UNIVERSITÄT HEIDELBERG
ZUKUNFT SEIT 1386

IRN Terascale, 26.10.2023

Diffusion Models

for LHC event generation

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arXiv: 2305.10475

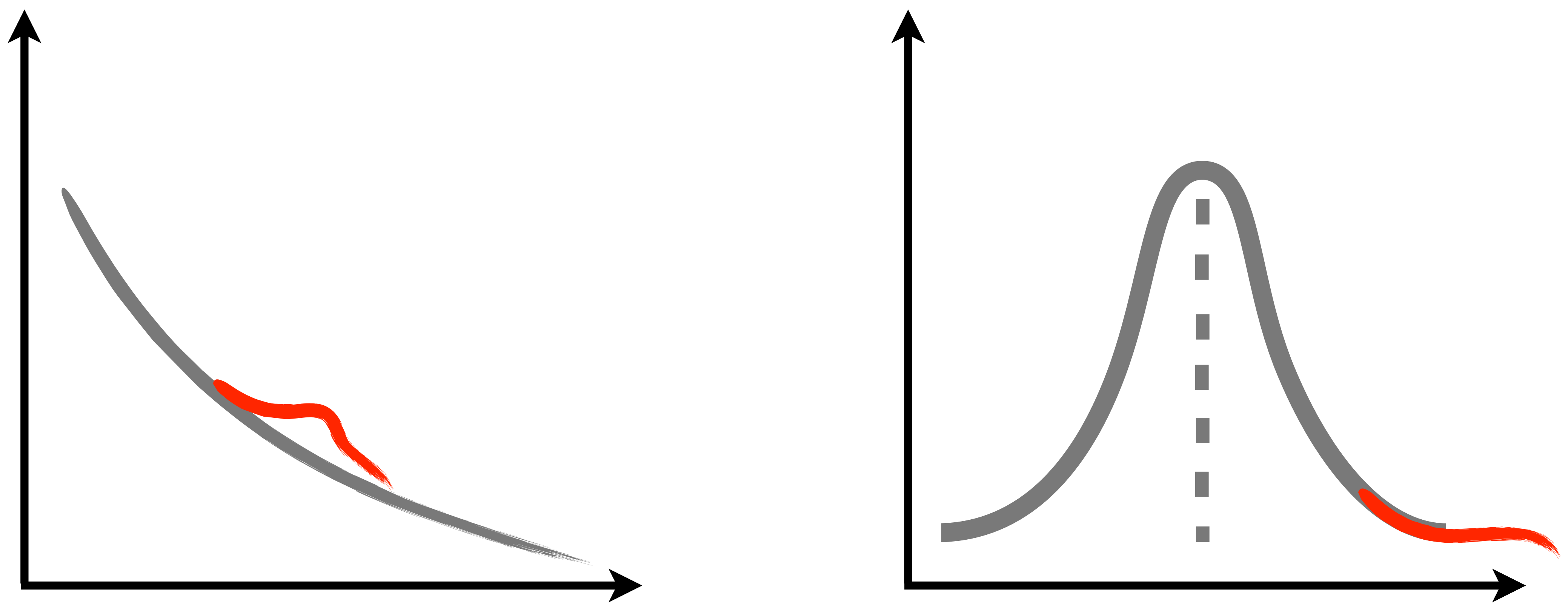
Why Event Generation?

Vast amount of data collected by collider experiments

Standard Model is probed

Theoretical predictions (simulation) needs to match experimental statistics

$5\,\sigma$?



Why ML Event Generation?

After high luminosity runs → ~ 5 times as much data

Theoretical predictions needs to be even more precise (include higher correction terms)

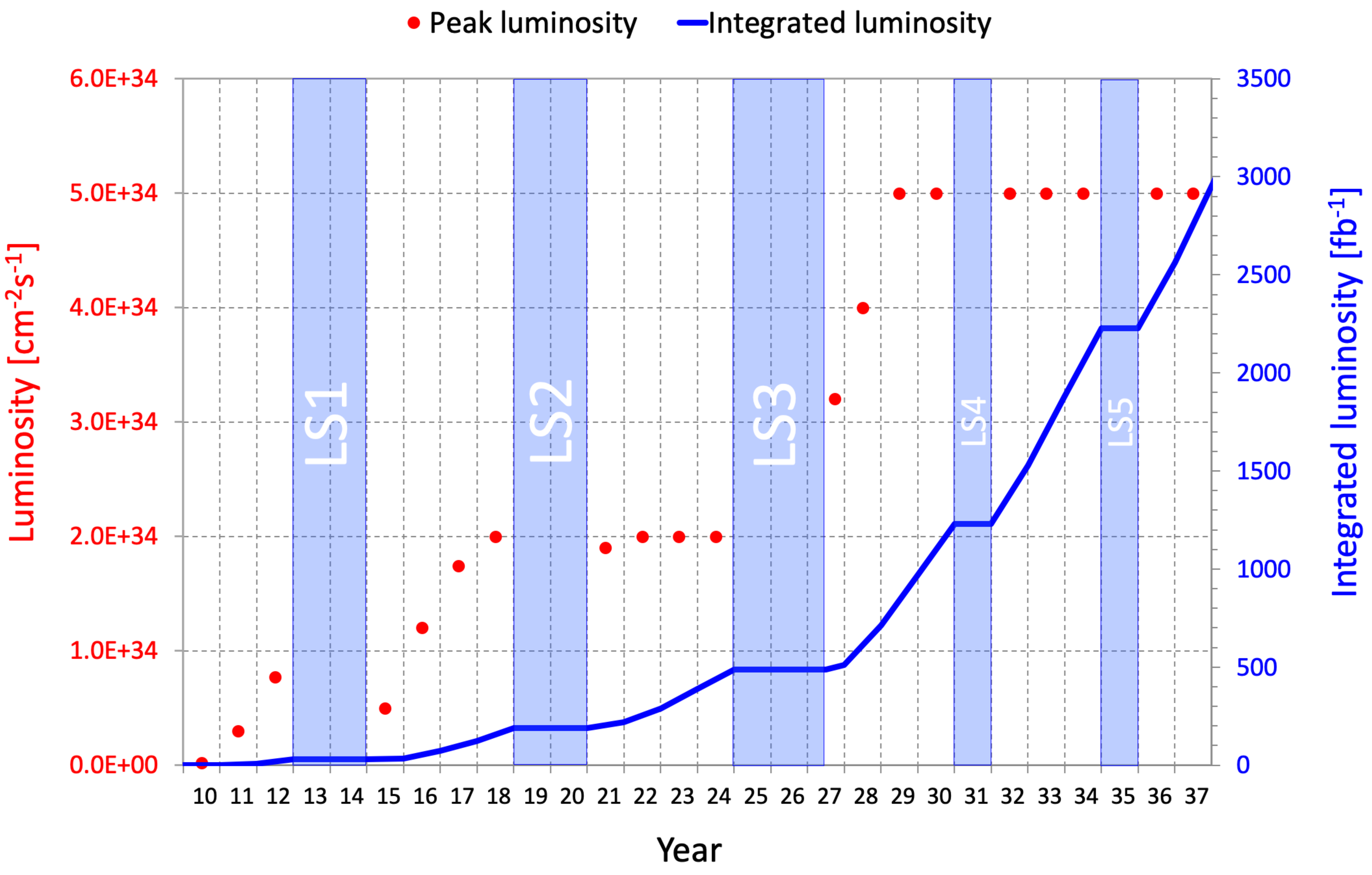


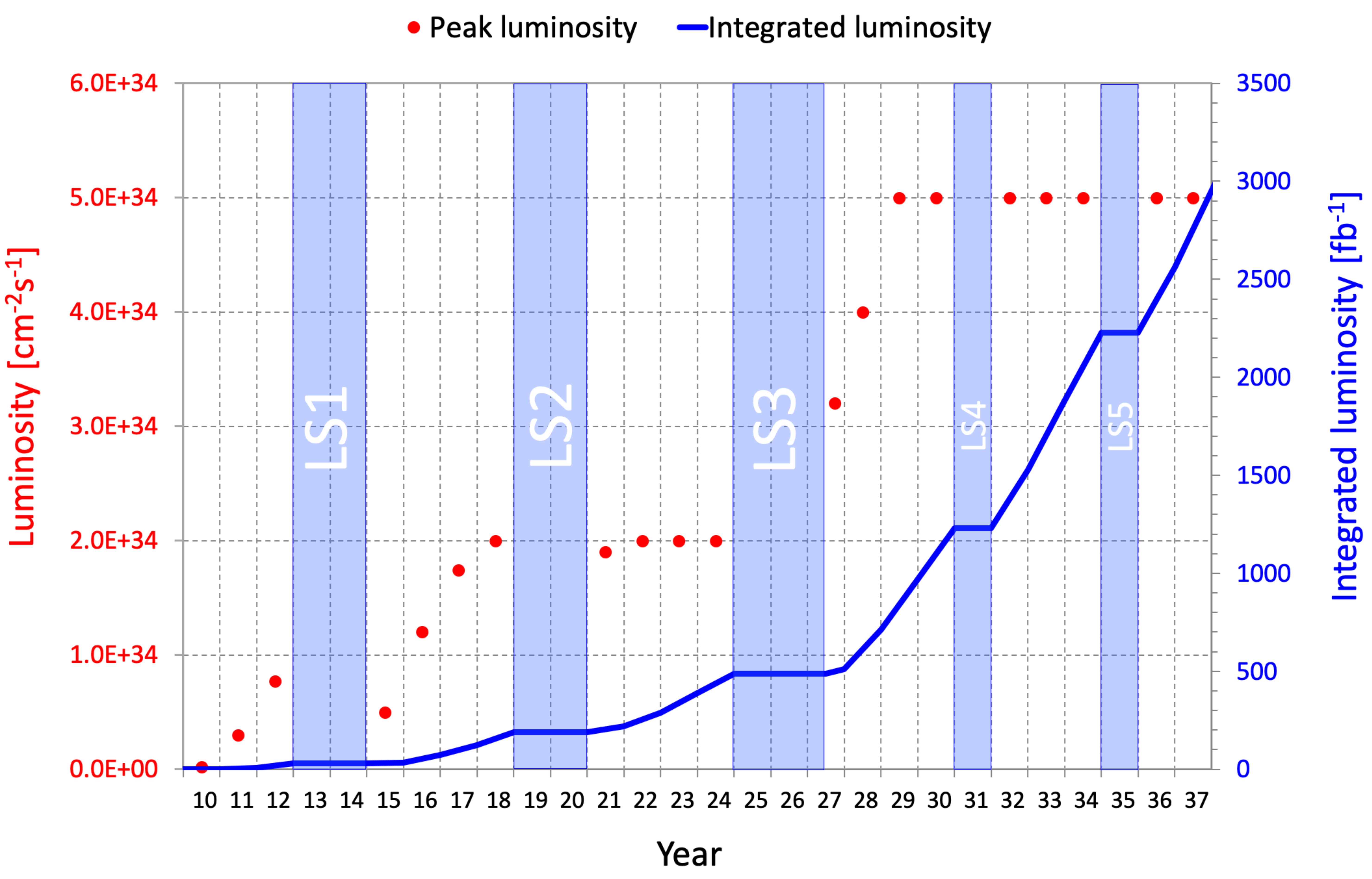
Figure from https://web.archive.org/web/20220706170326/https://lhc-commissioning.web.cern.ch/schedule/images/LHC-nominal-lumi-projection.png

Why ML Event Generation?

After high luminosity runs → ~ 5 times as much data

Theoretical predictions needs to be even more precise (include higher correction terms)

But: Currently computational expensive



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Where ML Event Generation?

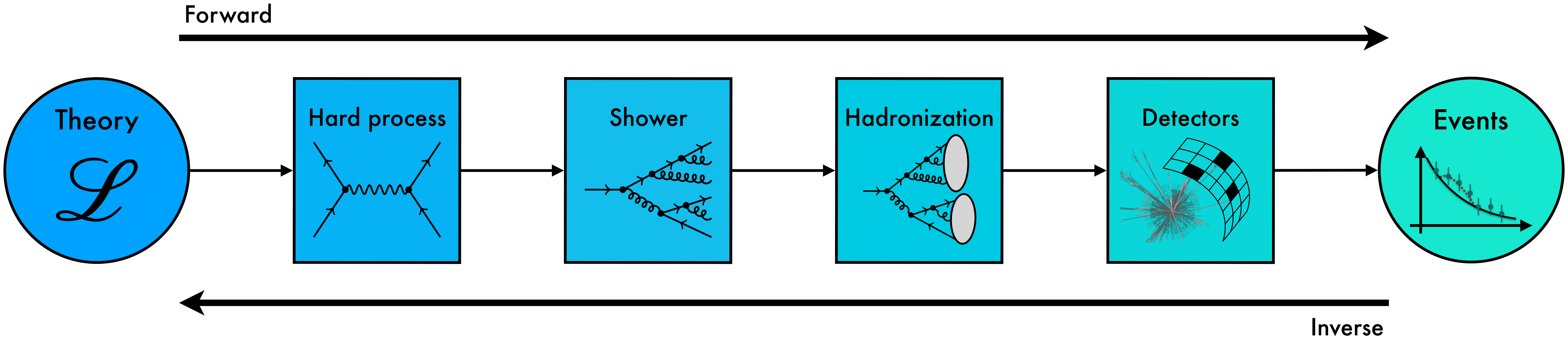
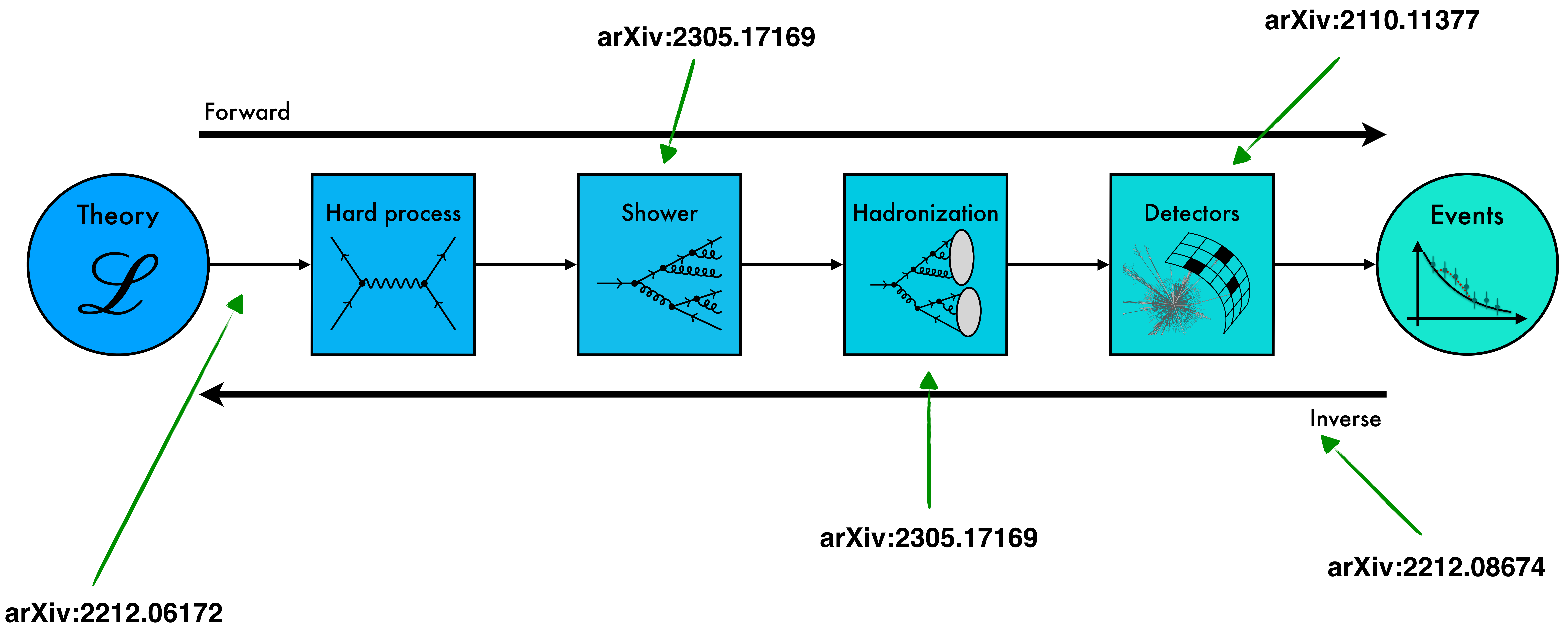


Figure from A. Butter et al.: arXiv:2203.07460, R. Winterhalder

Where ML Event Generation?



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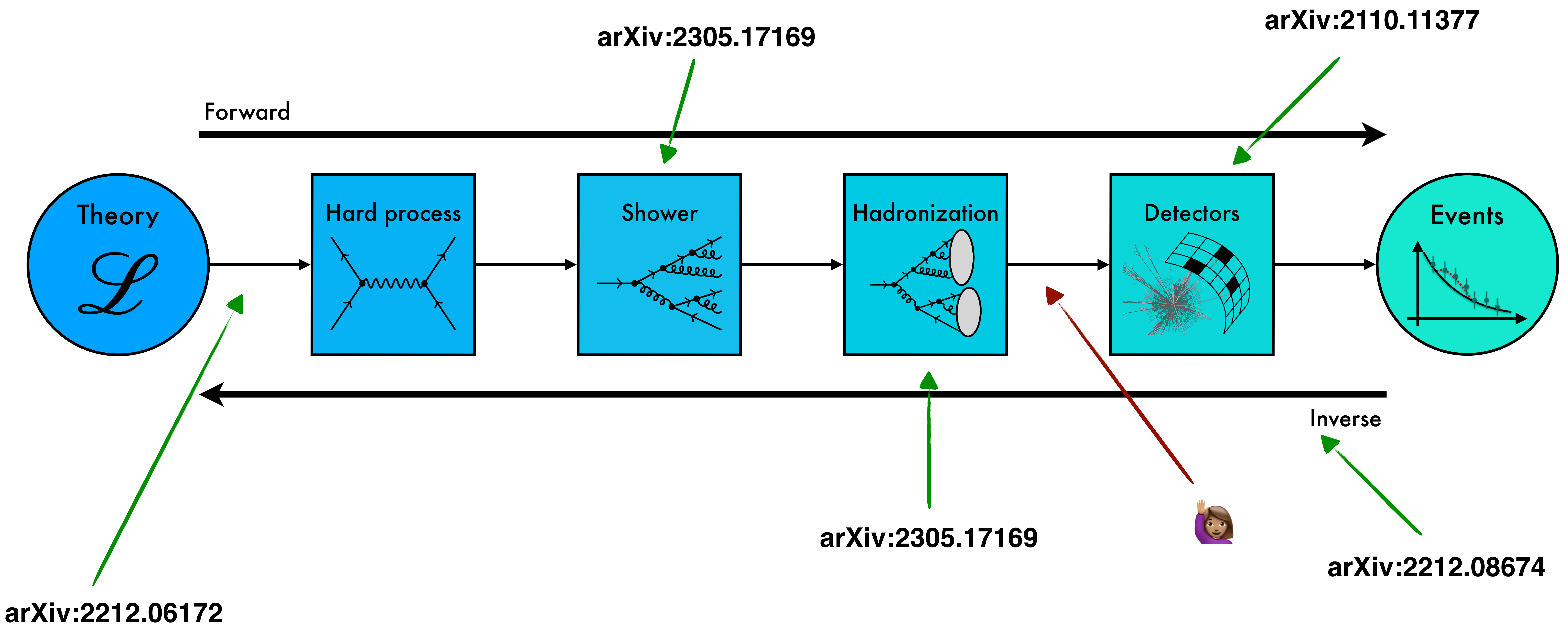

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How to be generative

Phase Space

$x \sim p(x)$

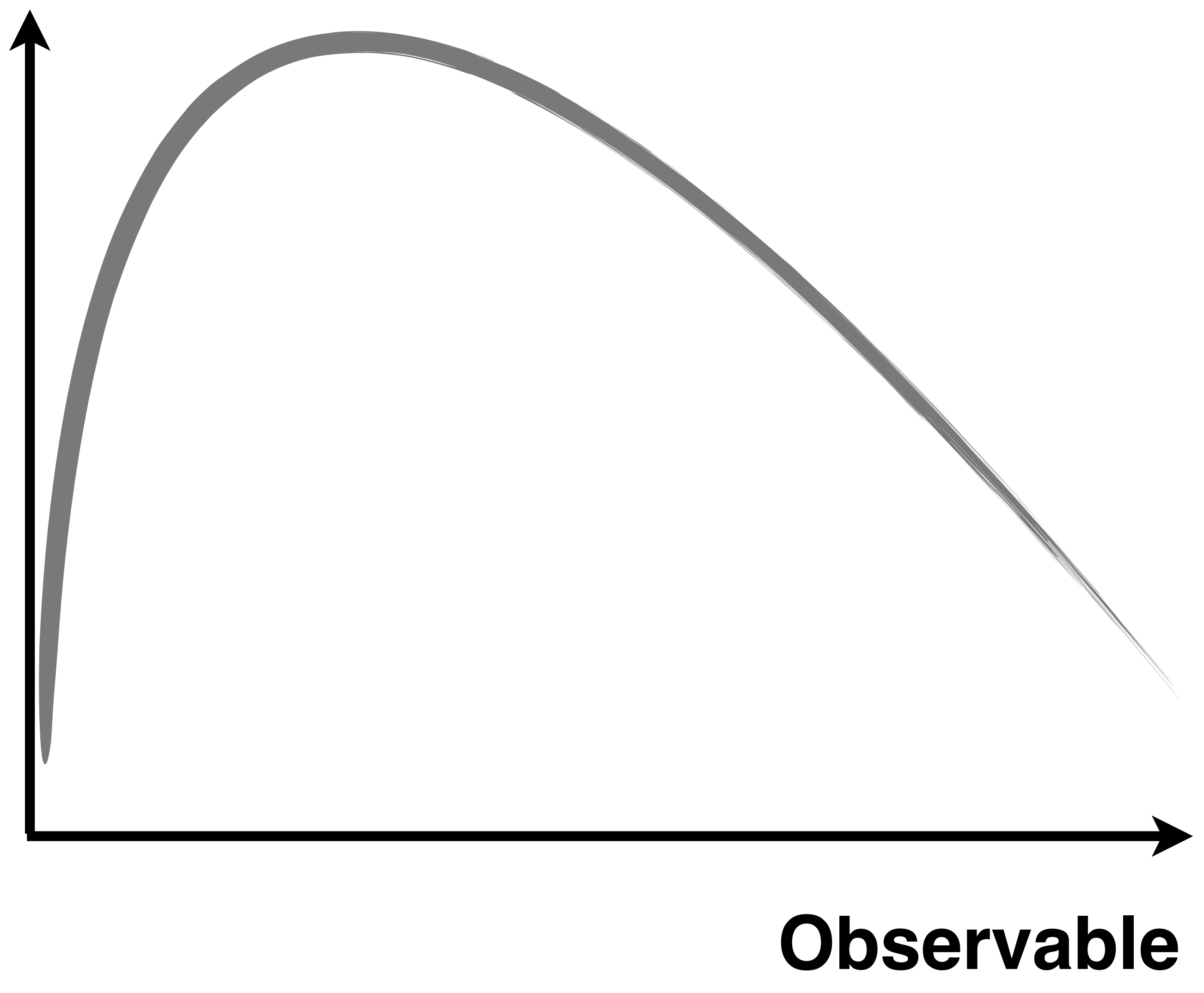
👎🏽 Difficult to sample from

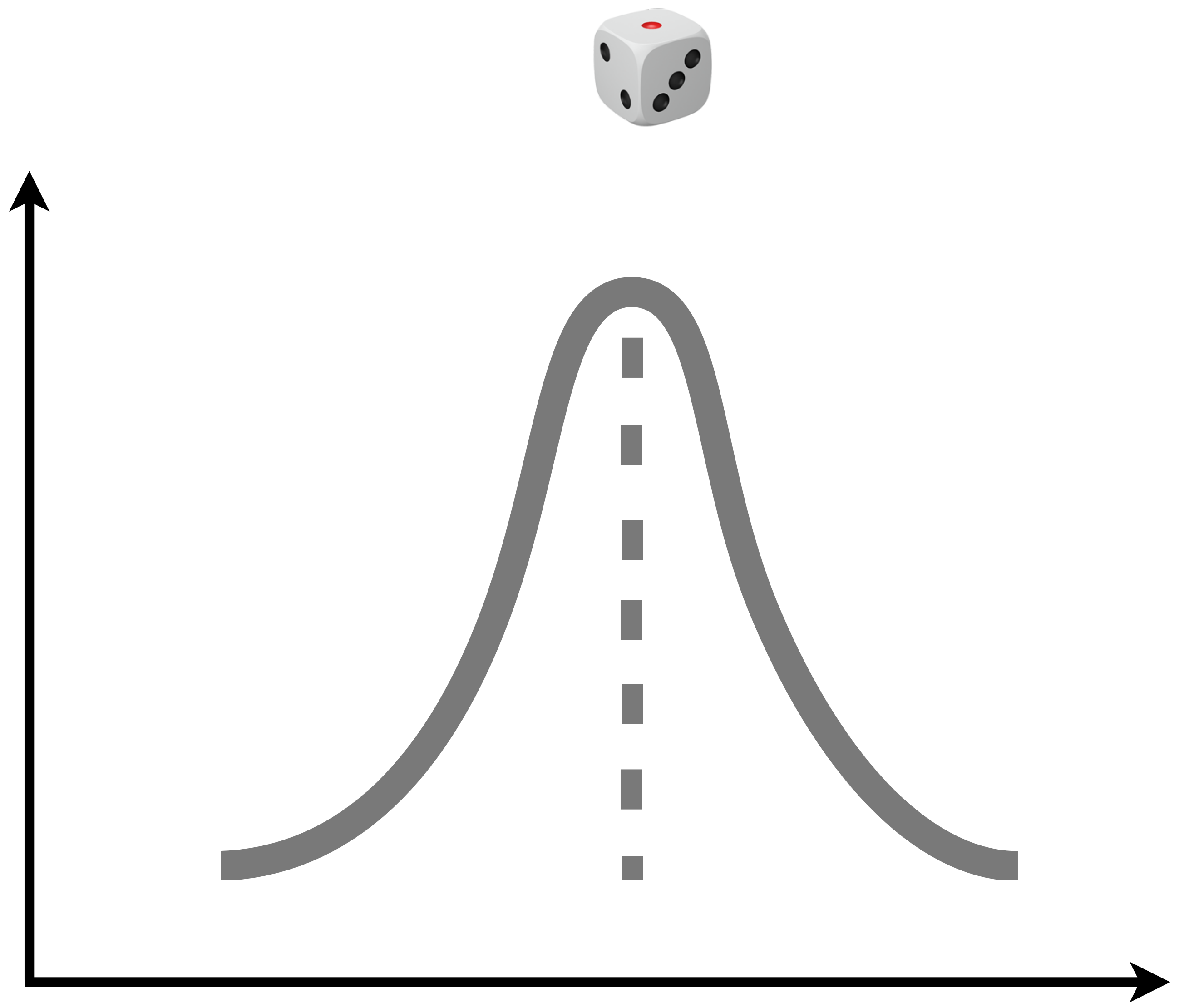
?

Latent Space

$z \sim \mathcal{N}(0,1)$

👍🏽 Easy to sample from





How to be generative

Phase Space

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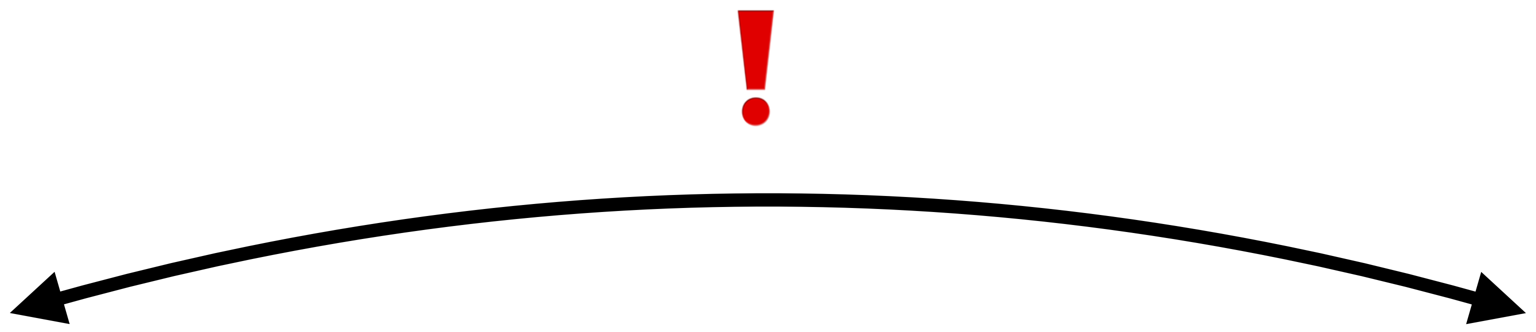
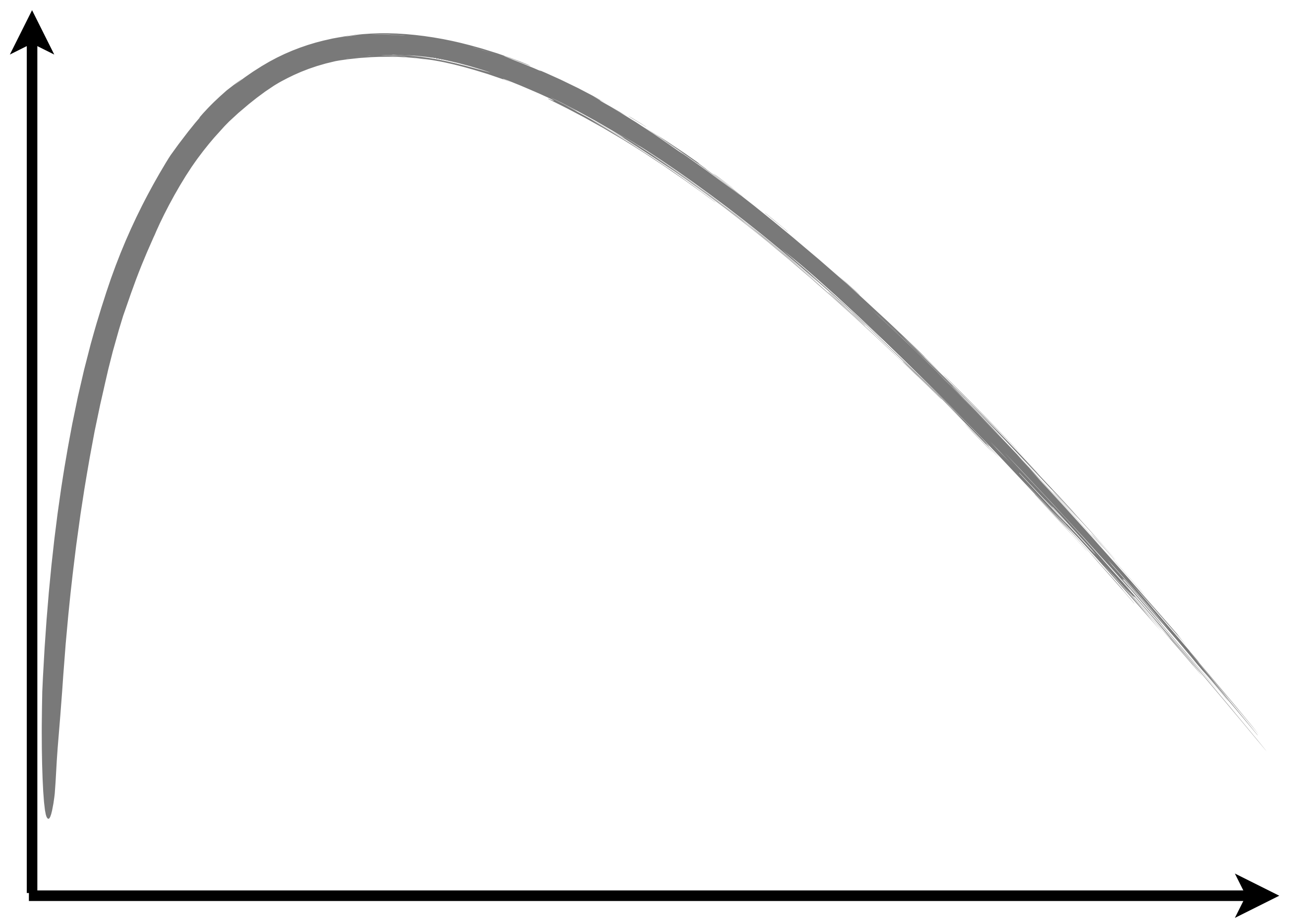


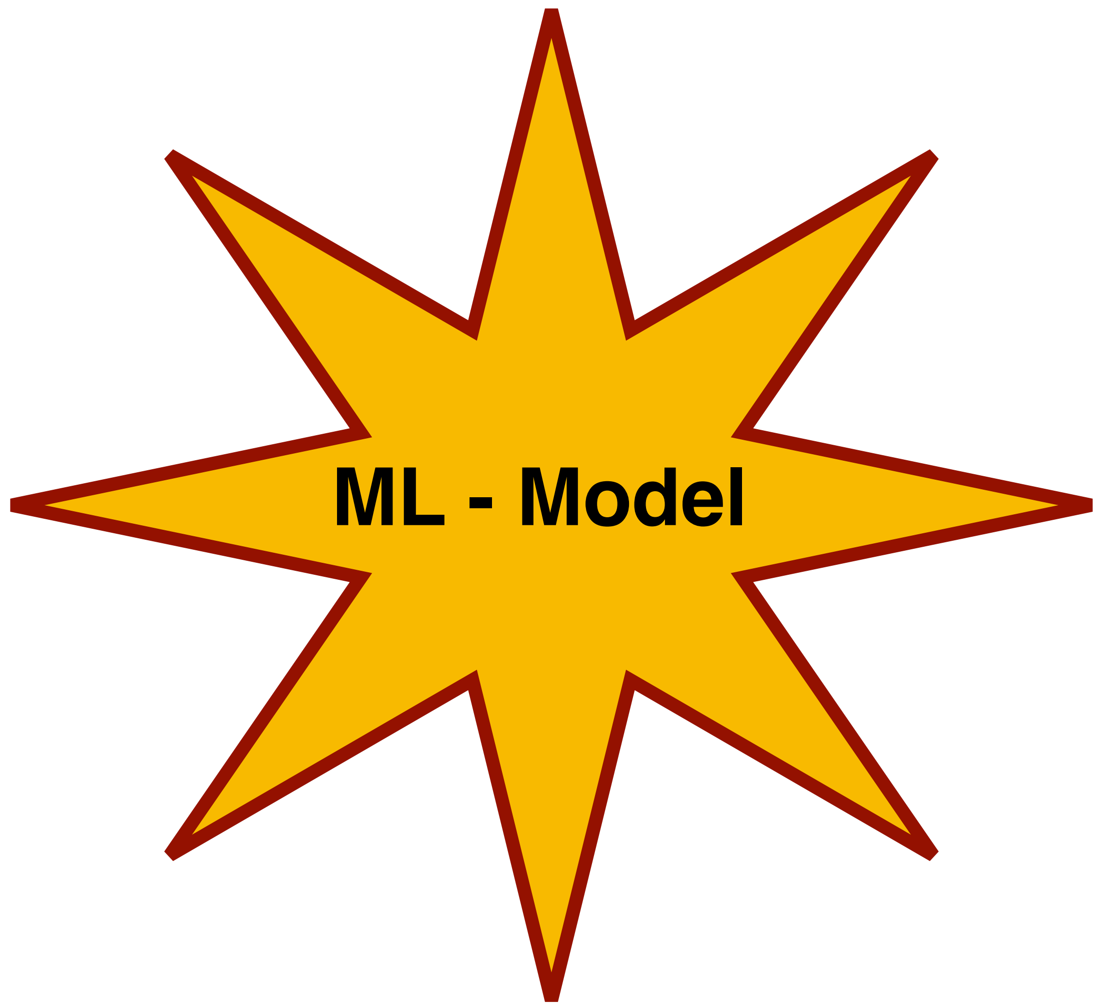
Latent Space

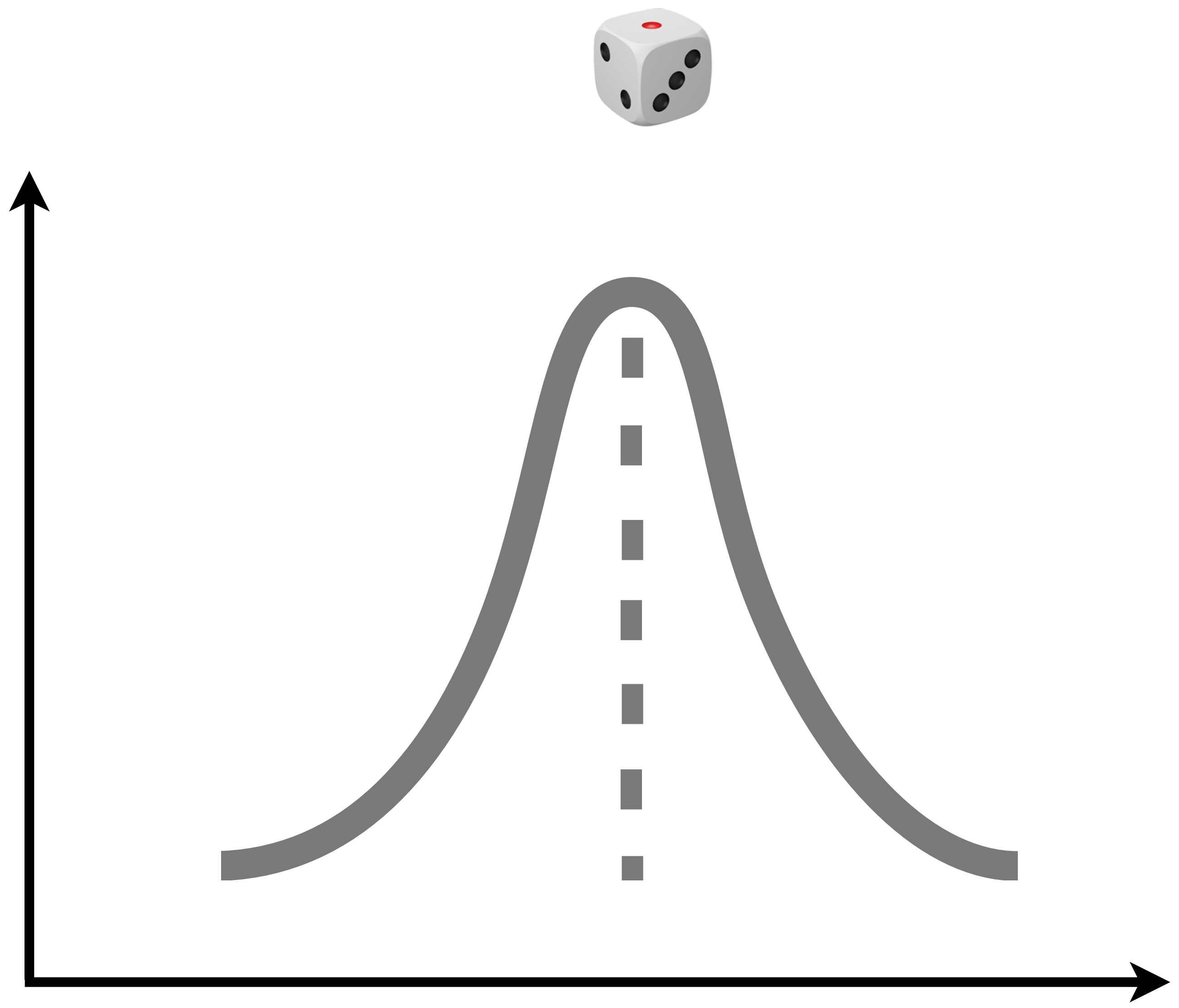
$z \sim \mathcal{N}(0,1)$

👍 Easy to sample from



Observable

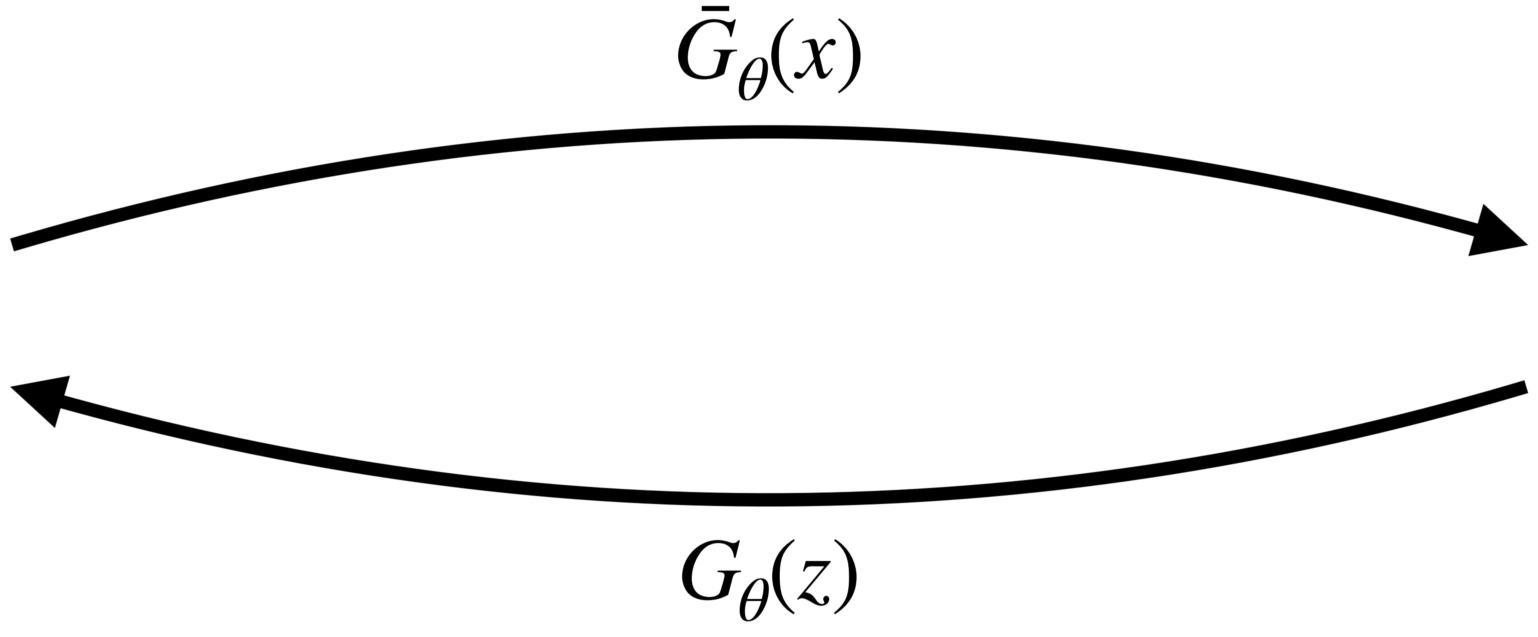




Invertible Neural Networks (INNs)

Phase Space

$x \sim p(x)$



Latent Space

$z \sim \mathcal{N}(0,1)$

Bijective mapping $G_\theta(x)$

$$p_\theta(x) = p(z)\frac{dz}{dx} = p(z)\left|\frac{\partial \bar{G}_\theta(x)}{\partial x}\right|$$

$$\mathscr{L}_{INN} = -\log p_\theta(x) = -\log p(\bar{G}_\theta(x)) - log\left|\frac{\partial \bar{G}_\theta(x)}{\partial x}\right|$$

Diffusion Models

Phase Space

$x_0 \sim p(x_0)$

Latent Space

$x_T \sim p(x_T)(= \mathcal{N}(0,1))$

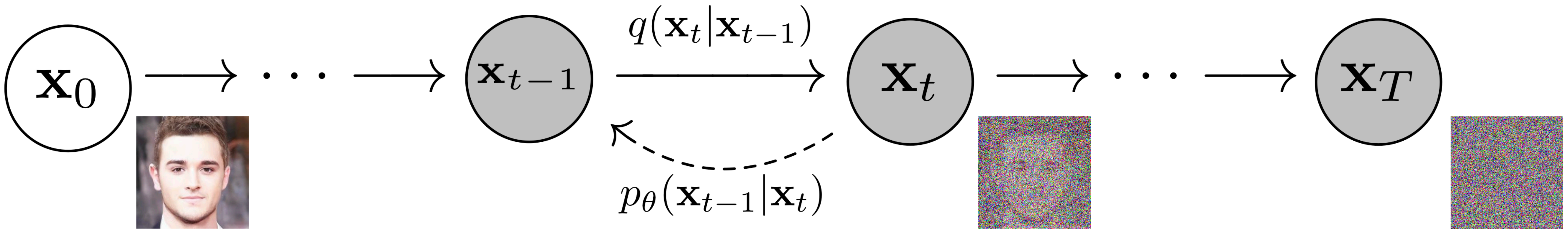
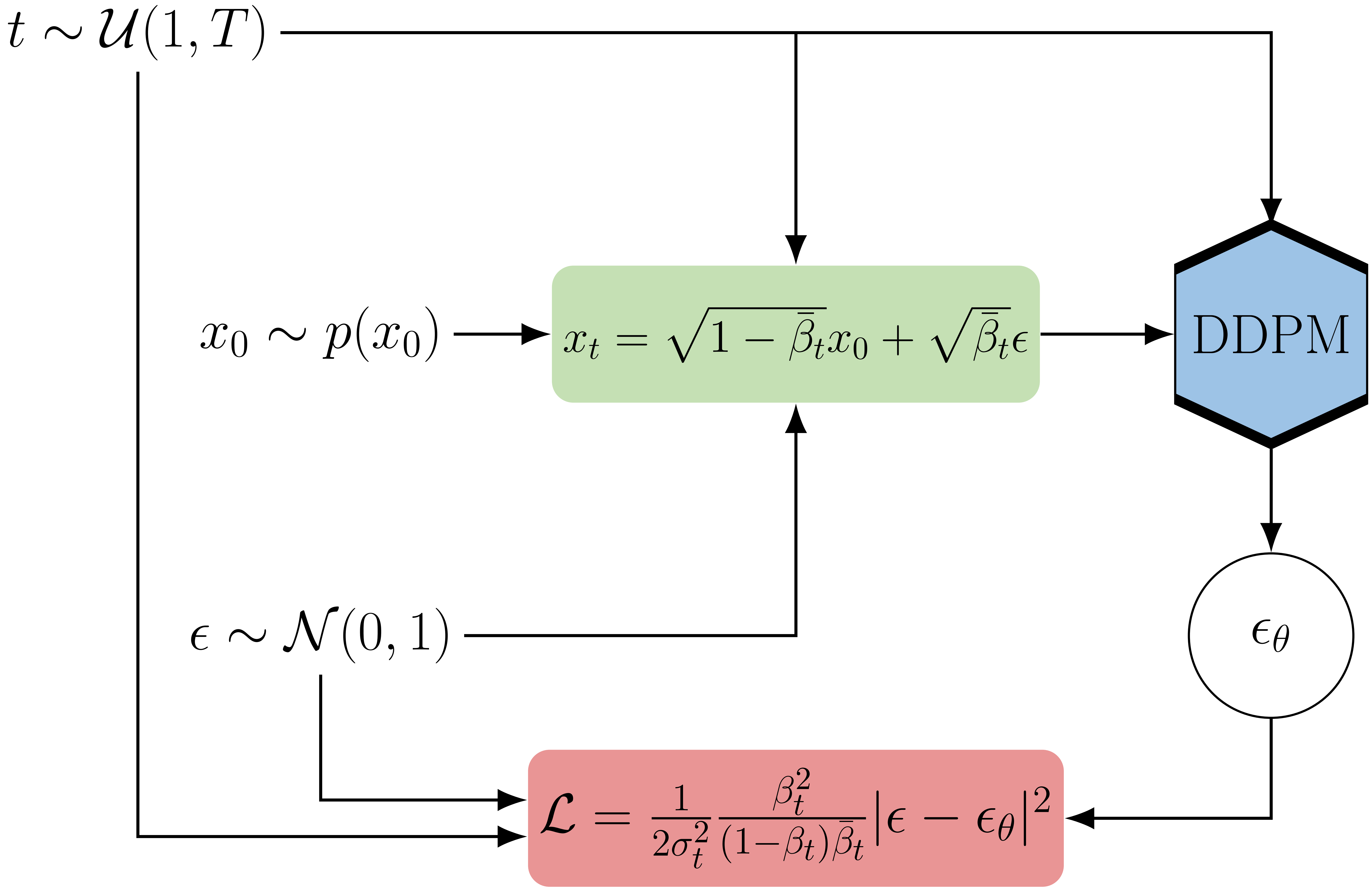


Figure from J.Ho et al.: arXiv:2006.11239

Diffusion Models (DDPM)



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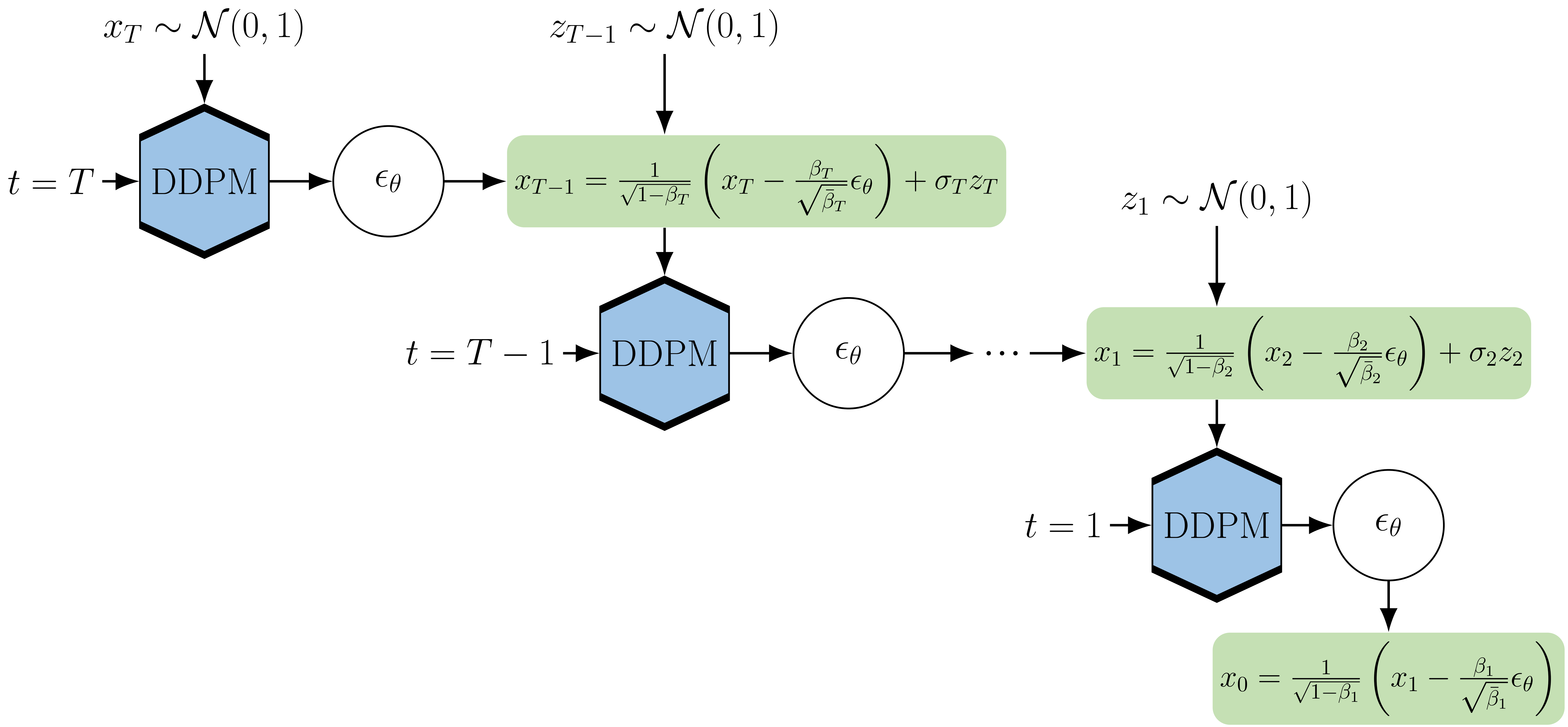


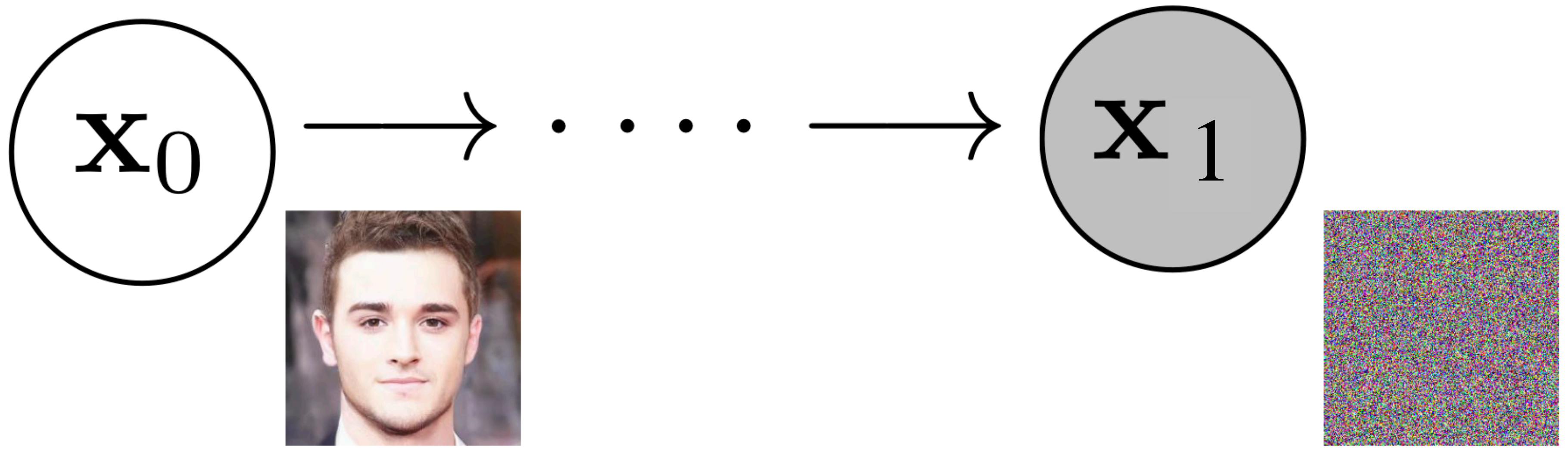
Diffusion Models (CFM)

Phase Space

$x_0 \sim p(x_0)$

Latent Space

$x_1 \sim p(x_1)(= \mathcal{N}(0,1))$

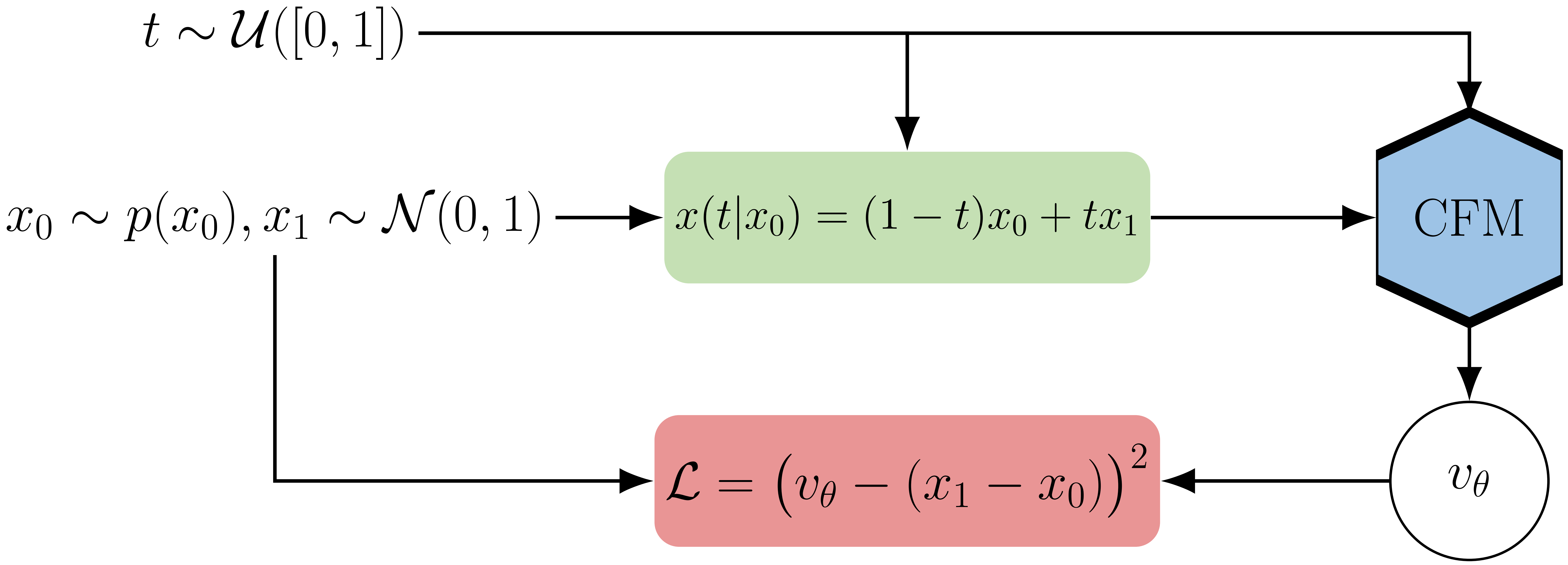


Continuous time evolution **t**

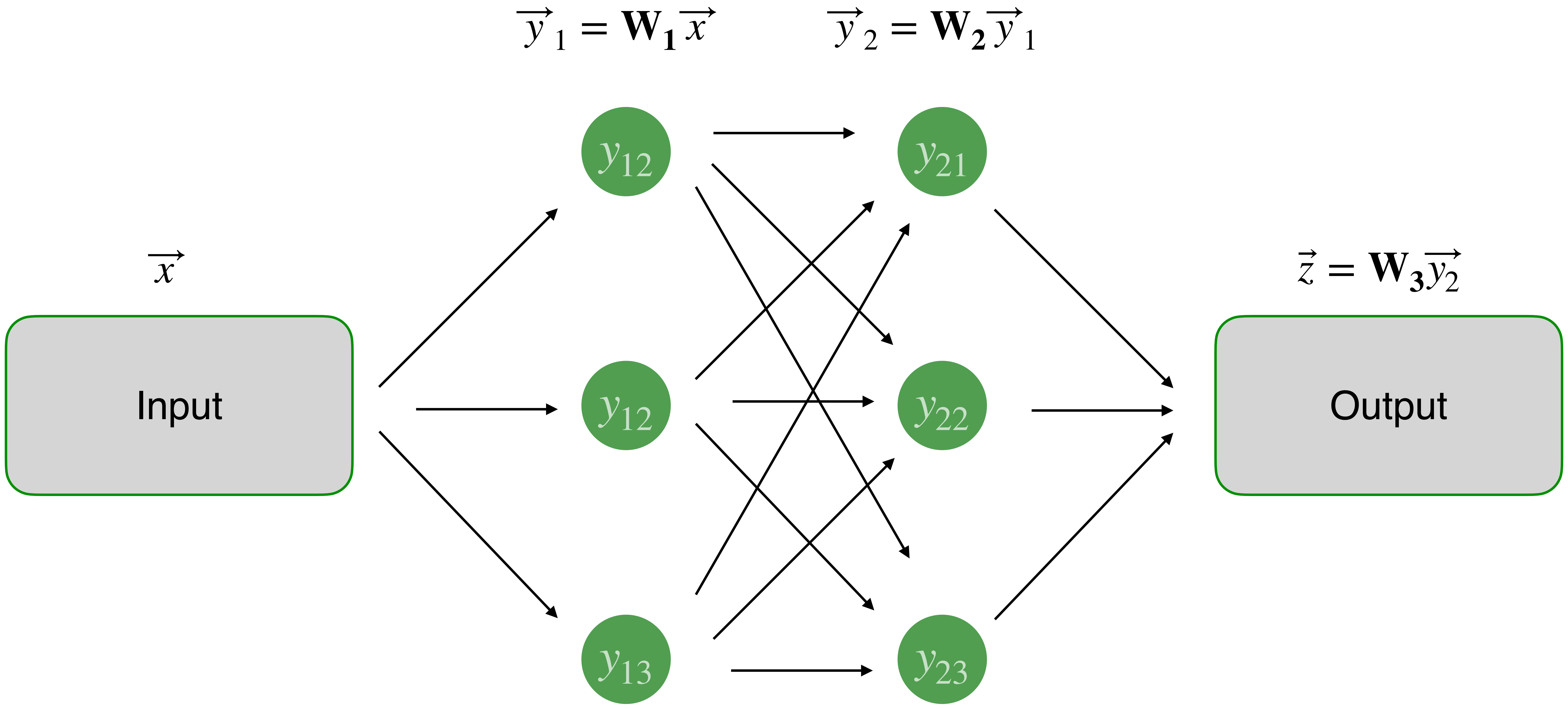
Evolution governed by $\frac{dx}{dt}$

Figure from J.Ho et al.: arXiv:2006.11239

Diffusion Models (CFM)

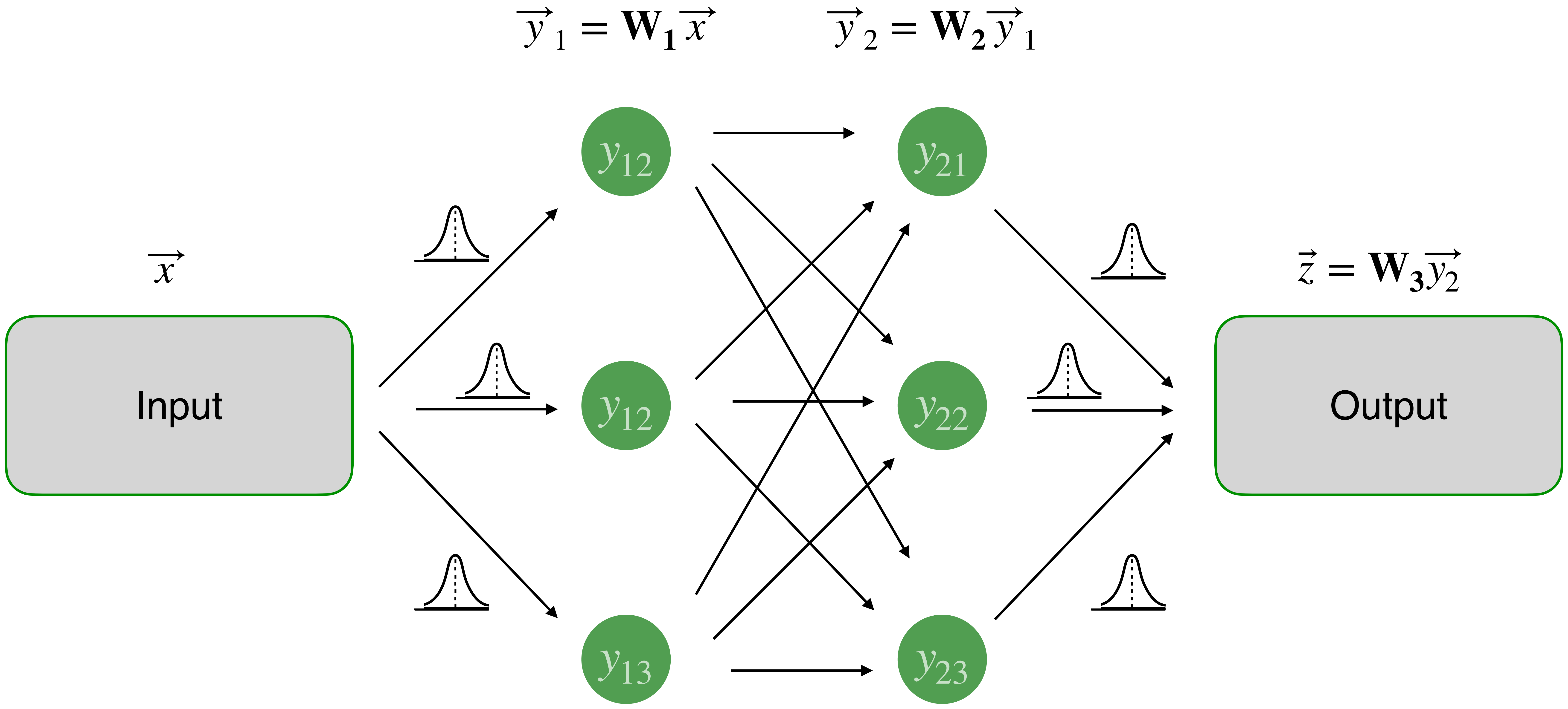


What about uncertainties?



Once training is done: $\mathbf{W_1}, \mathbf{W_2}, \mathbf{W_3}$ fixed (*"Network output is deterministic"*)

What about uncertainties?



Bayesianization: We draw each entry from $\mathbf{W_1}, \mathbf{W_2}, \mathbf{W_3}$ from distribution $q(w \,|\, \mu_\phi, \sigma_\phi)$

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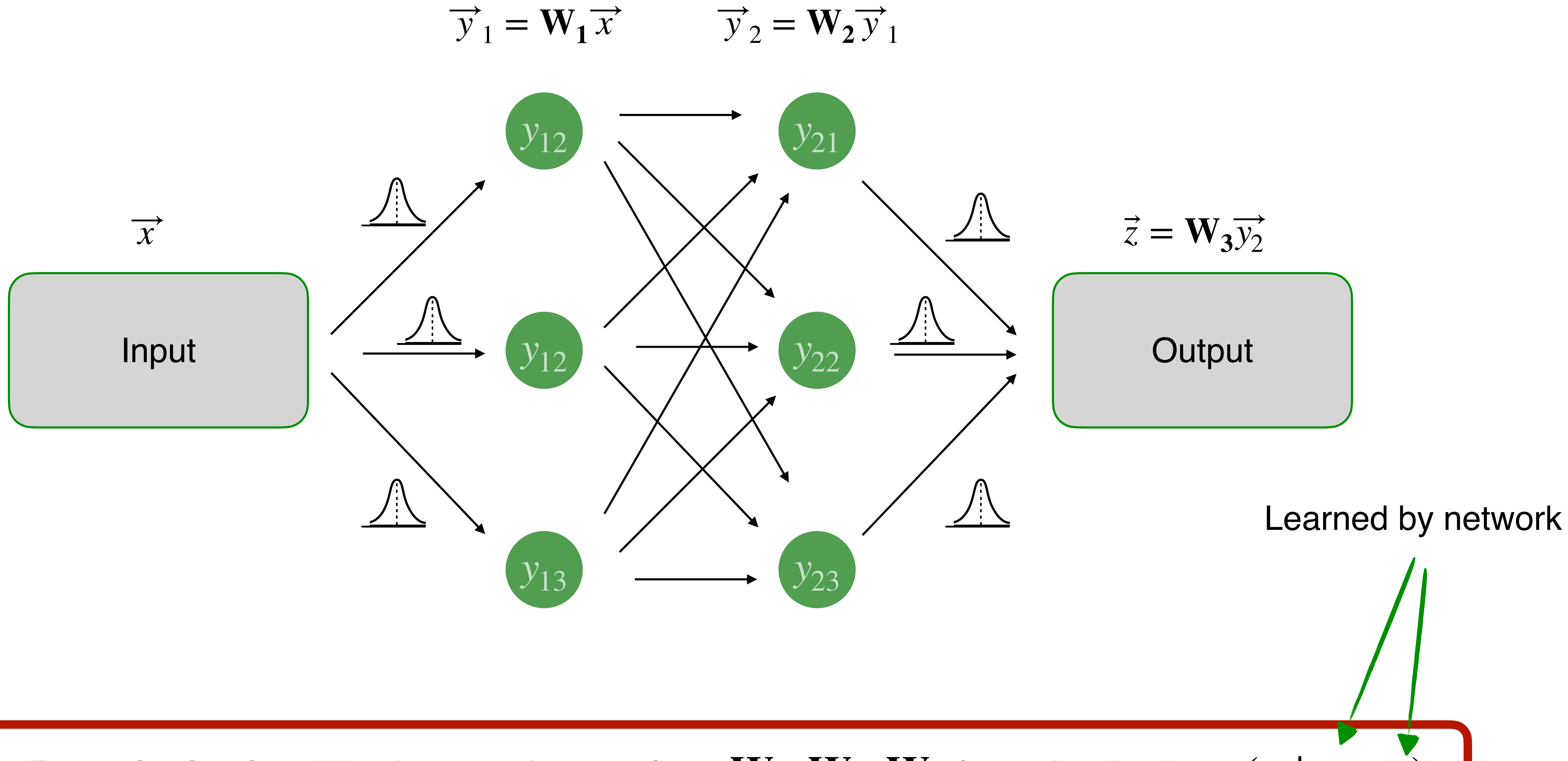

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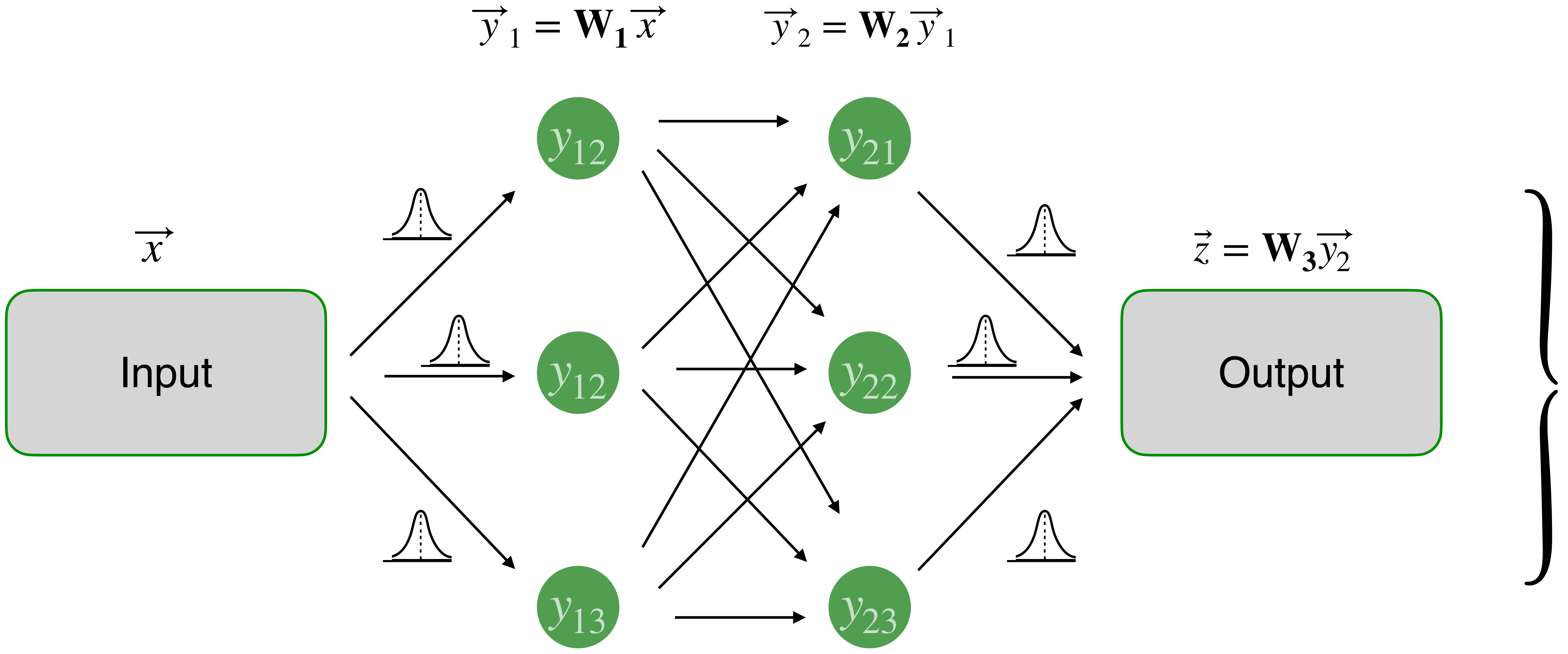
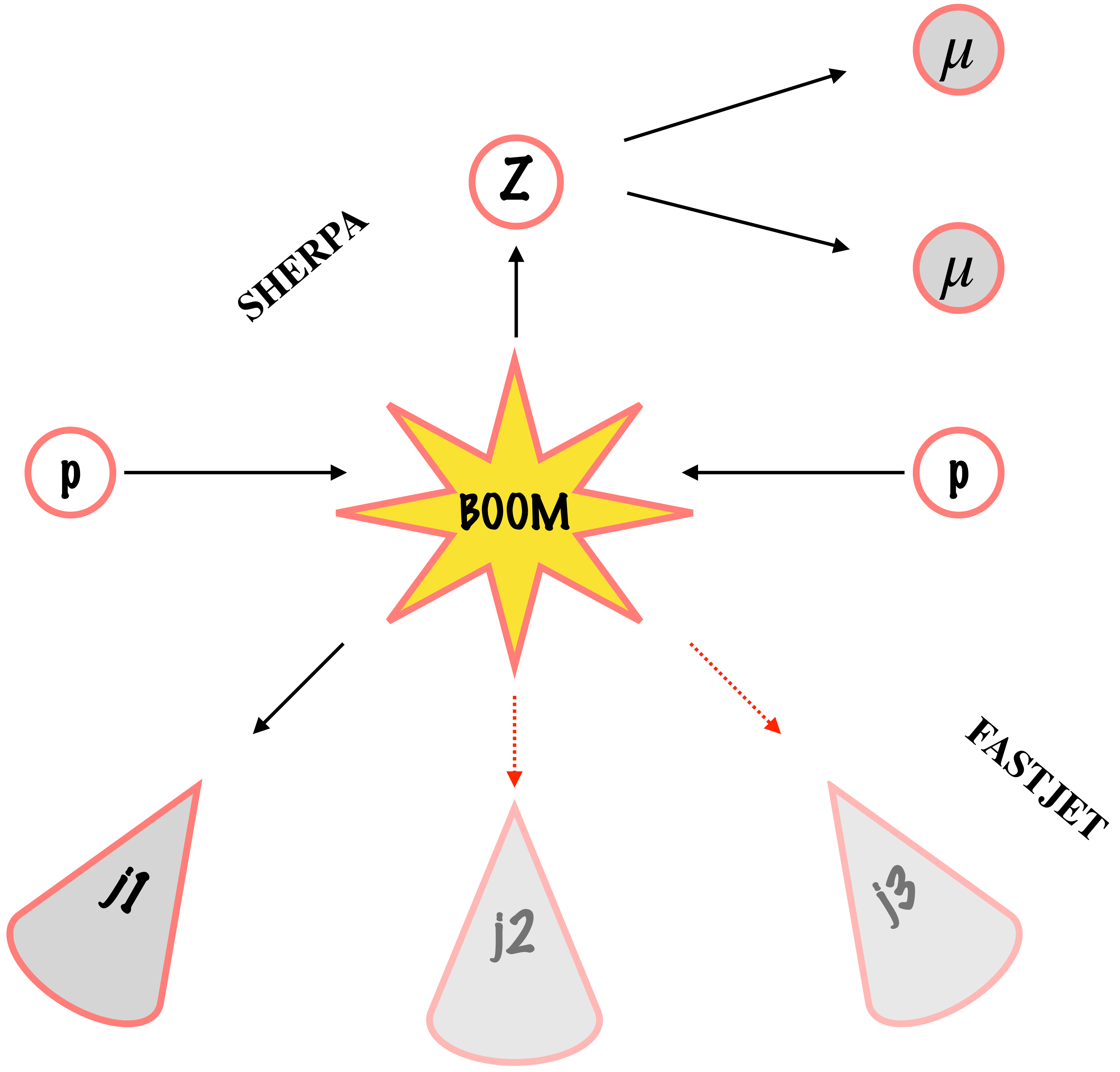


$$\langle \vec{z} \rangle = \frac{1}{N} \sum_i \vec{z}_i$$

$$\sigma^2_{pred} = \frac{1}{N} \sum_{i=1}^{N} \left(\langle \vec{z} \rangle - \vec{z}_i \right)^2$$

Concrete Application — LHC



<u>Z ($\rightarrow \mu\mu$) + jets:</u>

3 - 5 final state particles (including jets)

12 - 20 dimensional phase space

<u>Smart preprocessing:</u>

Global Phase Shift

Drop muon masses

$\rightarrow$ reduces phase space to 9 - 17 dimensions

To be precise

Previous studies showed: INNs can reach precision benchmark

Percent level precision (comparable to statistical uncertainty)

Uncertainty well defined

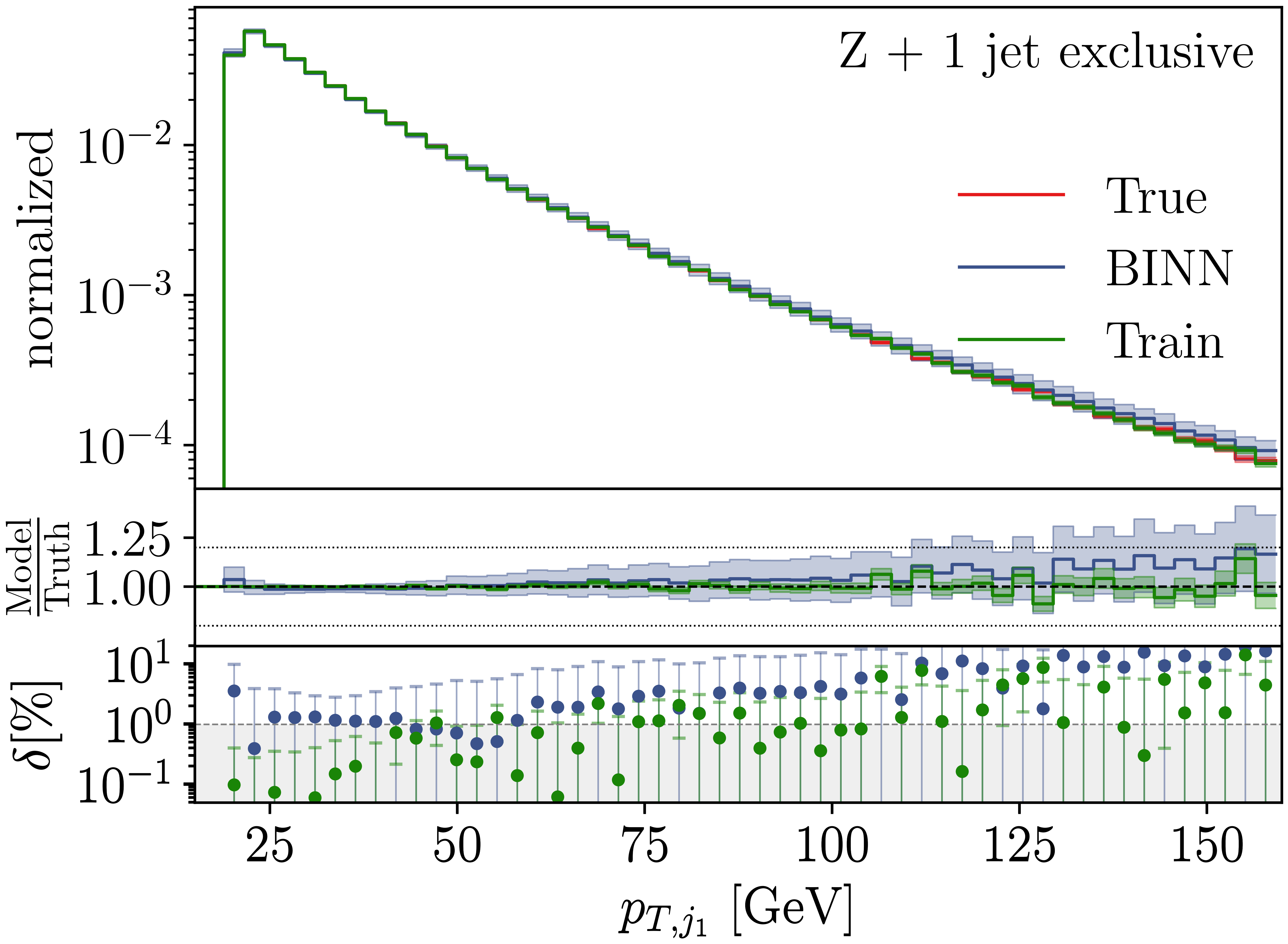


Figure from A. Butter et al.: arXiv:2110.13632

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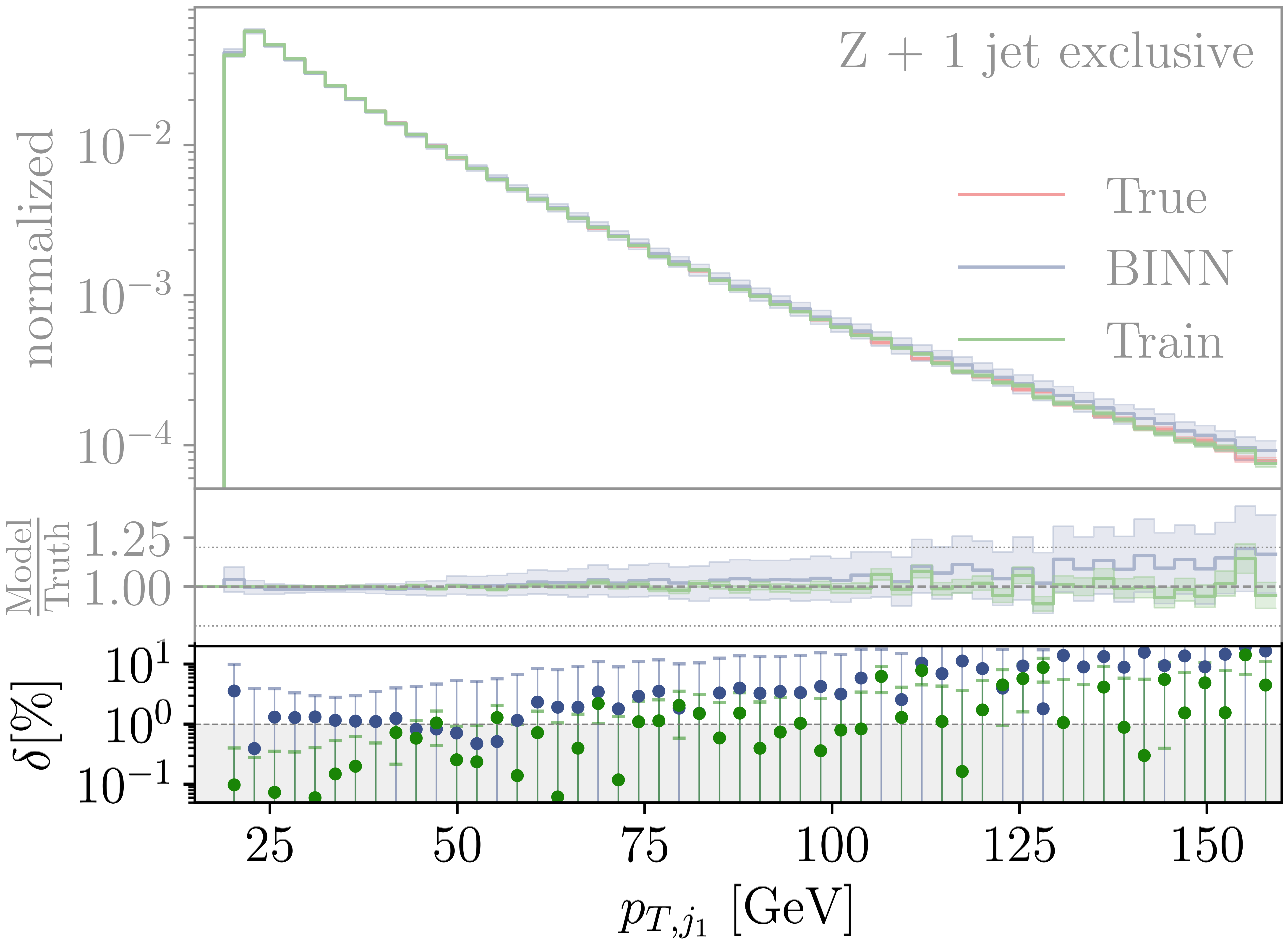

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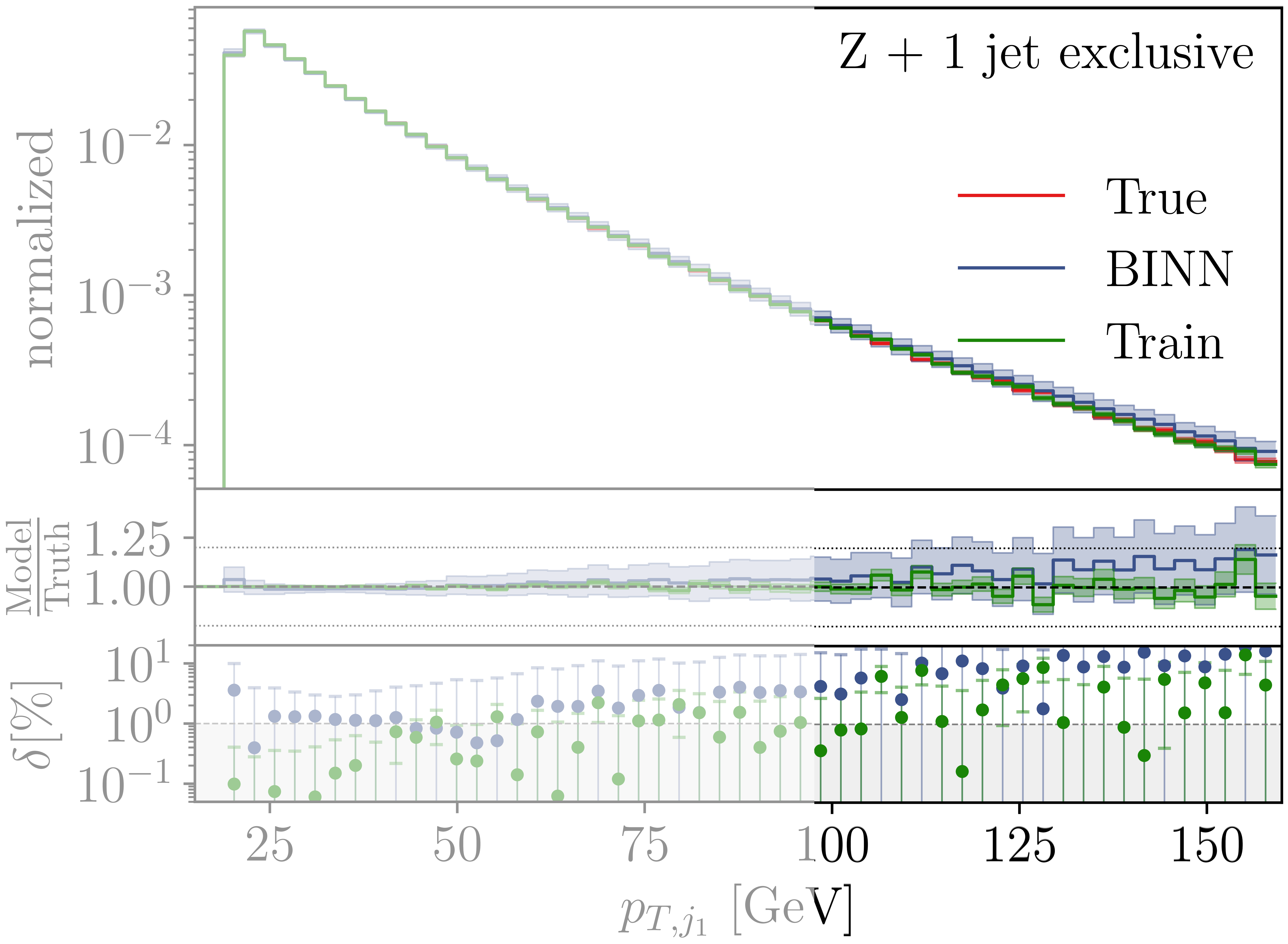

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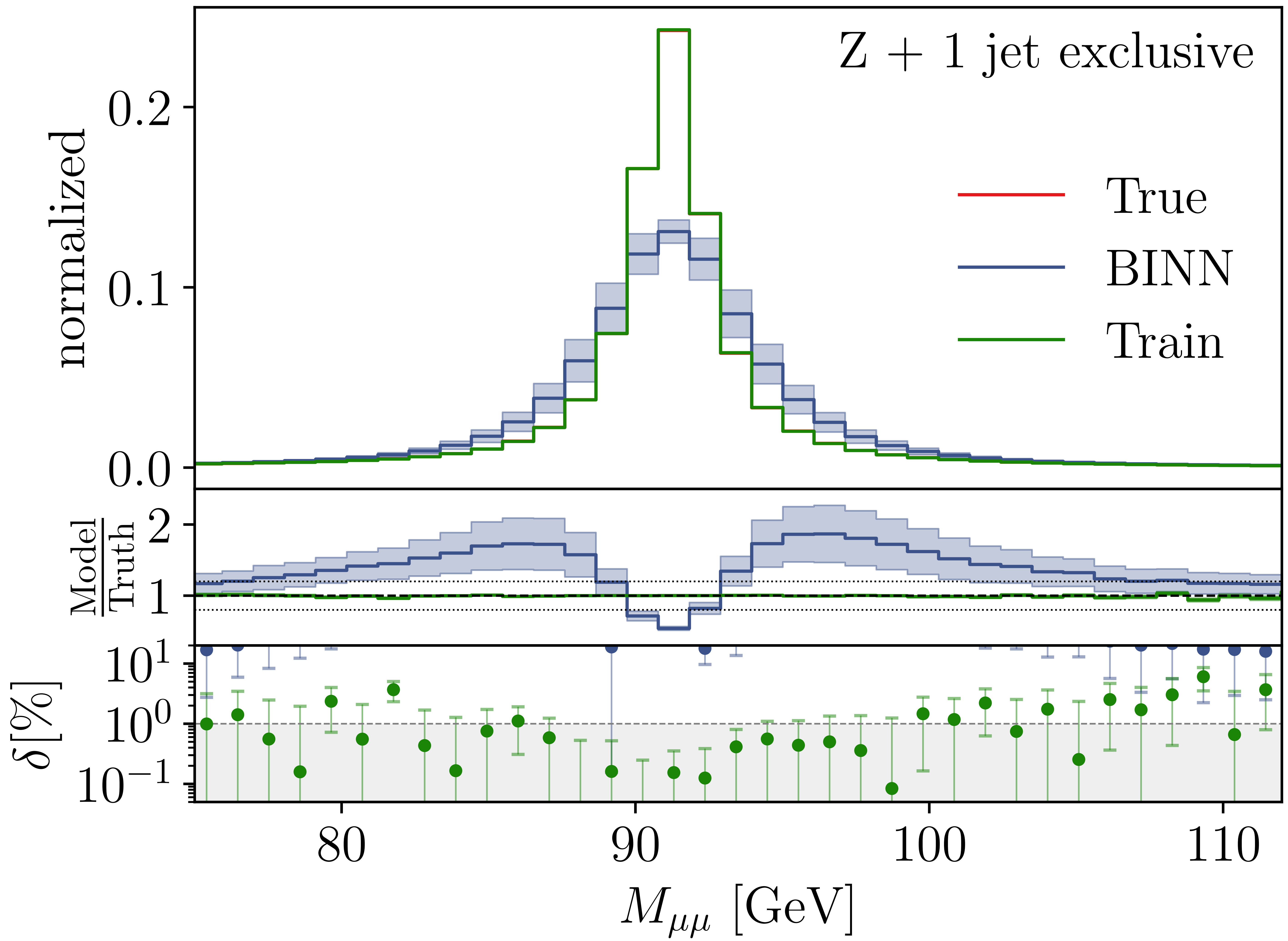
<u>BUT:</u> only in one dimensional marginal distributions



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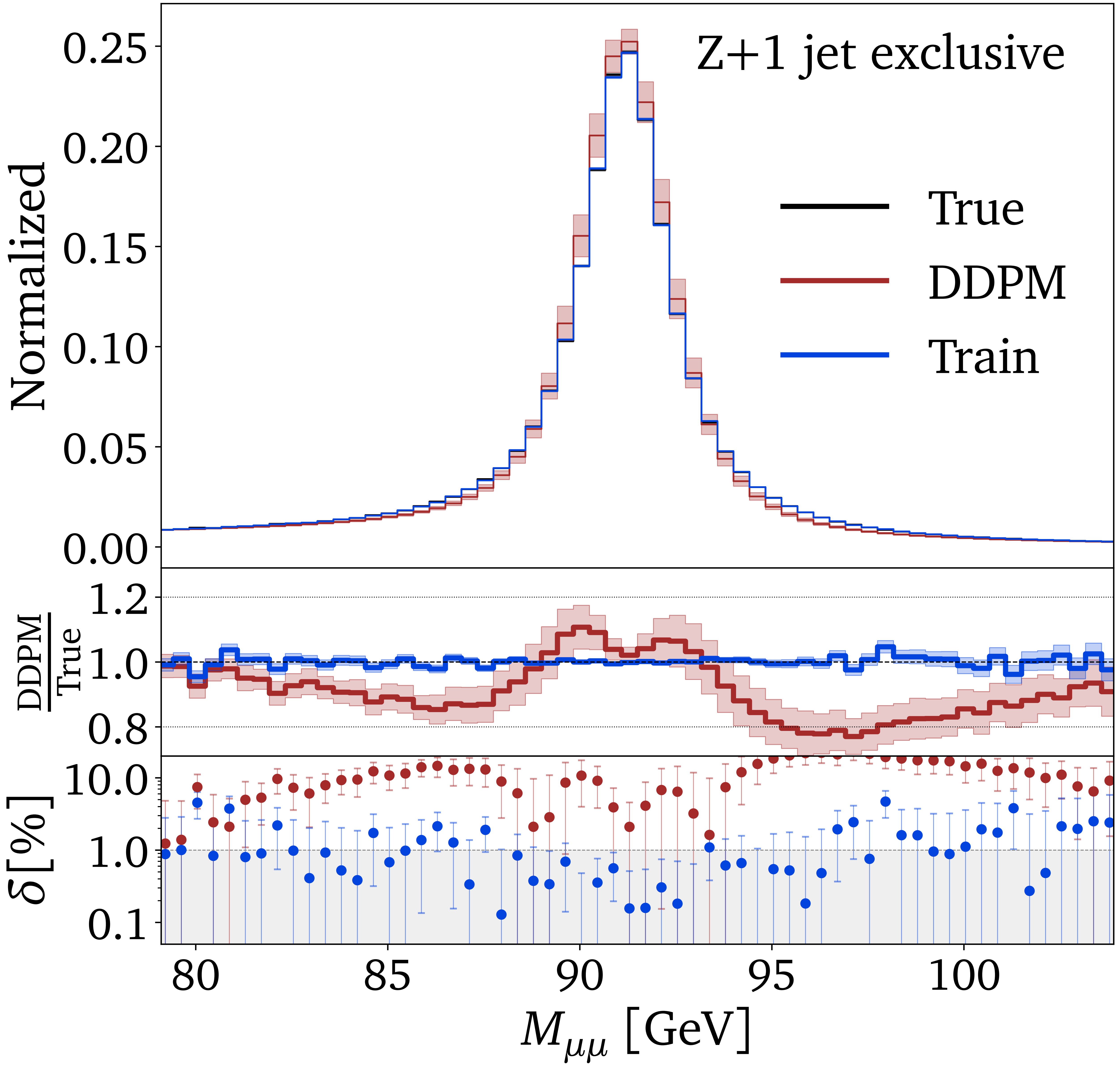

→ **Diffusion Models surpass precision**

To be precise

Previous studies showed: INNs can reach precision benchmark

Percent level precision (comparable to statistical uncertainty)

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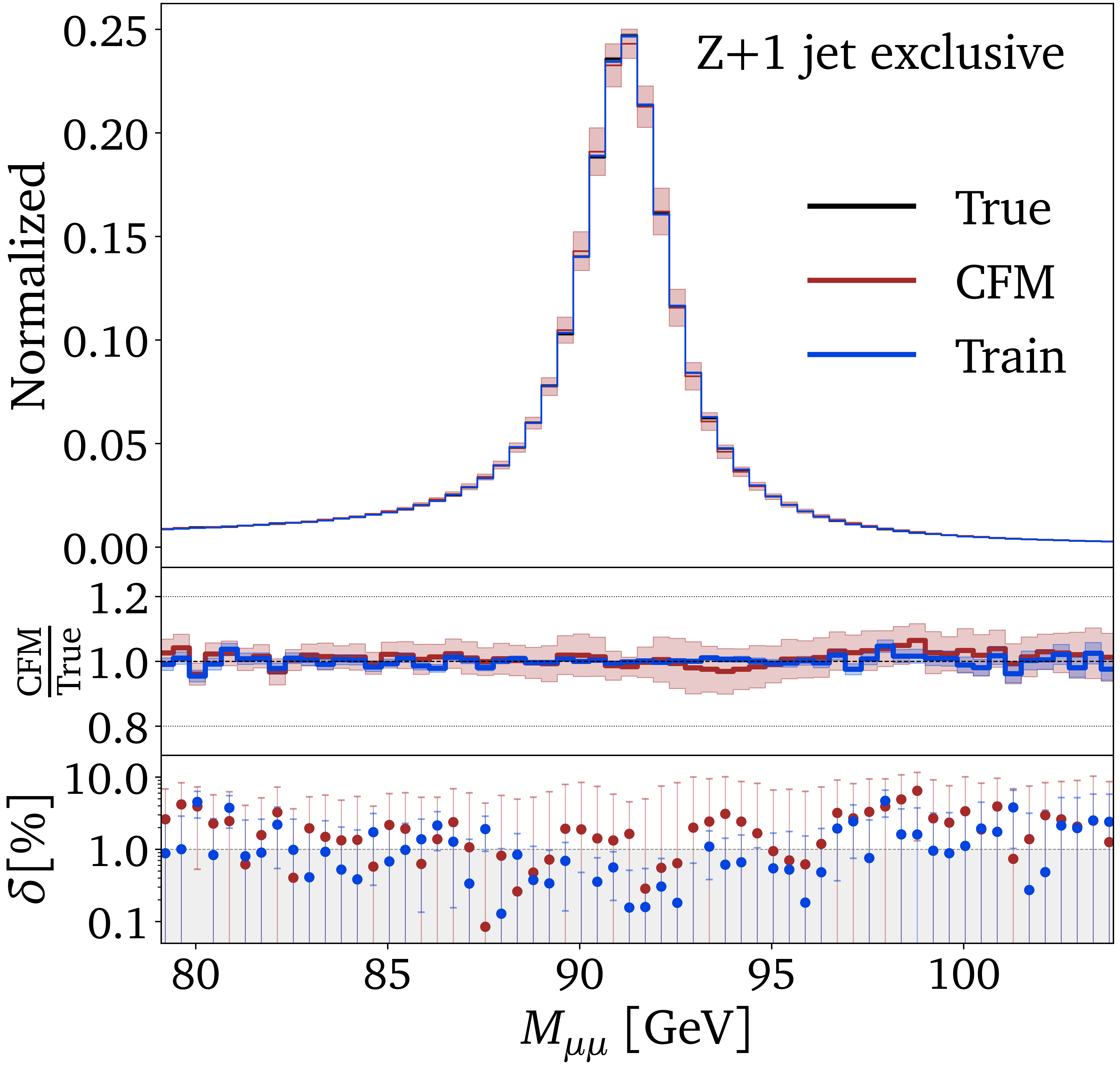
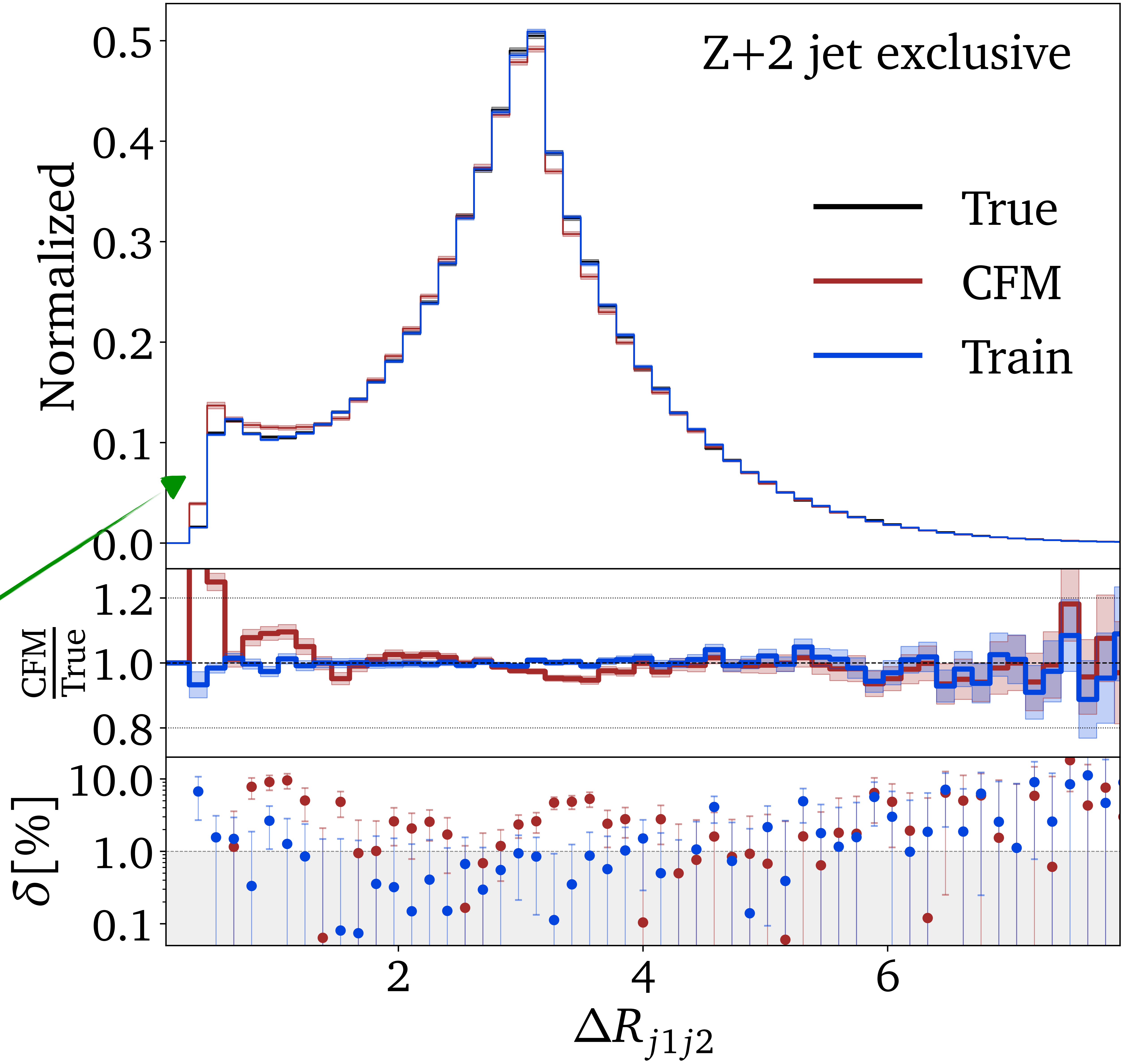
<u>BUT:</u> only in one dimensional marginal distributions



Diffusion Models surpass precision

To be precise

For all non-autoregressiv models: Difficult is to learn **sharp cuts** in correlations

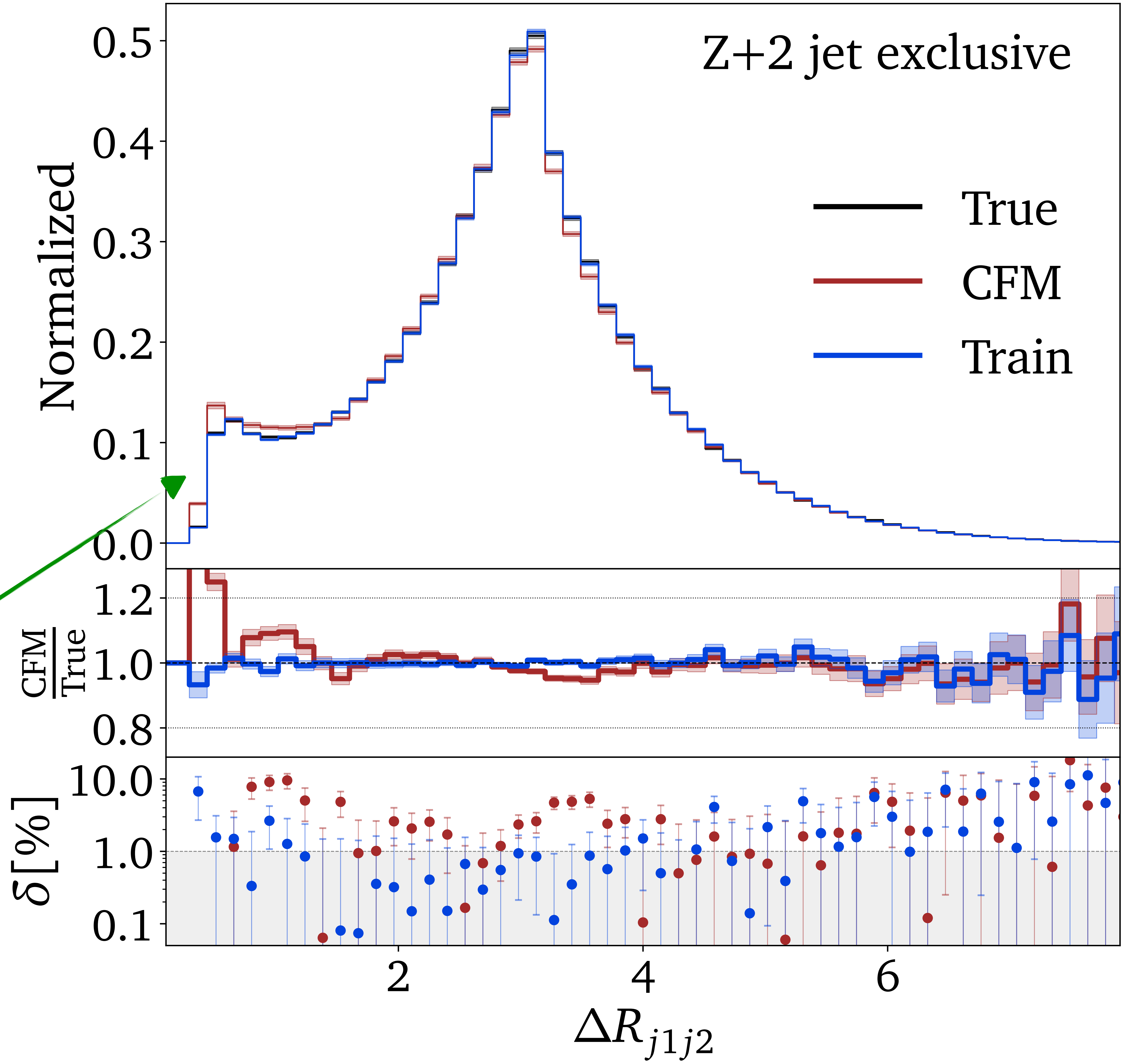


Some tricks already applied

To be precise

For all non-autoregressiv models: Difficult is to learn **sharp cuts** in correlations

Could an autoregressiv model help?



Some tricks already applied

And now what?

New, “hyped” ML-Models can compete with current benchmark

All of them come with their own advantages and disadvantages

A lot of on-going research (generation speed up, precision, etc.)

→ Diffusion models show potential to be applied to particle physics tasks

Backup

Diffusion Models (DDPM)

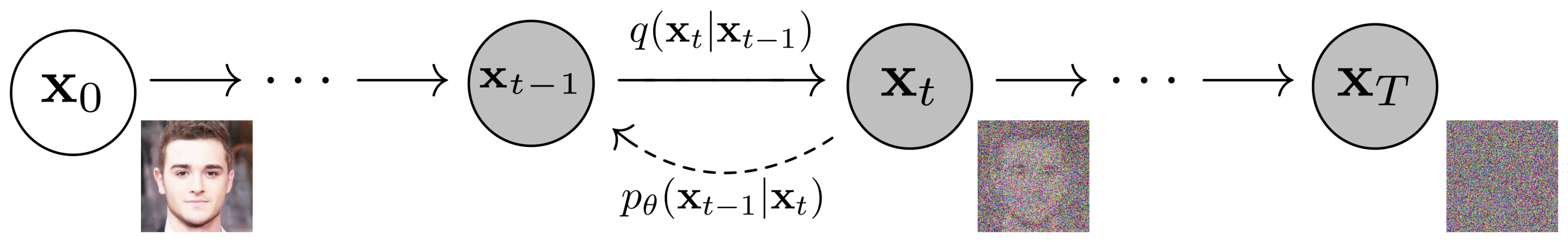
Forwards

Phase Space

$x_0 \sim p(x_0)$

Latent Space

$x_T \sim p(x_T)(= \mathcal{N}(0,1))$



$$q(x_1, \ldots, x_T | x_0) = \prod_{t=1}^{T} q(x_t | x_{t-1})$$

$$q(x_t | x_{t-1}) = \mathcal{N}(x_t; \sqrt{1-\beta_t} x_{t-1}, \beta_t)$$

where β_t follows noise scheduler

Figure from J.Ho et al.: arXiv:2006.11239

Diffusion Models (DDPM)

Phase Space

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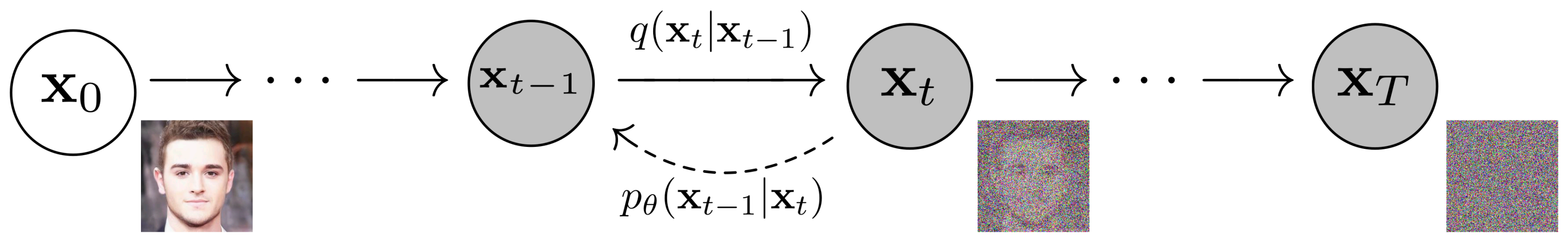
Backwards

Latent Space

$x_T \sim p(x_T)(= \mathcal{N}(0,1))$



To reverse: $q(x_{t-1} | x_t) = \dfrac{q(x_t | x_{t-1}) q(x_{t-1})}{q(x_t)}$

…but we don't know $q(x_t)$ & $q(x_{t-1})$ 🙎‍♀️ 🤷‍♀️

Figure from J.Ho et al.: arXiv:2006.11239

Diffusion Models (DDPM)

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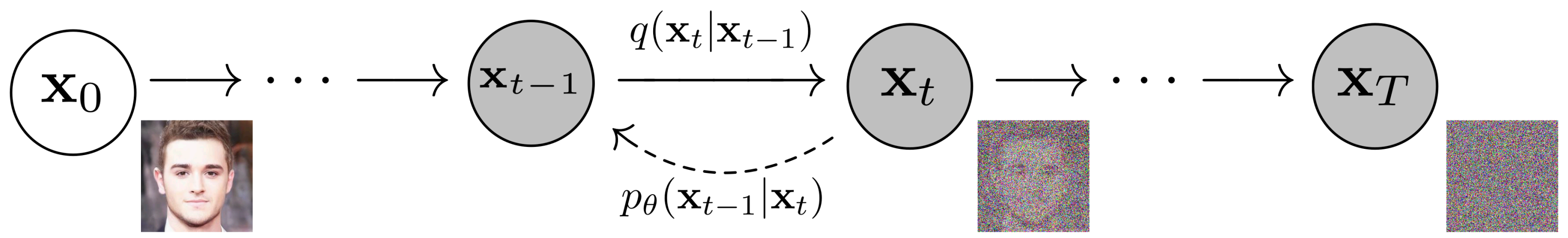

Instead, learn: $p_\theta(x_{t-1} \,|\, x_t) = \mathcal{N}(x_{t-1}; \mu_\theta(x_t, t), \sigma_\theta^2(x_t, t))$

$$p(x_0, \ldots, x_T \,|\, \theta) = p(x_T) \prod_{t=1}^{T} p_\theta(x_{t-1} \,|\, x_t)$$

Figure from J.Ho et al.: arXiv:2006.11239

Diffusion Models (DDPM)

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Latent Space

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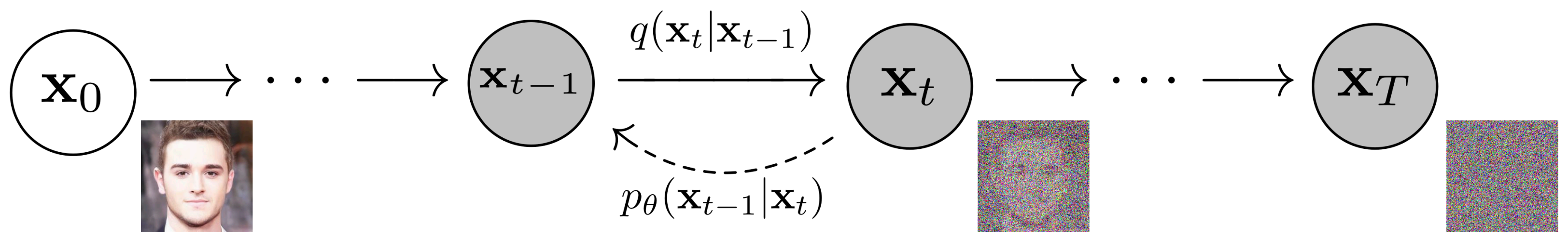

$$\mathscr{L}_{DDPM} = -\log p_\theta(x_0) \approx \frac{1}{2\sigma_t^2}\frac{\beta_t^2}{(1-\beta_t)\bar{\beta}_t}\,|\,\epsilon(t) - \epsilon_\theta(t)\,|^2$$

Figure from J.Ho et al.: arXiv:2006.11239

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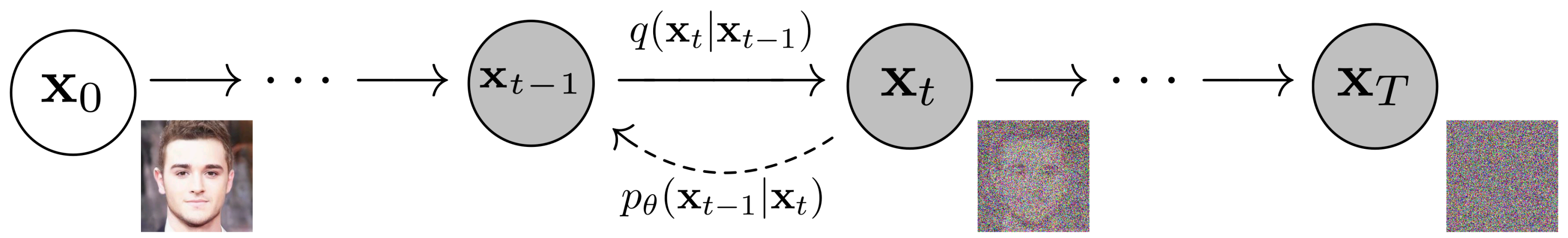

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 :

- Reparametrization
- Estimation
- …

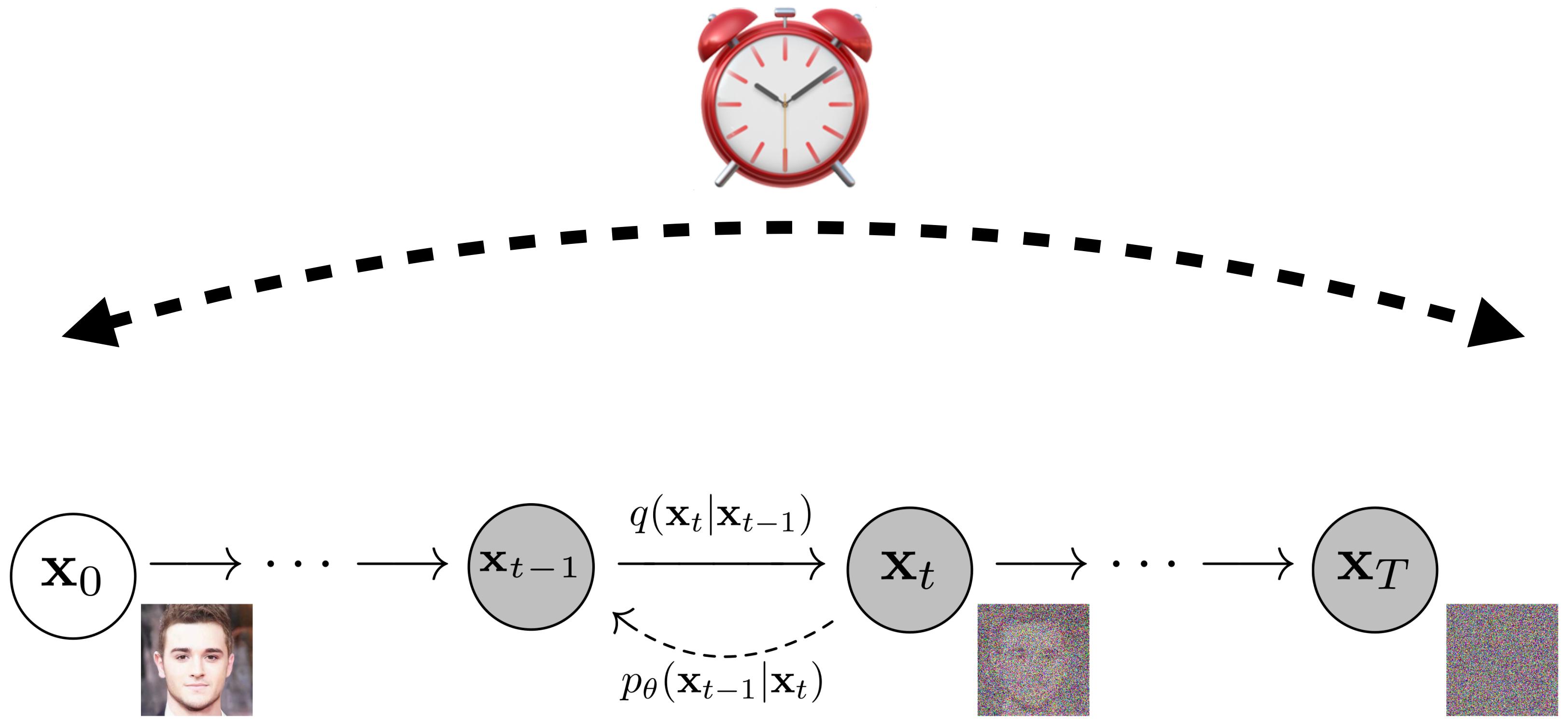
Predicted and actual noise added at time t

Figure from J.Ho et al.: arXiv:2006.11239

Diffusion Models (DDPM)

Phase Space

$x_0 \sim p(x_0)$



Latent Space

$x_T \sim p(x_T)(= \mathcal{N}(0,1))$

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Denoising

Figure from J.Ho et al.: arXiv:2006.11239

Diffusion Models (CFM)

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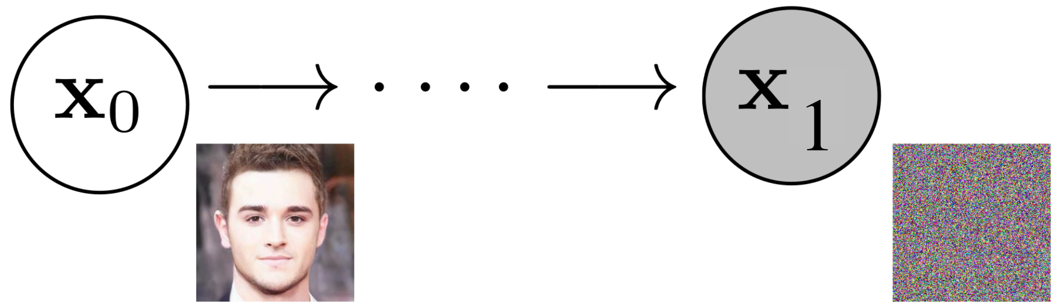
Latent Space

$x_1 \sim p(x_1)(= \mathcal{N}(0,1))$



1. Connect x_0 with x_1 by a linear trajectory: $x(t\,|\,x_0) = (1-t)x_0 + tx_1$

2. Derive: $\frac{d}{dt}x(t\,|\,x_0) = (x_1 - x_0) \equiv v_\theta(x_1, x_0)$

3. Solve for x_0 (ODE): $x_0 = x_t - \int_0^1 v_\theta(x(t), t)dt$

Figure from J.Ho et al.: arXiv:2006.11239

Diffusion Models (CFM)

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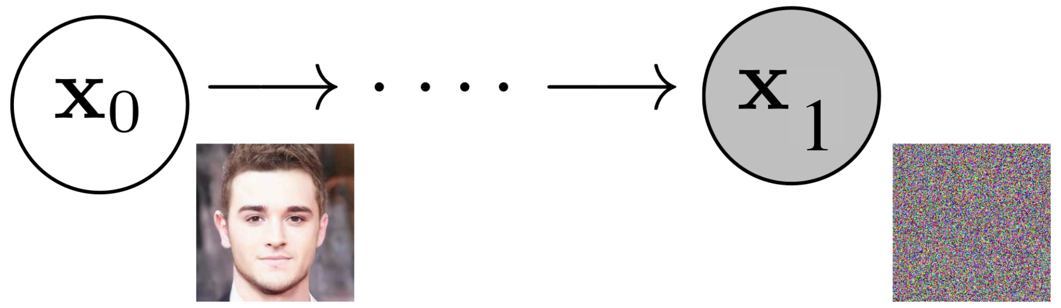
Latent Space

$x_1 \sim p(x_1)(=\mathcal{N}(0,1))$



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How to Bayesianize

1. Replace each linear layer with a *Bayesian* layer

2. Add additional regularisation term to loss