{\mathbf{z}\hat{\mathbf{z}}}(\hat{\mathbf{z}})$$

Total loss:

$$\bar{\mathcal{L}}^{\text{Turbo}}(\phi, \theta) = \bar{\mathcal{L}}^{\text{Direct}}(\phi, \theta) + \gamma \bar{\mathcal{L}}^{\text{Reverse}}(\phi, \theta)$$

Turbo-Sim: losses

Direct and reverse losses:

Adversarial AutoEncoder (AAE)

$$\bar{\mathcal{L}}^{\text{Direct}}(\phi, \theta) = \mathcal{L}_{\tilde{\mathbf{z}}}(\mathbf{z}, \tilde{\mathbf{z}}) + \mathcal{D}_{\tilde{\mathbf{z}}\tilde{\mathbf{z}}}(\tilde{\mathbf{z}}) + \alpha \mathcal{L}_{\hat{\mathbf{x}}}(\mathbf{x}, \hat{\mathbf{x}}) + \alpha \mathcal{D}_{\mathbf{x}\hat{\mathbf{x}}}(\hat{\mathbf{x}})$$

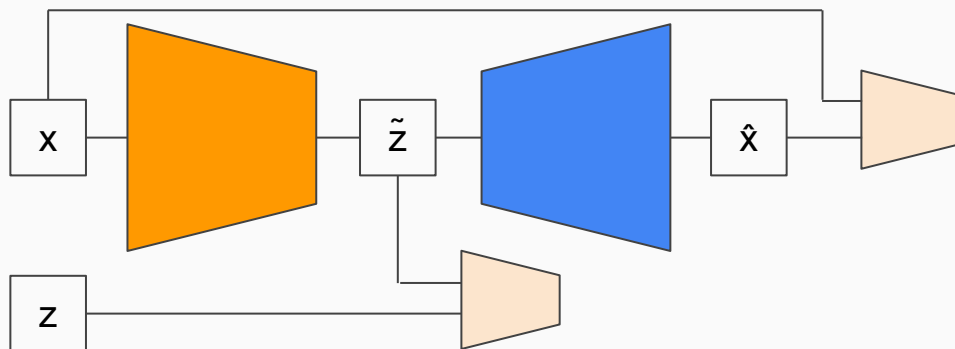
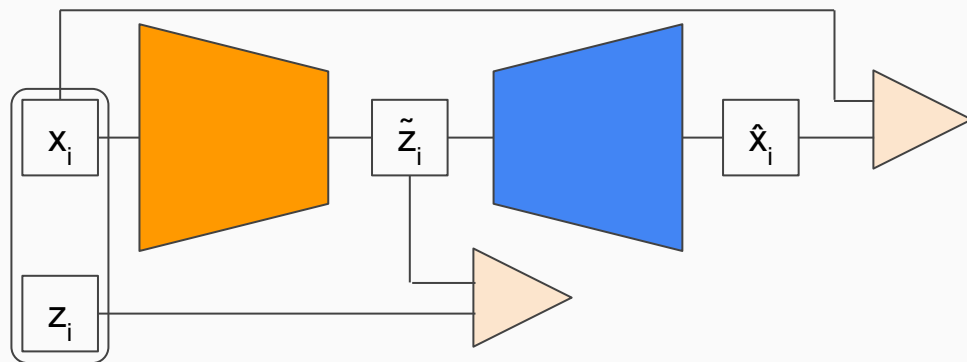
$$\bar{\mathcal{L}}^{\text{Reverse}}(\phi, \theta) = \mathcal{L}_{\tilde{\mathbf{x}}}(\mathbf{x}, \tilde{\mathbf{x}}) + \mathcal{D}_{\mathbf{x}\tilde{\mathbf{x}}}(\tilde{\mathbf{x}}) + \beta \mathcal{L}_{\hat{\mathbf{z}}}(\mathbf{z}, \hat{\mathbf{z}}) + \beta \mathcal{D}_{\mathbf{z}\hat{\mathbf{z}}}(\hat{\mathbf{z}})$$

Generative Adversarial Network (GAN)

Total loss:

$$\bar{\mathcal{L}}^{\text{Turbo}}(\phi, \theta) = \bar{\mathcal{L}}^{\text{Direct}}(\phi, \theta) + \gamma \bar{\mathcal{L}}^{\text{Reverse}}(\phi, \theta)$$

Training scheme



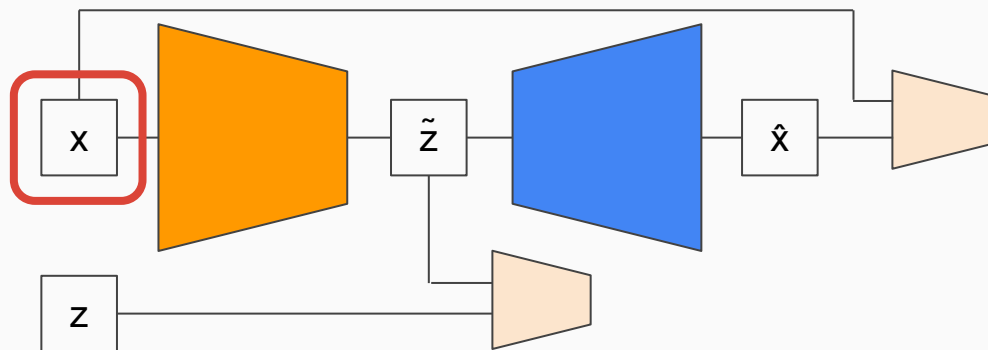
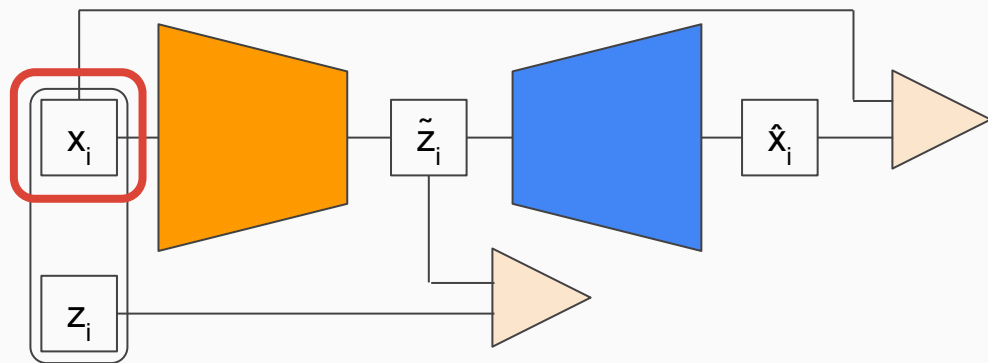
Direct

- A minibatch of $\{x_i\}$ and $\{x\}$ is passed through the network
- **Supervised losses** are computed between $\{z_i, x_i\}$ and $\{\tilde{z}_i, \hat{x}_i\}$
- **Unsupervised losses** are computed between $\{z, x\}$ and $\{\tilde{z}, \hat{x}\}$
- **Random noise** is added to the input of both the encoder and the decoder

Reverse:

- The same is done swapping $x \leftrightarrow z$

Training scheme



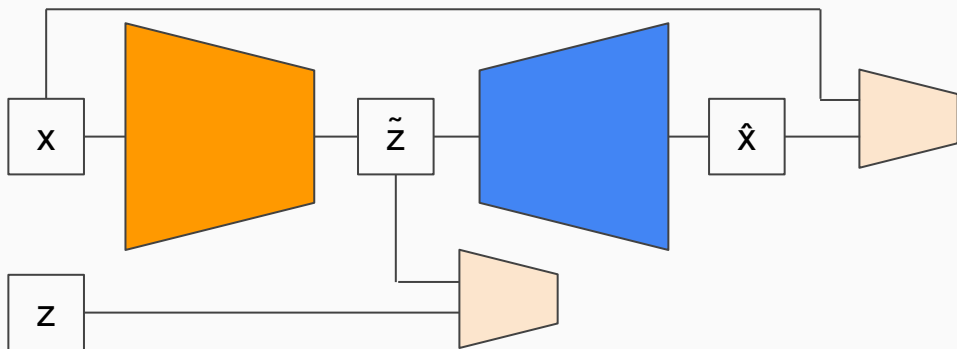
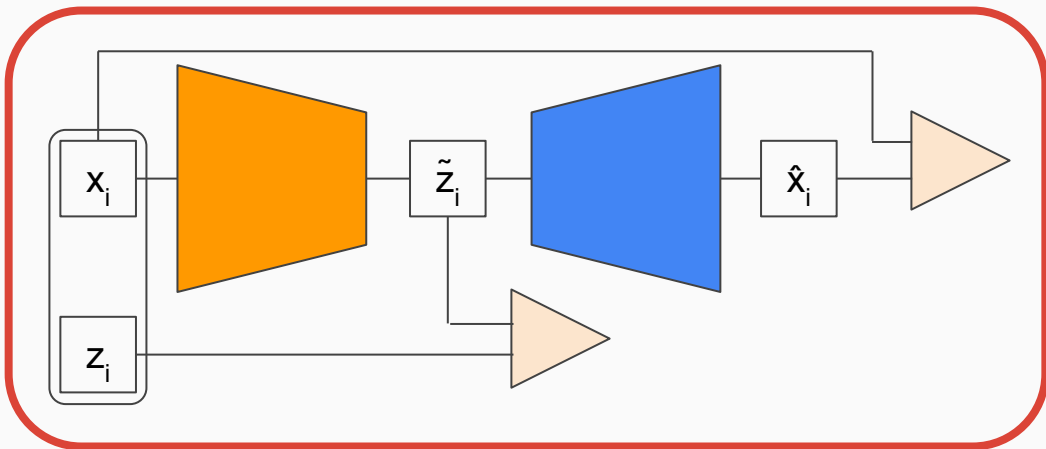
Direct

- A minibatch of $\{x_i\}$ and $\{z_i\}$ is passed through the network
- **Supervised losses** are computed between $\{z_i, x_i\}$ and $\{\tilde{z}_i, \hat{x}_i\}$
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- The same is done swapping $x \leftrightarrow z$

Training scheme



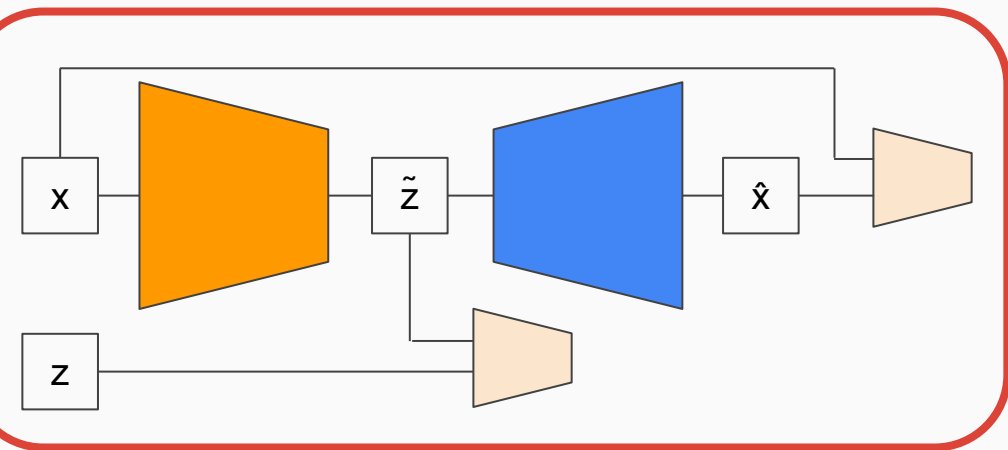
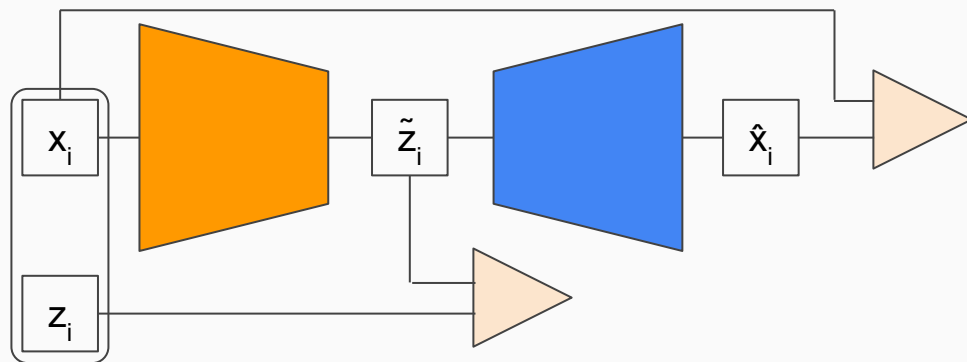
Direct

- A minibatch of $\{x_i\}$ and $\{x\}$ is passed through the network
- **Supervised losses** are computed between $\{z_i, x_i\}$ and $\{\tilde{z}_i, \hat{x}_i\}$
- **Unsupervised losses** are computed between $\{z, x\}$ and $\{\tilde{z}, \hat{x}\}$
- **Random noise** is added to the input of both the encoder and the decoder

Reverse:

- The same is done swapping $x \leftrightarrow z$

Training scheme



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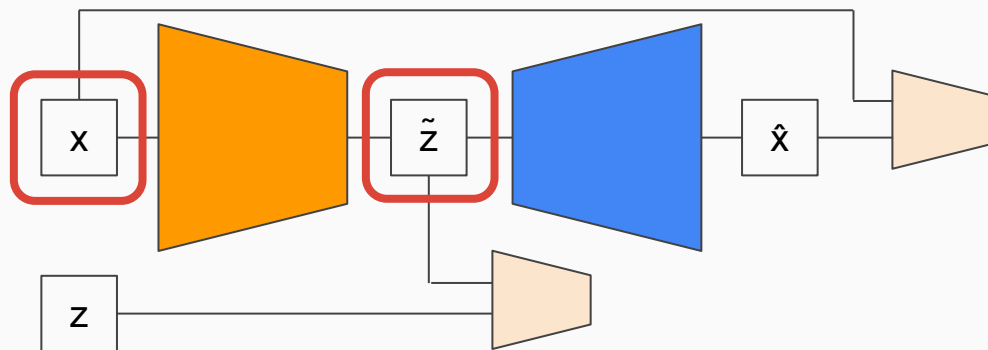
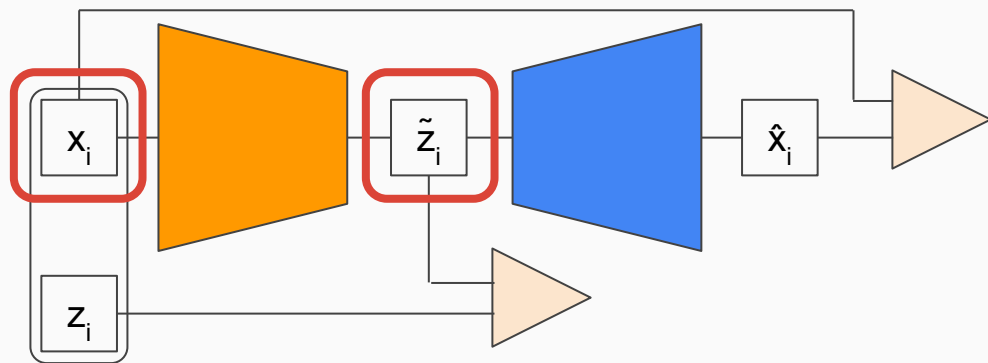
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Training scheme



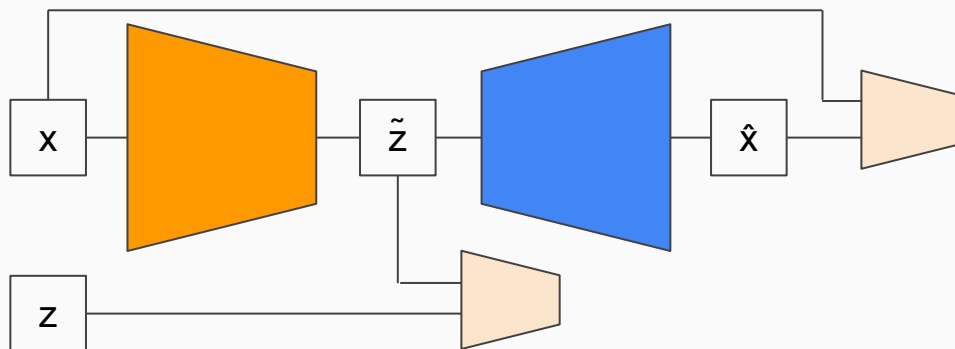
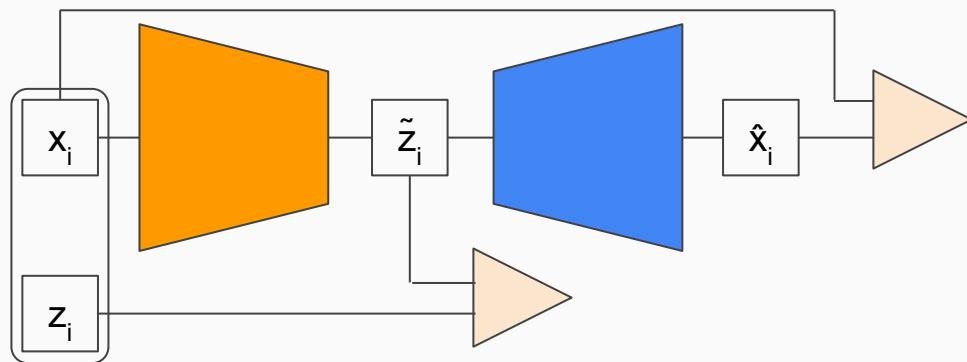
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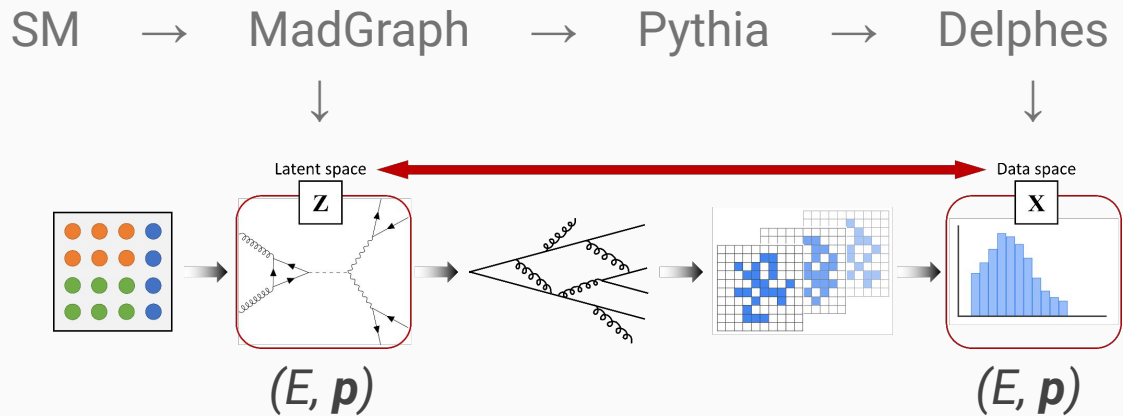
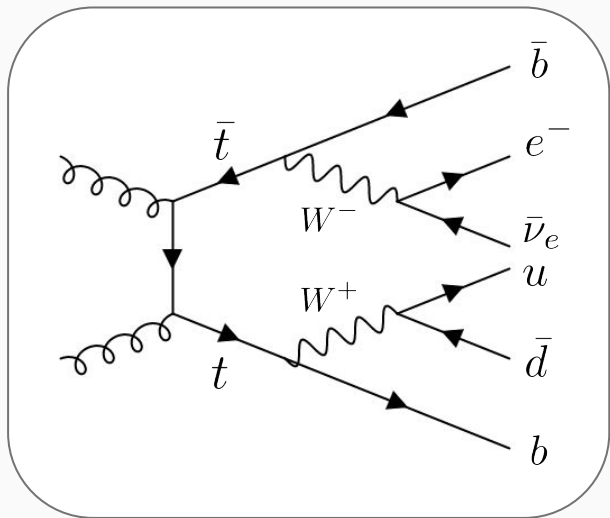
Reverse:

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HEP experiment

Dataset and results

Dataset

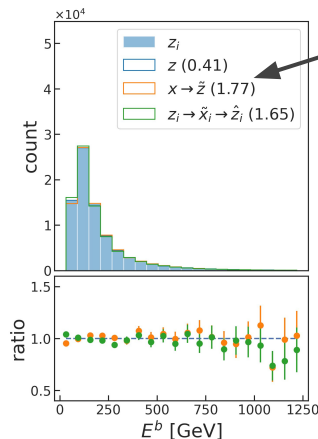


$$z = \{E_{e^-}, \mathbf{p}_{e^-}, E_{\bar{\nu}_e}, \mathbf{p}_{\bar{\nu}_e}, E_b, \mathbf{p}_b, E_{\bar{b}}, \mathbf{p}_{\bar{b}}, E_u, \mathbf{p}_u, E_{\bar{d}}, \mathbf{p}_{\bar{d}}\}$$

$$x = \{E_{e^-}, \mathbf{p}_{e^-}, E_{\text{miss}}, \mathbf{p}_{\text{miss}}, E_1, \mathbf{p}_1, E_2, \mathbf{p}_2, E_3, \mathbf{p}_3, E_4, \mathbf{p}_4\}$$

Legend

- **Input data**
 $\{z, x\}$ pairs and $\{z\}, \{x\}$ marginals
(KS for the dataset itself)
- **Generated data**
 i.e. simulation and unfolding
- **Reconstructed data**
 i.e. autoencoder output



Distributions of several observables

Trained on:

- (E, \mathbf{p}) of final state particles
- (E, \mathbf{p}) of reconstructed particles

Not trained on:

- *mass of underlying particles (W, t)*

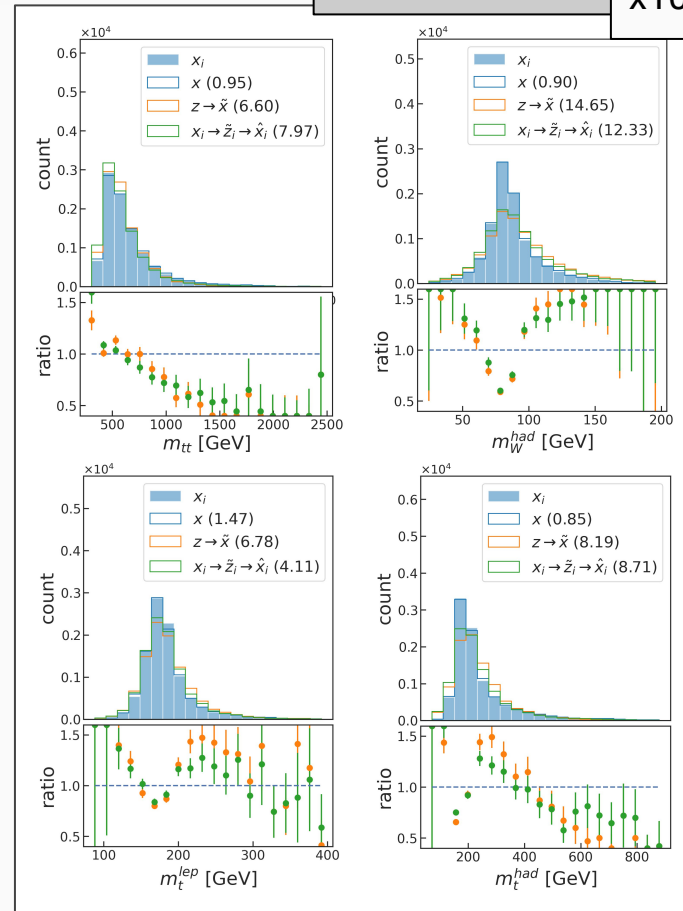
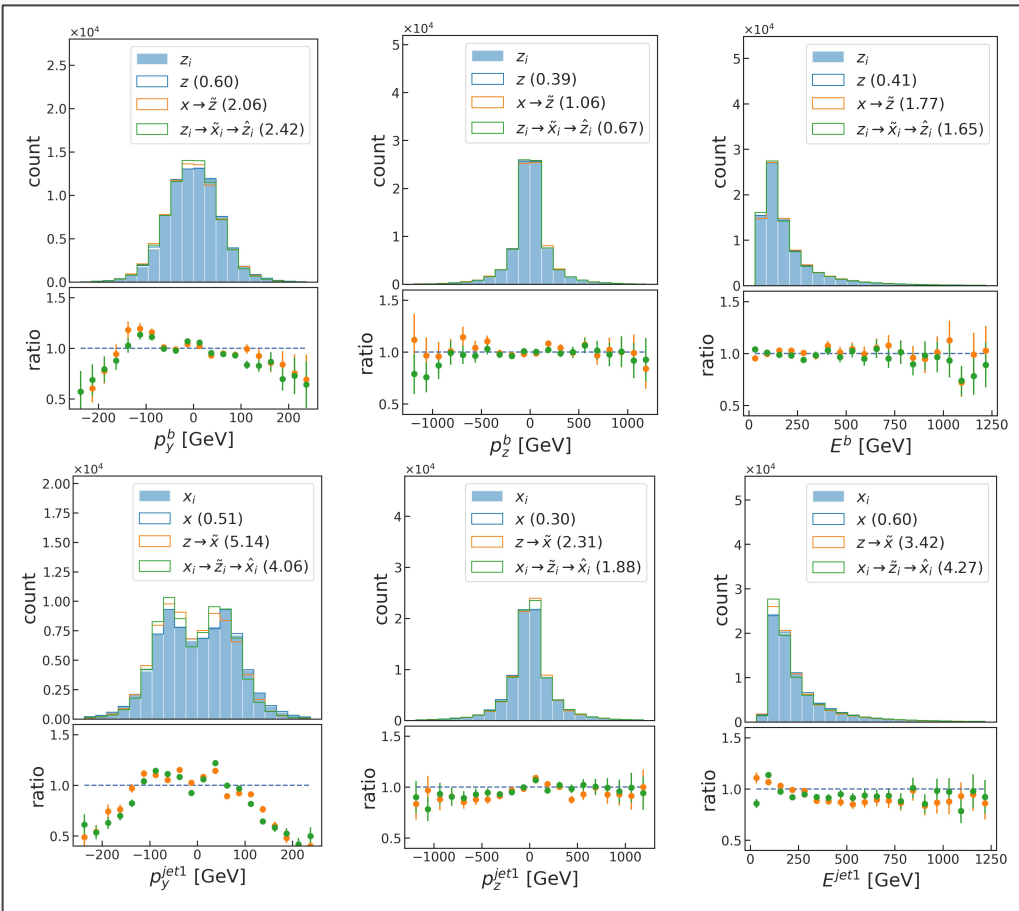
In parenthesis:

Kolmogorov-Smirnov distance to truth (the lower the better)

Results

Kolmogorov-Smirnov

$\times 10^{-2}$



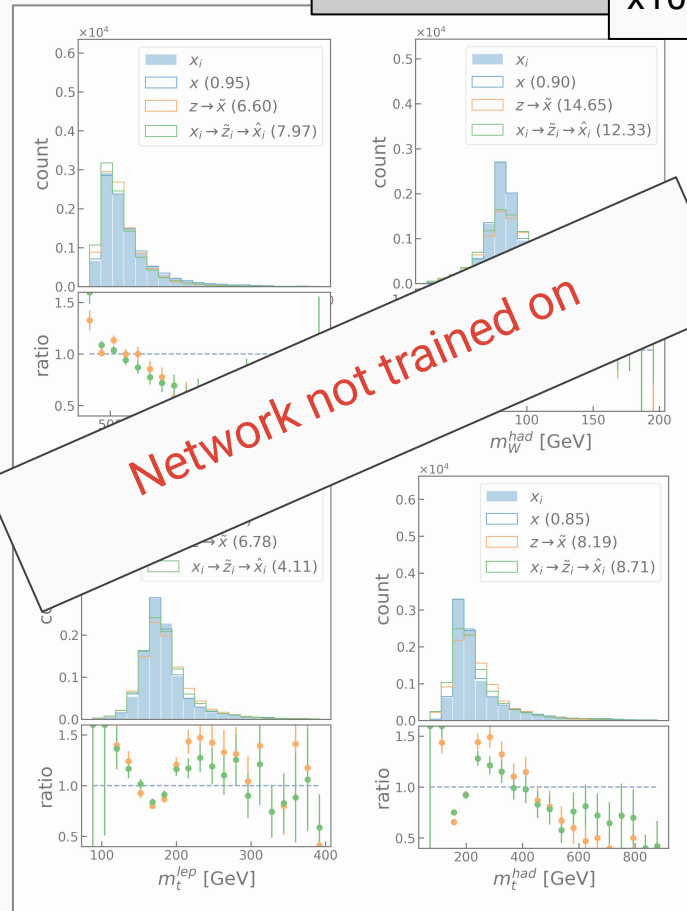
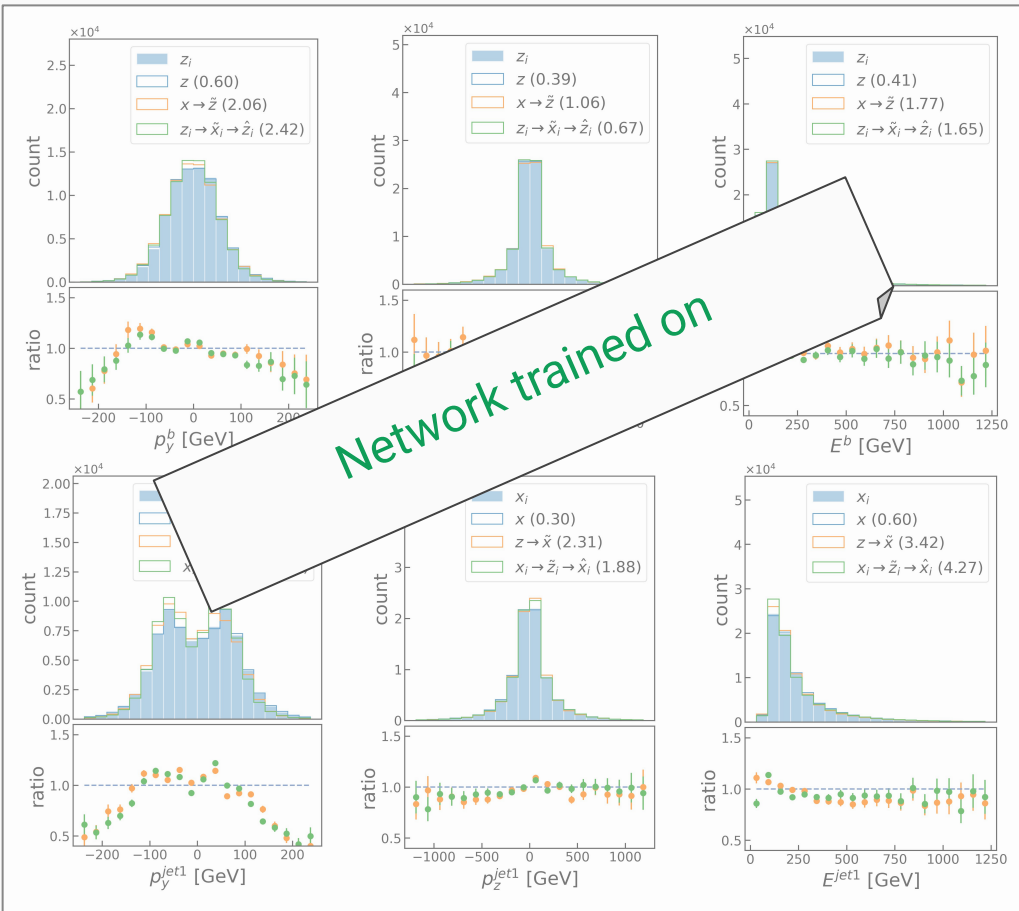
Results

Kolmogorov-Smirnov

$\times 10^{-2}$

Network trained on

Network not trained on

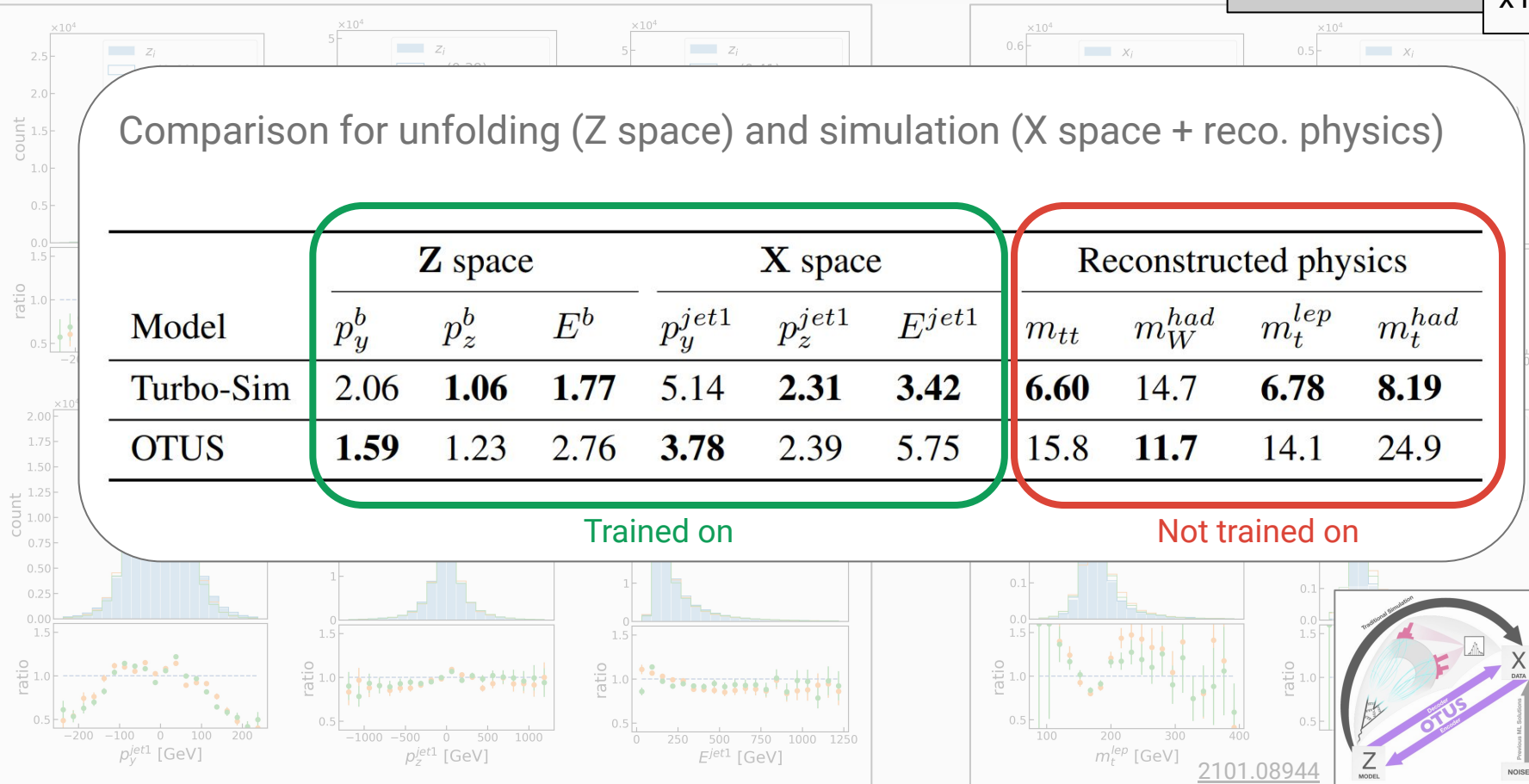


Comparison for unfolding (Z space) and simulation (X space + reco. physics)

Model	Z space			X space			Reconstructed physics			
	p_y^b	p_z^b	E^b	p_y^{jet1}	p_z^{jet1}	E^{jet1}	m_{tt}	m_W^{had}	m_t^{lep}	m_t^{had}
Turbo-Sim	2.06	1.06	1.77	5.14	2.31	3.42	6.60	14.7	6.78	8.19
OTUS	1.59	1.23	2.76	3.78	2.39	5.75	15.8	11.7	14.1	24.9

Trained on

Not trained on



2101.08944

Conclusion

Summary and outlook

Summary

- **Generalised autoencoder** based on information theory principles
 - Maximise mutual information between input and latent space
 - Give an interpretation to several architecture (AAE, GAN, etc.)

- Applied to **HEP simulation and unfolding**
 - Transform four-momenta from hard scattering to detector reconstruction
 - Achieve very good results with basic building blocks

Outlook

- Other scattering processes
- Improve **stochasticity** (*more expressive network*)
- **Permutation invariance** (*input ordering \neq output ordering*)
 - Graph/attention based architecture
- **Transform distributions** (*specialised architecture*)
 - Conditional Normalising Flow (see yesterday [talk](#))
- but **variable dimensionality** (*of input/output*)
 - Funnels (see next [talk](#))

Thanks!