Amplitudes for Accuracy and Uncertainty Estimation in ML

Nina Elmer

COMETA - Uncertainty Quantification in Machine Learning
27. January 2025

arXiv: 2412.12069

with H. Bahl, L. Favaro, M. Haußmann, T. Plehn, and R. Winterhalder

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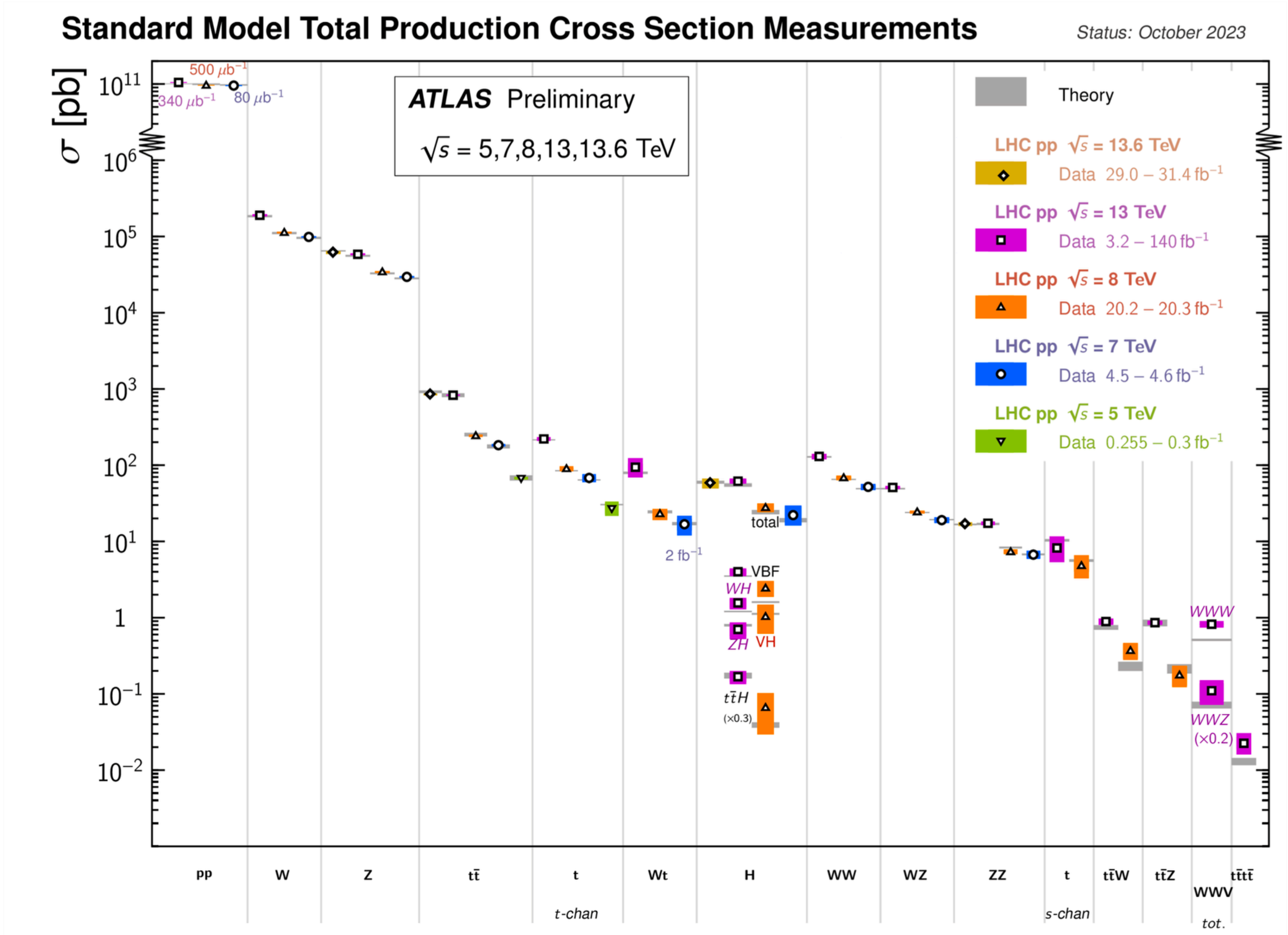
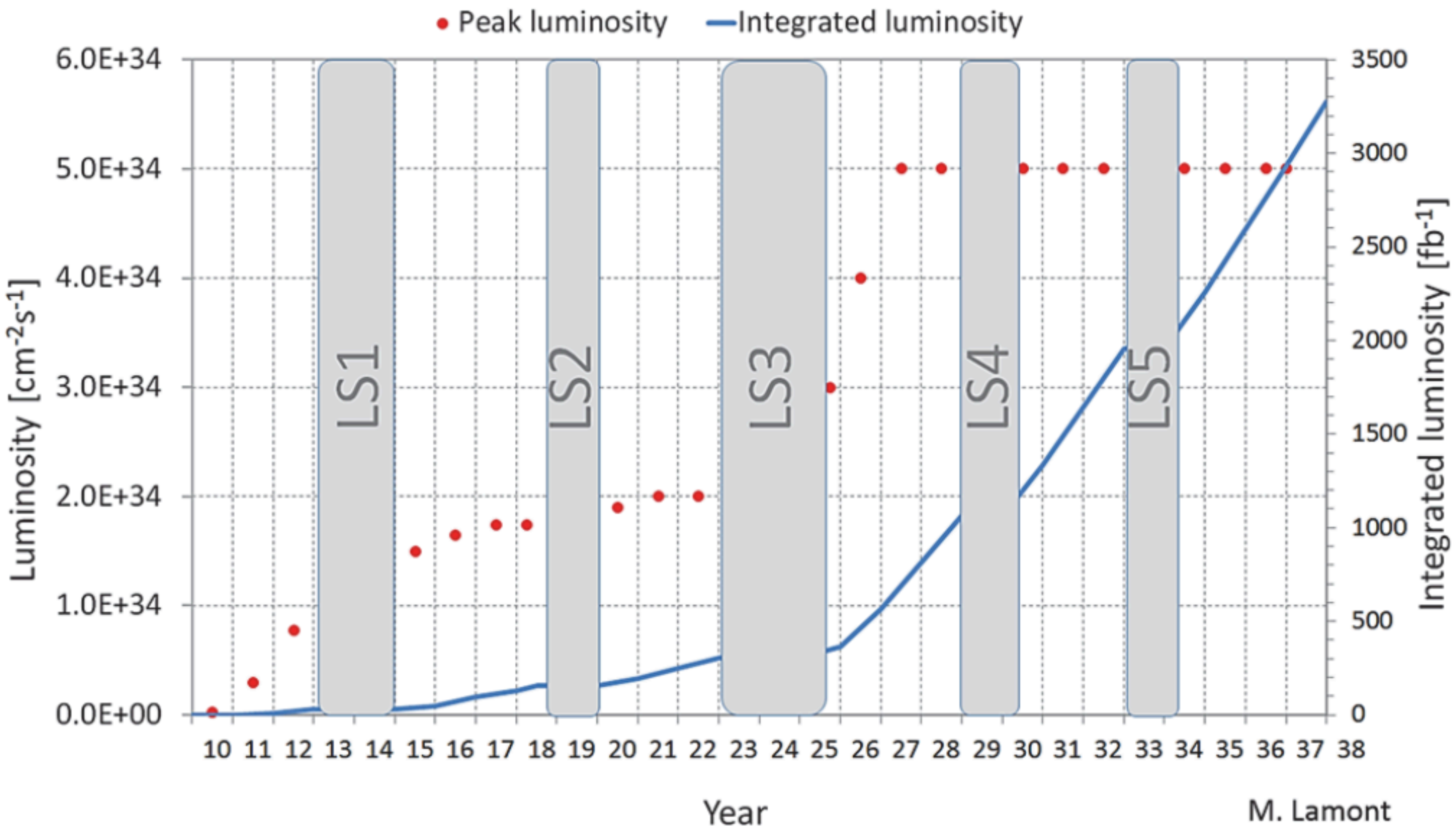
IMPRS
for Precision Tests of
Fundamental Symmetries
INTERNATIONAL MAX PLANCK
RESEARCH SCHOOL

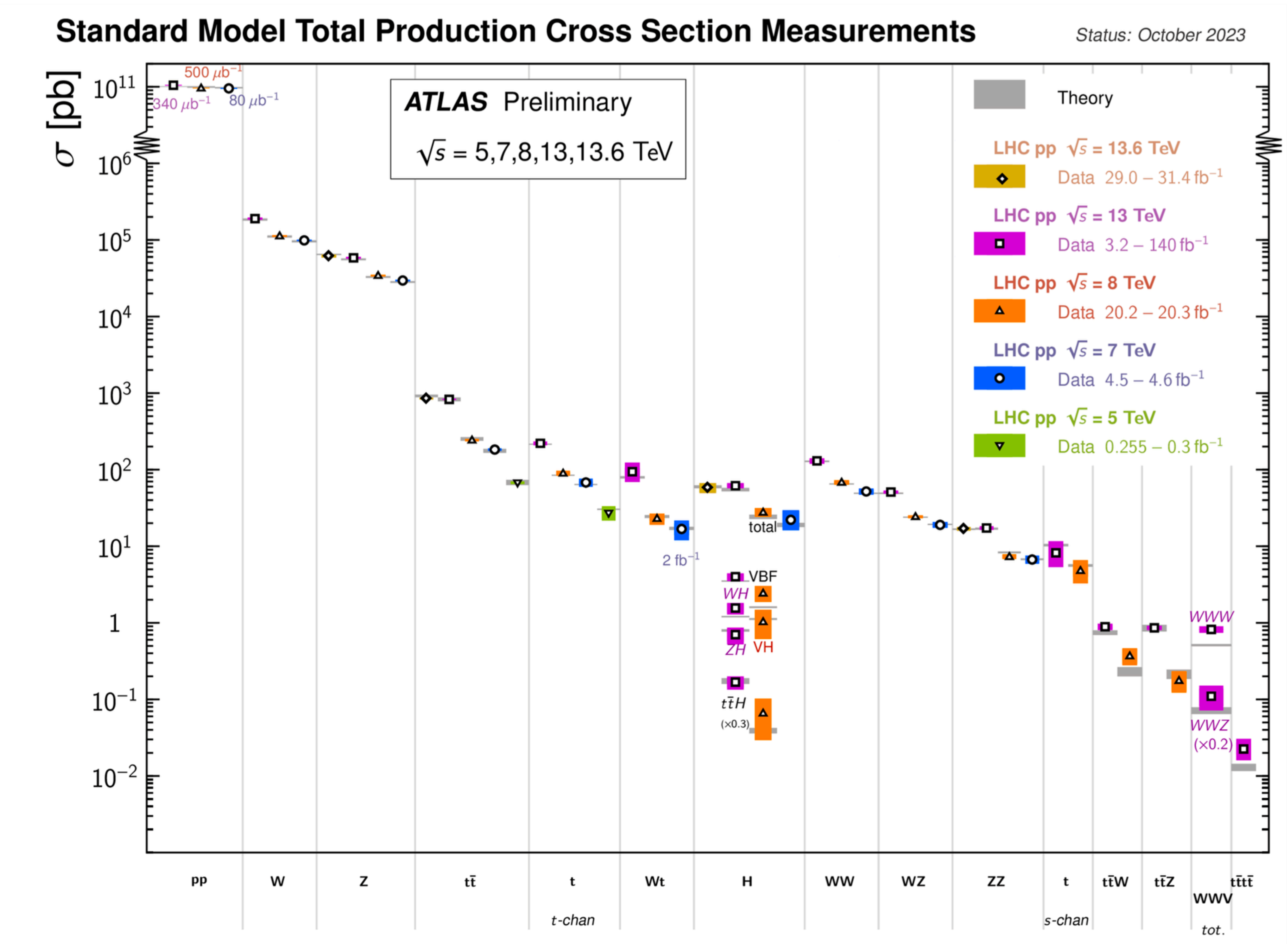
Entering the precision era

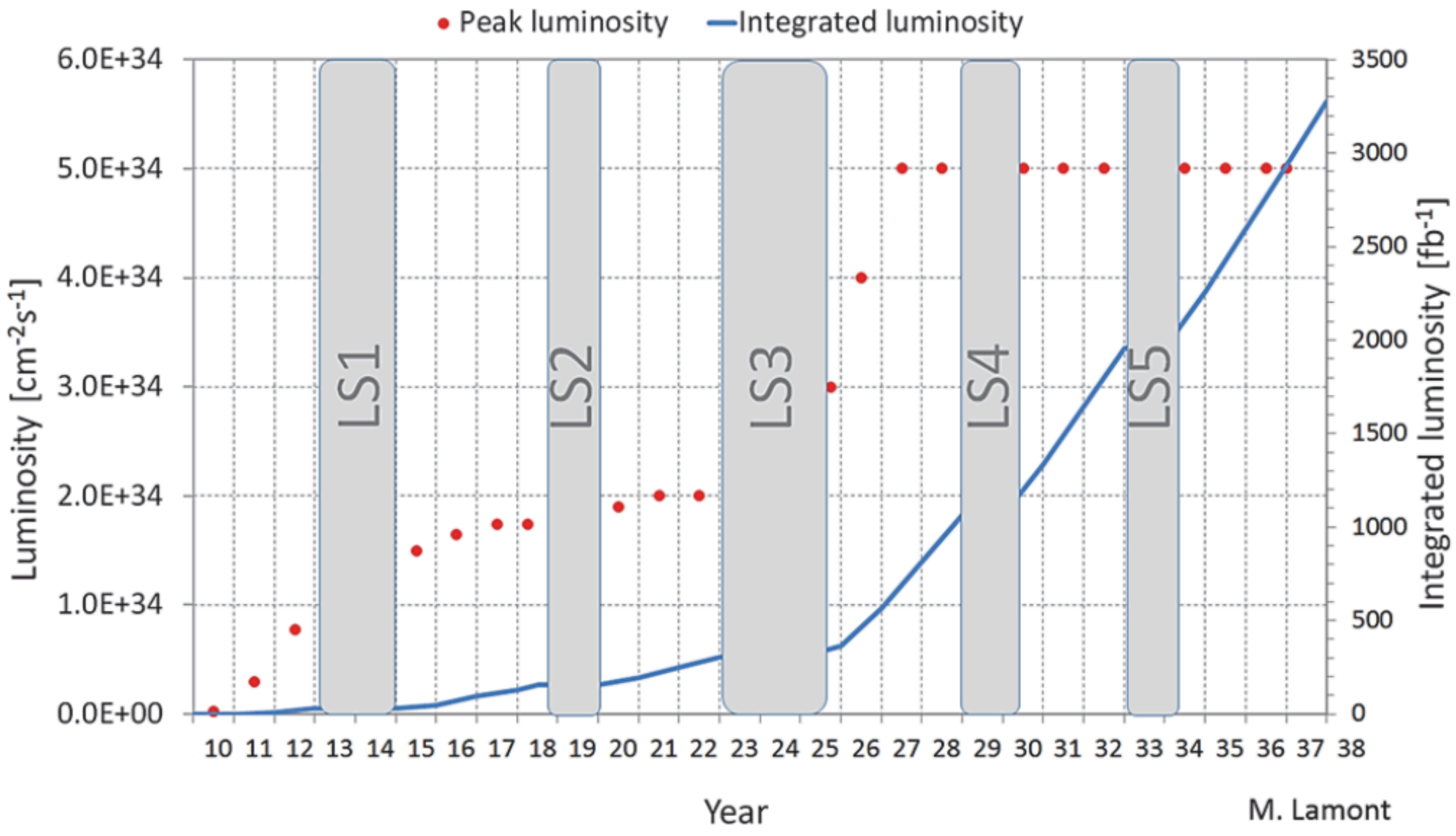




Entering the precision era

➡ Precision is central aspect of LHC physics





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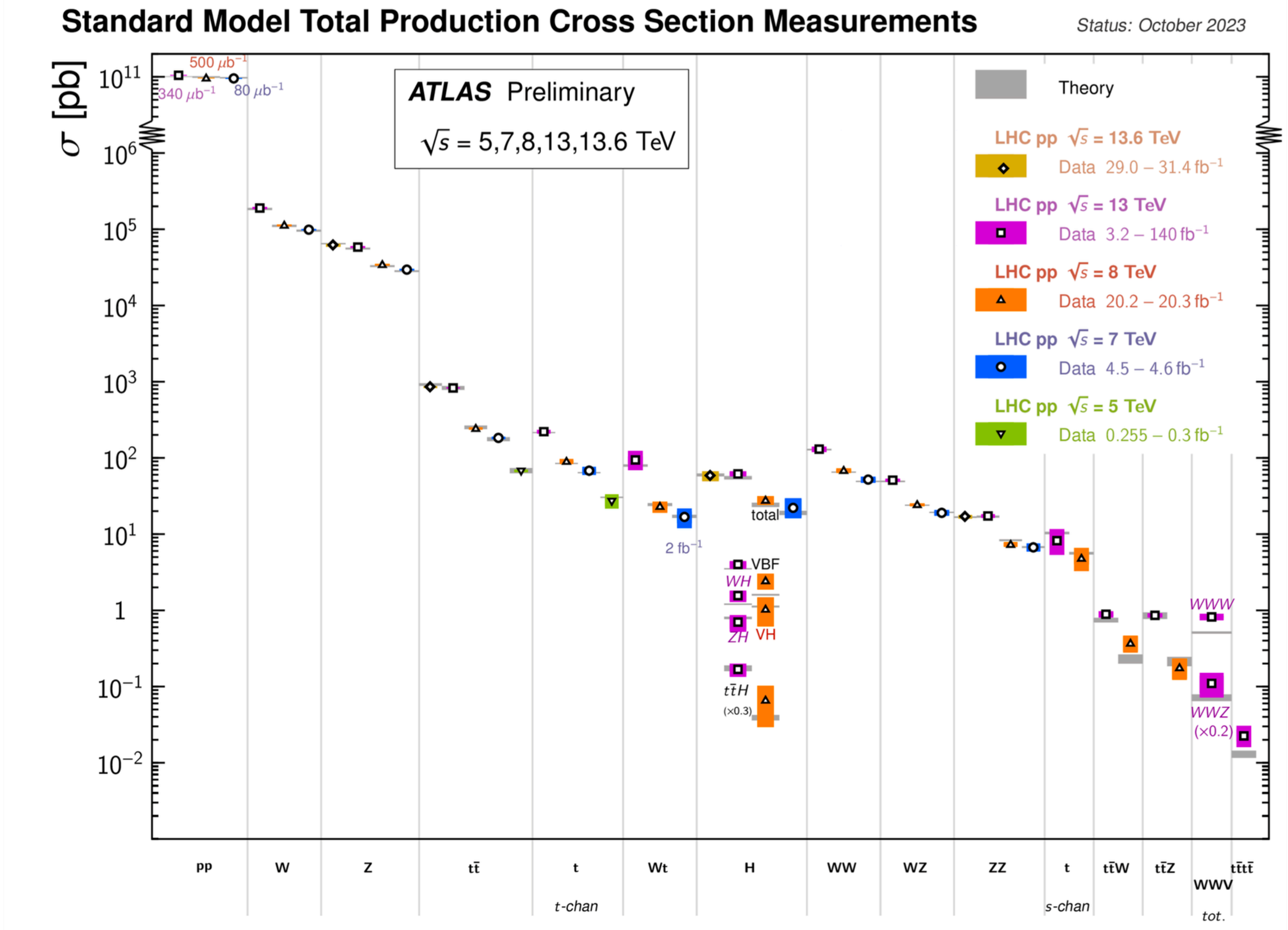
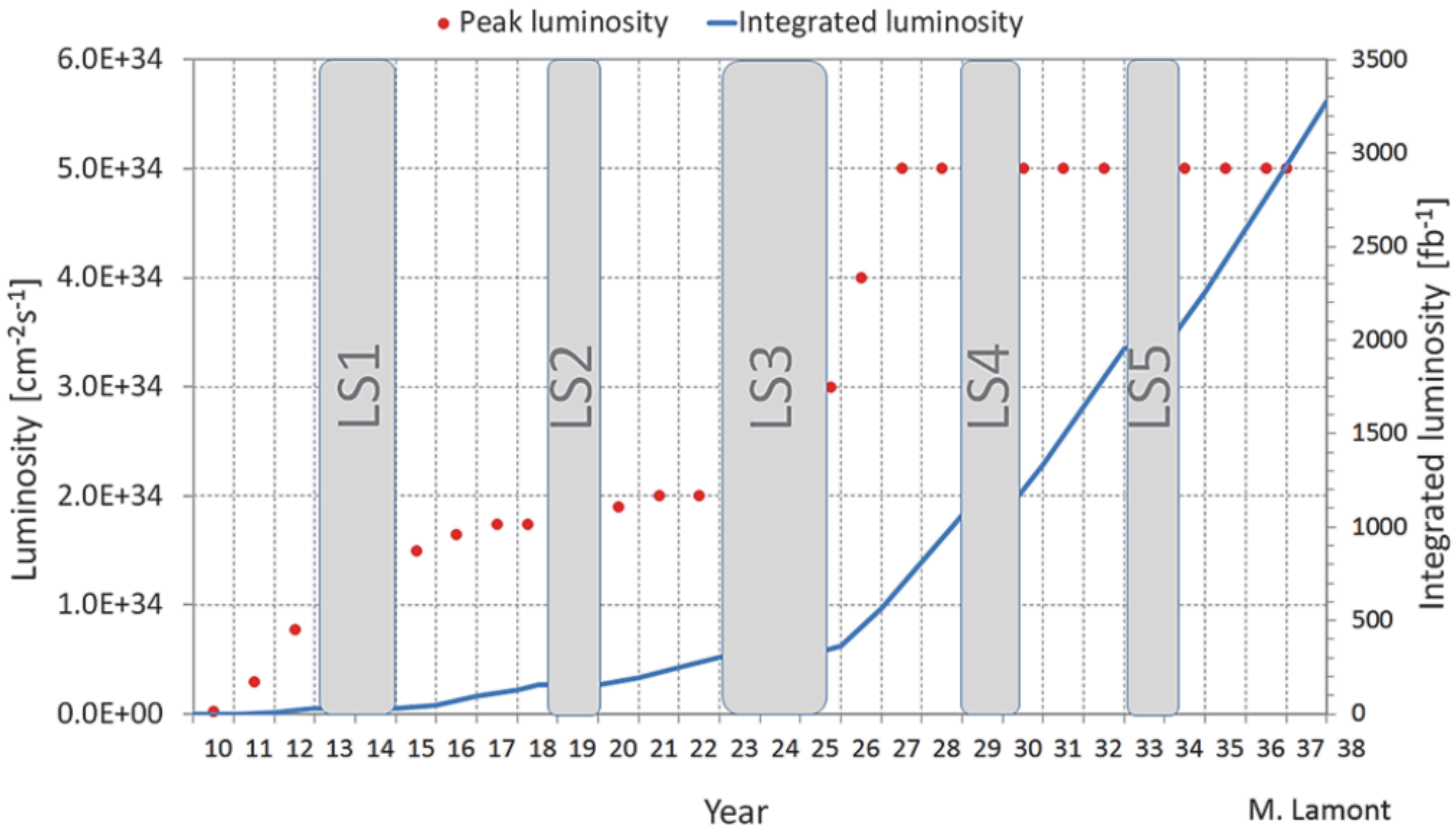
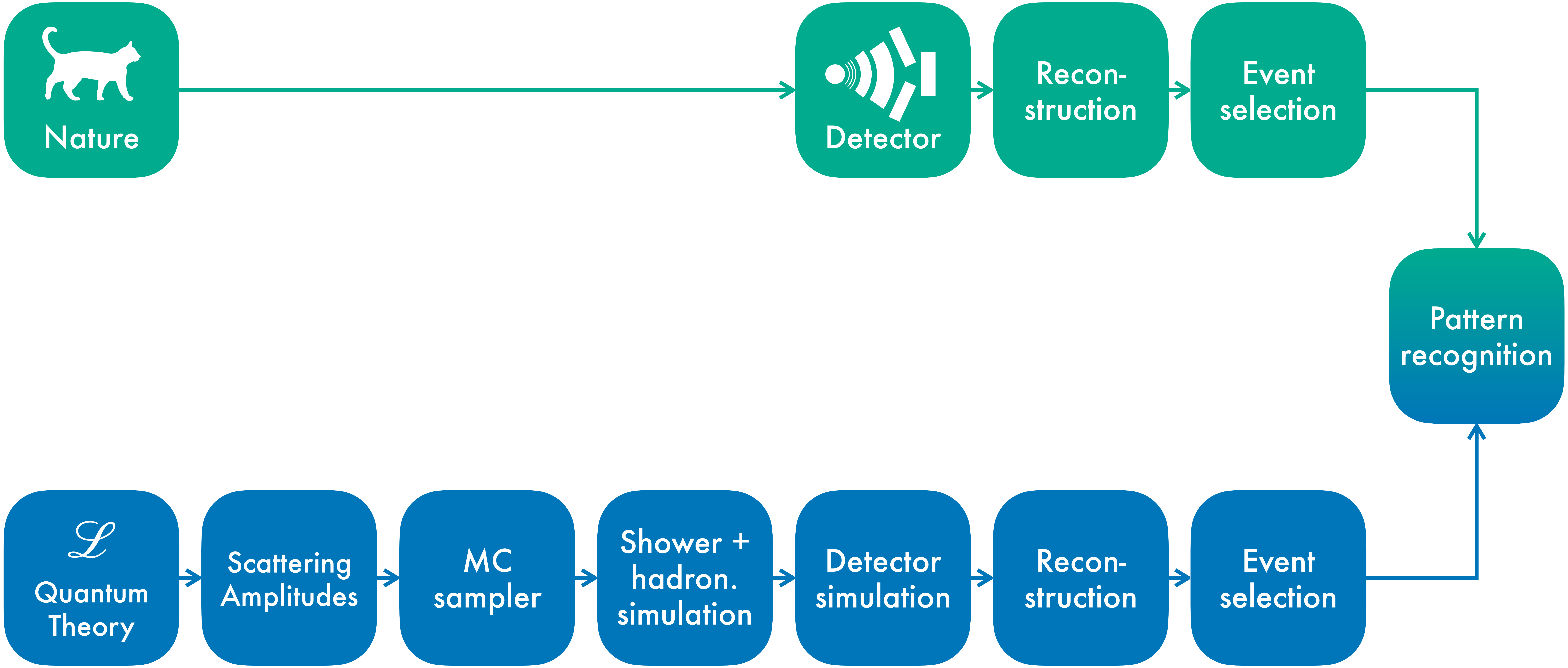




- ML tools for processing and evaluating the data

LHC physics and machine learning



Nature

Detector

Recon-struction

Event selection

Pattern recognition

$\mathscr{L}$

Quantum Theory

Scattering Amplitudes

MC sampler

Shower + hadron. simulation

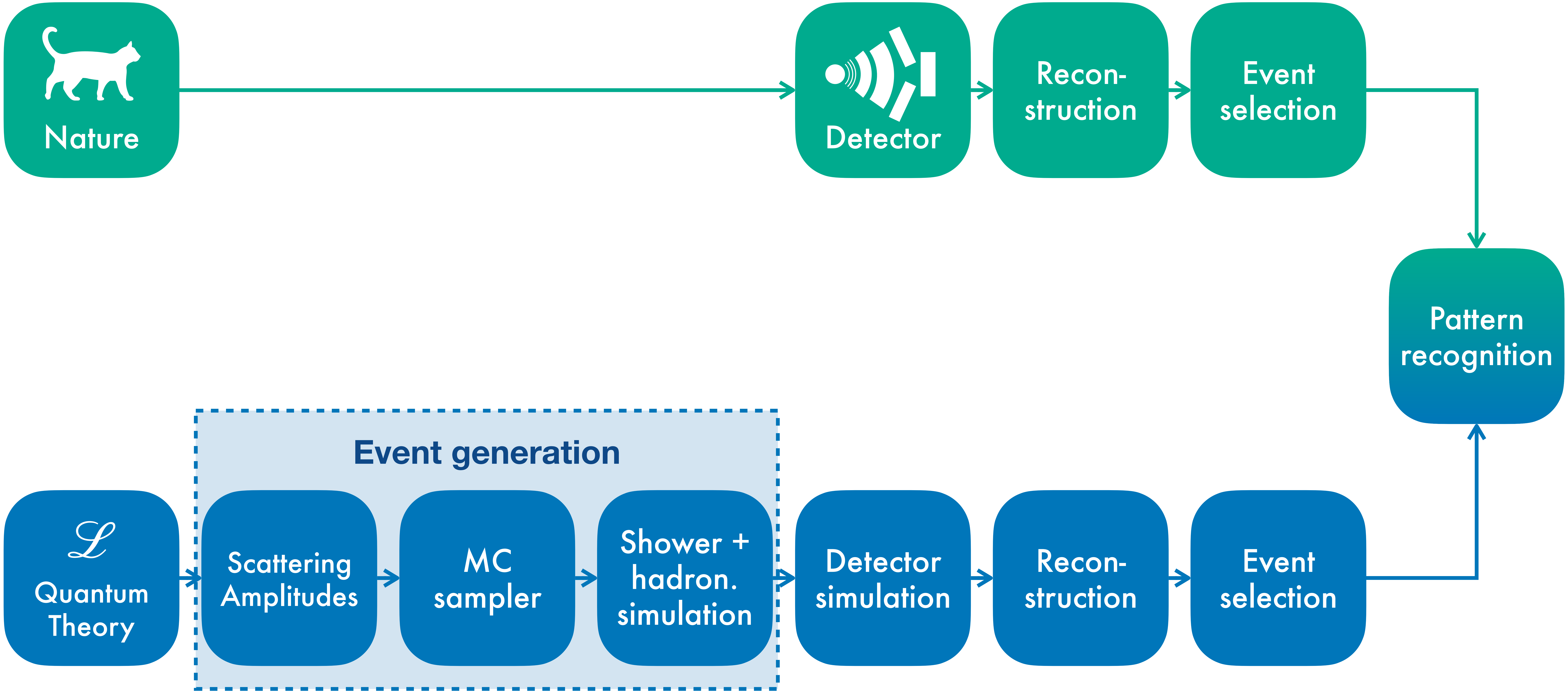
Detector simulation

Recon-struction

Event selection

Credits: R. Winterhalder

LHC physics and machine learning



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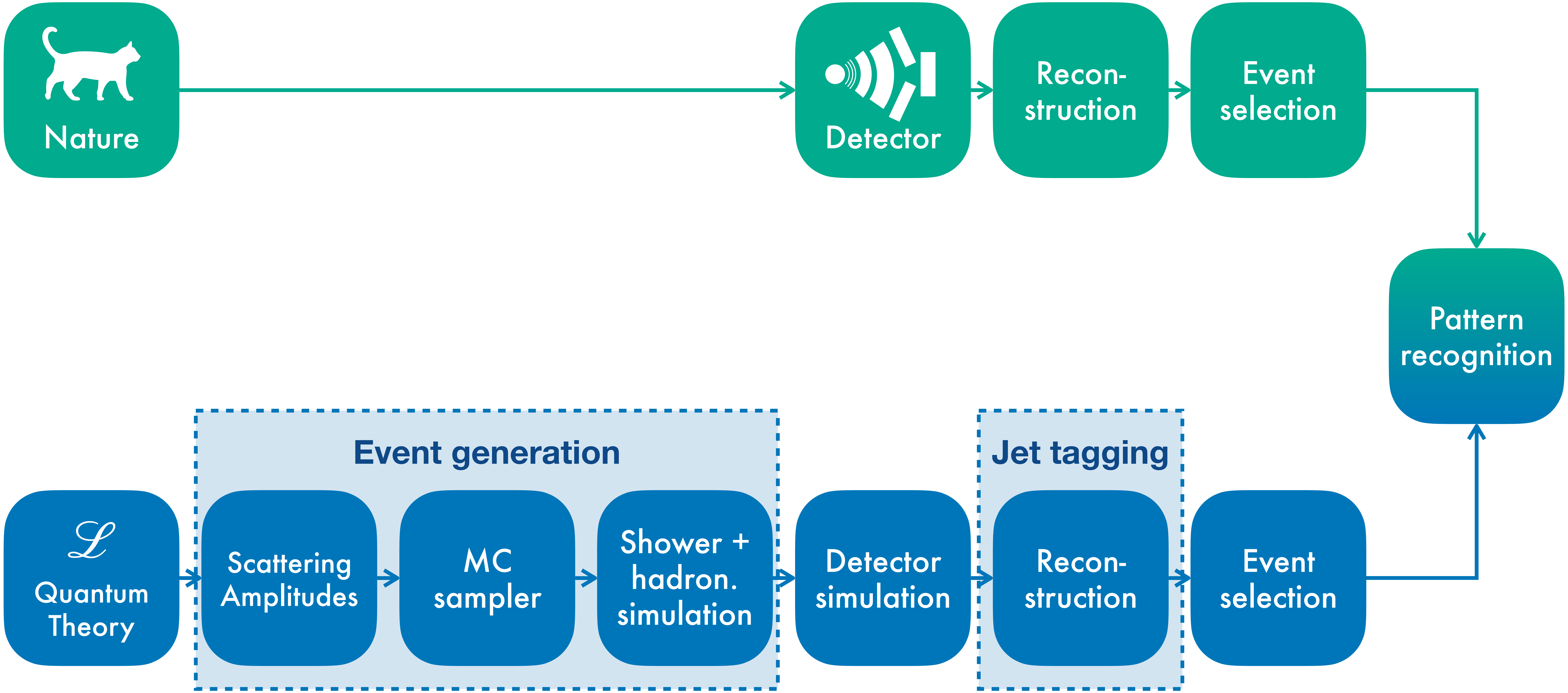

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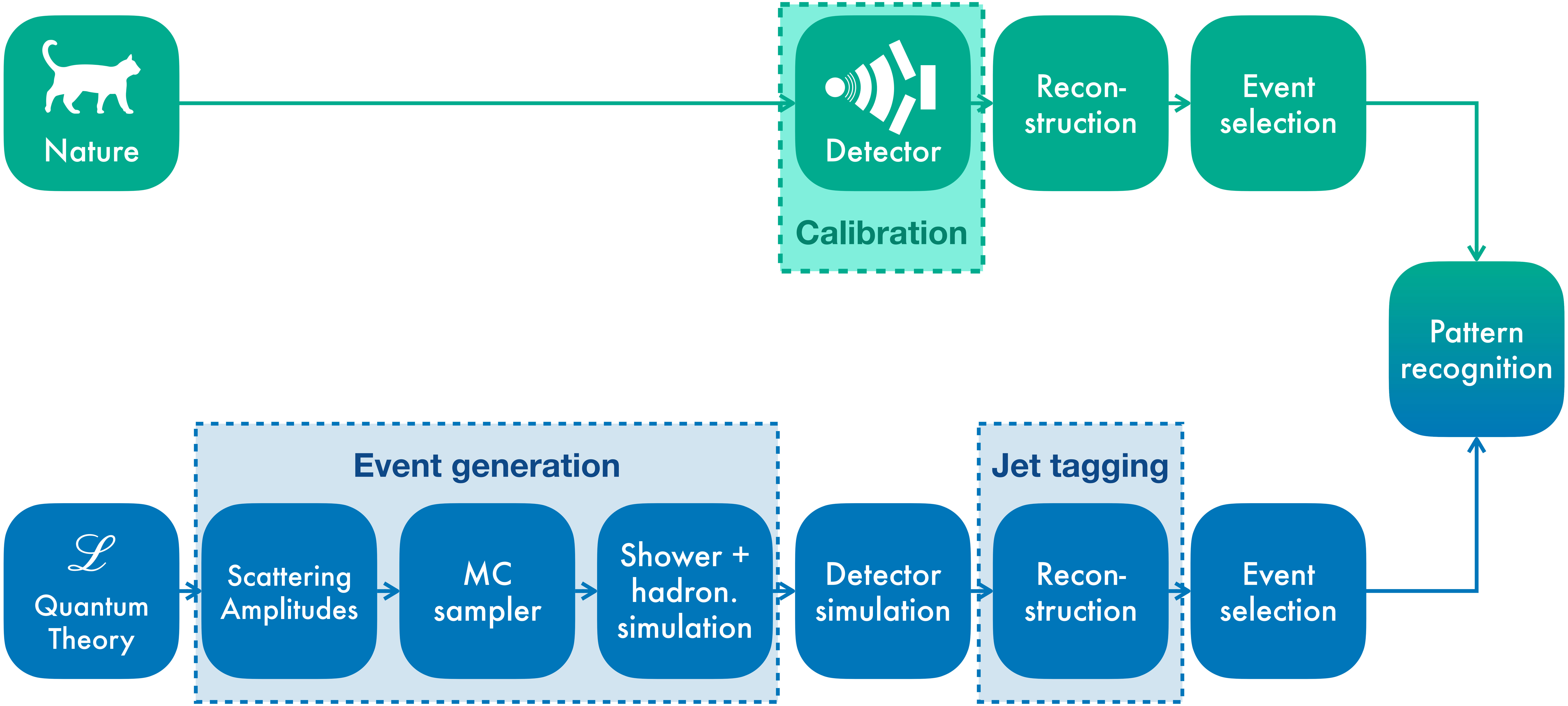

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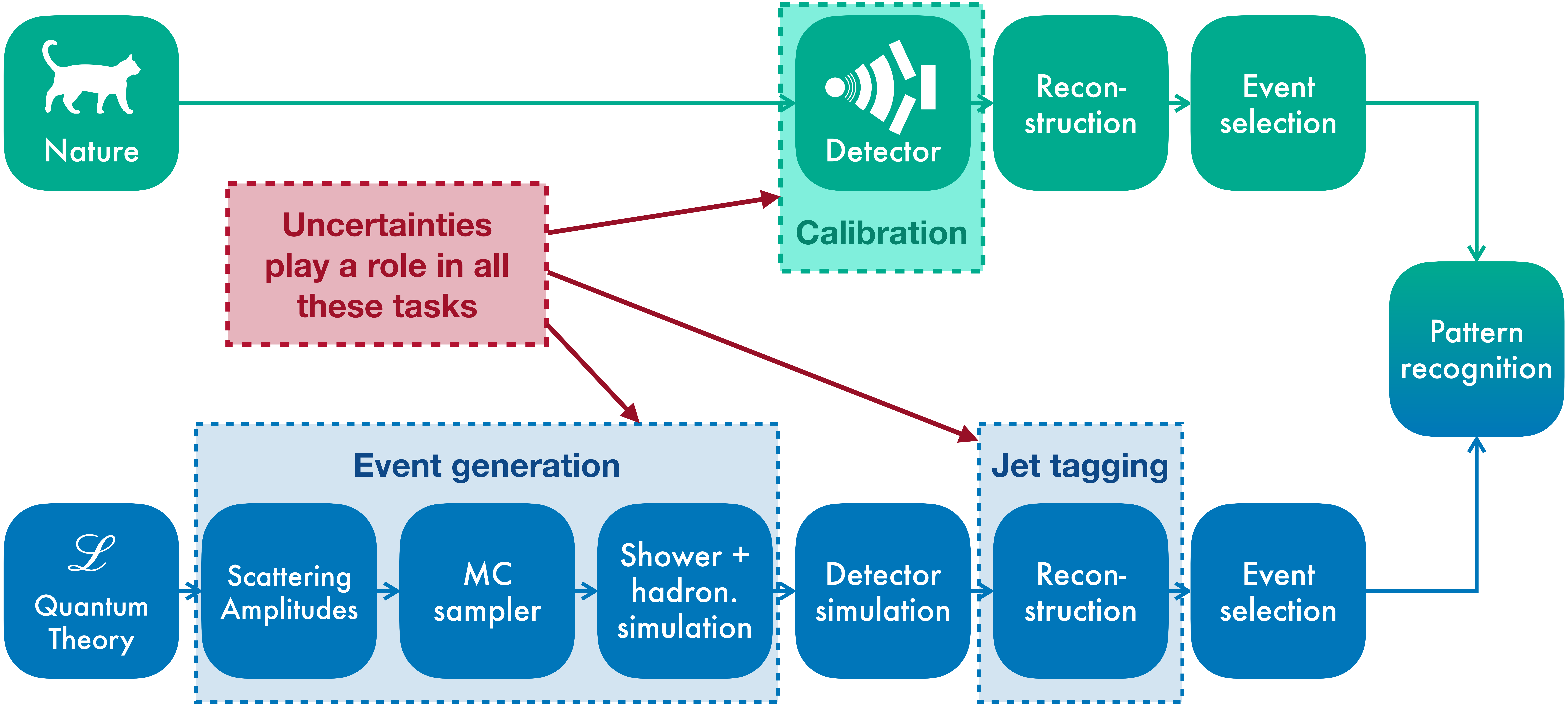

Nature

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Uncertainties play a role in all these tasks

Event generation

Jet tagging

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- Can they be controlled?
- Two types of uncertainties:
  - **Systematic**: Plateaus for perfect training (epistemic uncertainty)
  - **Statistical**: Vanishes for perfect training (aleatoric uncertainty)

Outline

Part I: **Different networks and architectures**

Part II: Systematic uncertainties

Part III: Statistical uncertainties

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- Fit set of Amplitudes $A(x)$ with training data: $\{x, A(x)\}$

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network distribution

network output

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network distribution

network output

- Standard heteroscedastic loss:

$$\mathscr{L}_{\text{heteroscedastic}} = \sum_i \frac{|f(x_i) - f_\theta(x_i)|^2}{2\sigma(x_i)^2} + \log \sigma(x_i) + \ldots$$

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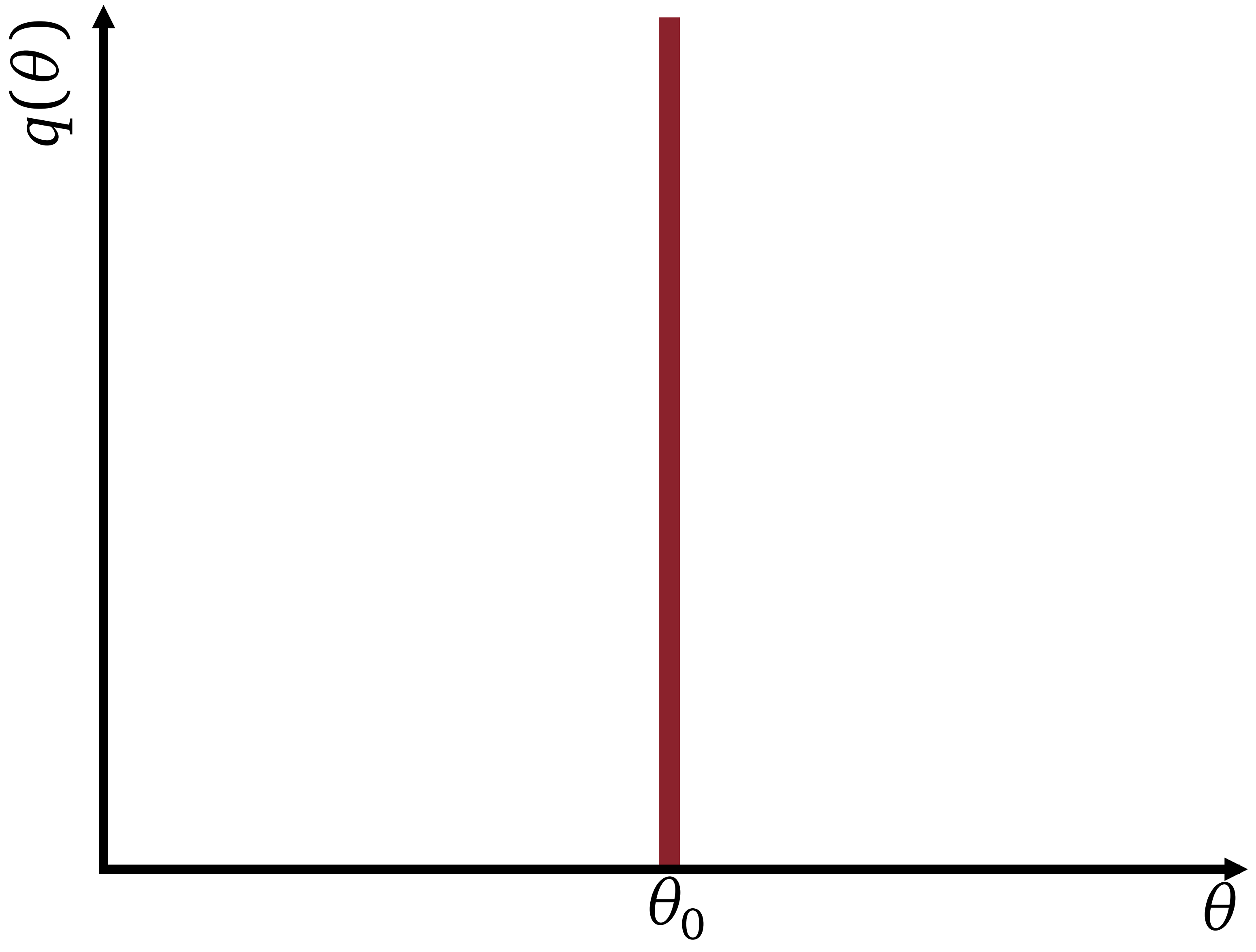
- Additional statistical uncertainty:

$$\sigma_{\text{tot}}^2(x) \equiv \langle (A - \langle A \rangle)^2 \rangle = \int \mathrm{d}A \, \left(A - \langle A \rangle\right)^2 \, p(A \,|\, x) = \int \mathrm{d}\theta \, q(\theta) \left(\overline{A^2}(x, \theta) - \bar{A}(x, \theta)^2 \right) + \int \mathrm{d}\theta \, q(\theta) \left(\bar{A}(x, \theta) - \langle A \rangle \right)^2$$

Bayesian neural networks (BNNs)

Neural network



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$$\theta = \theta_0$$

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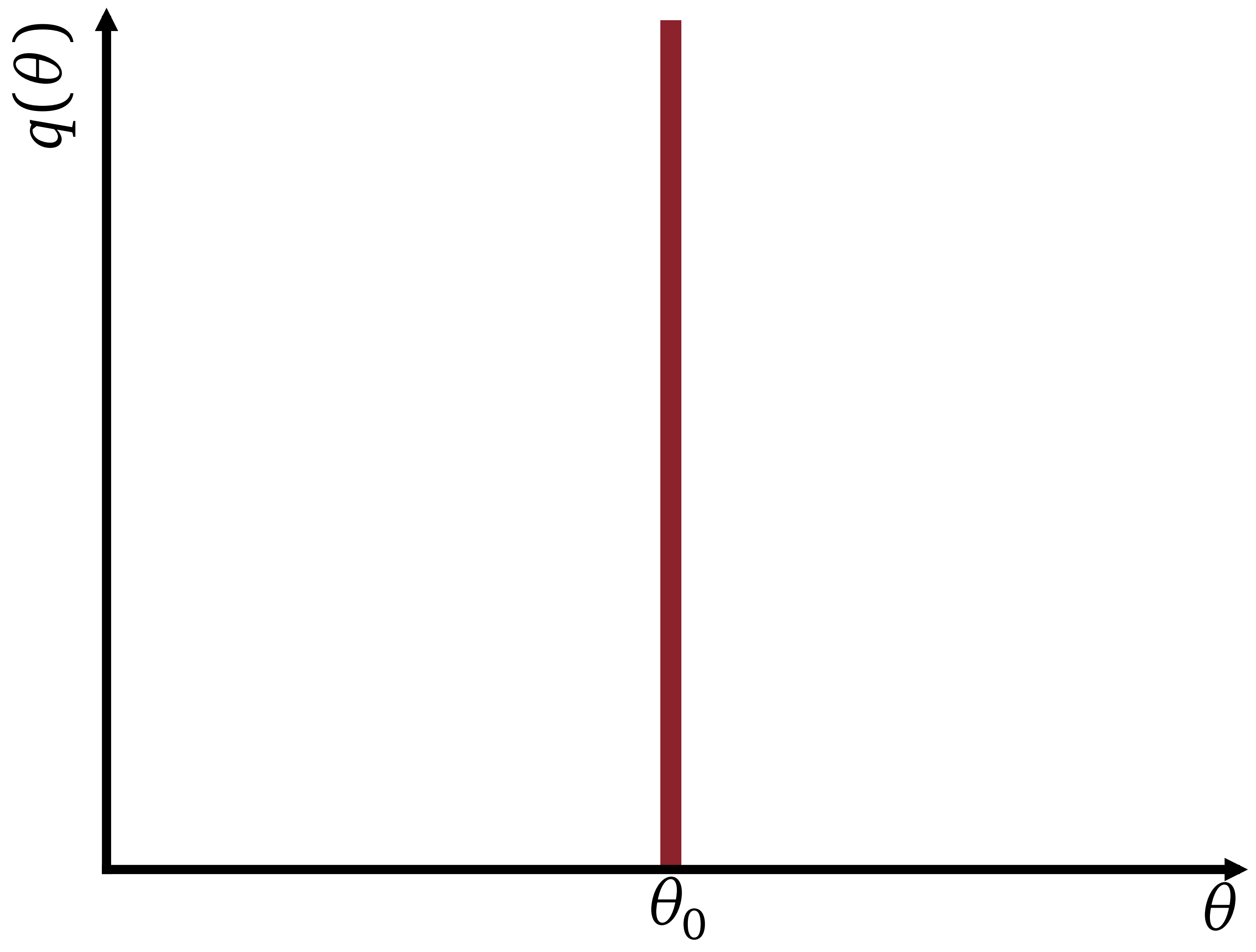

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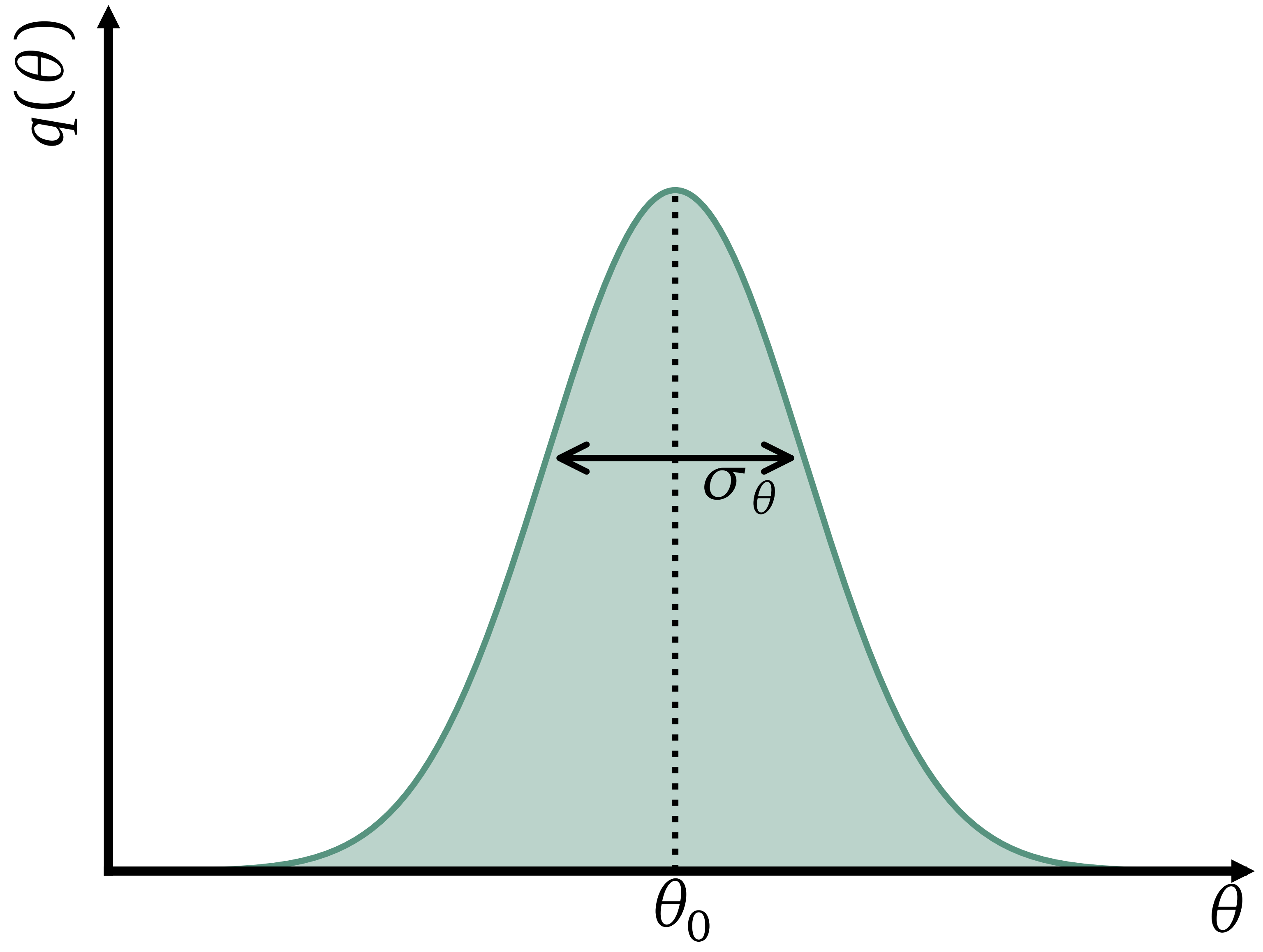

Network weights are drawn from distribution

$$\theta \sim q(\theta)$$

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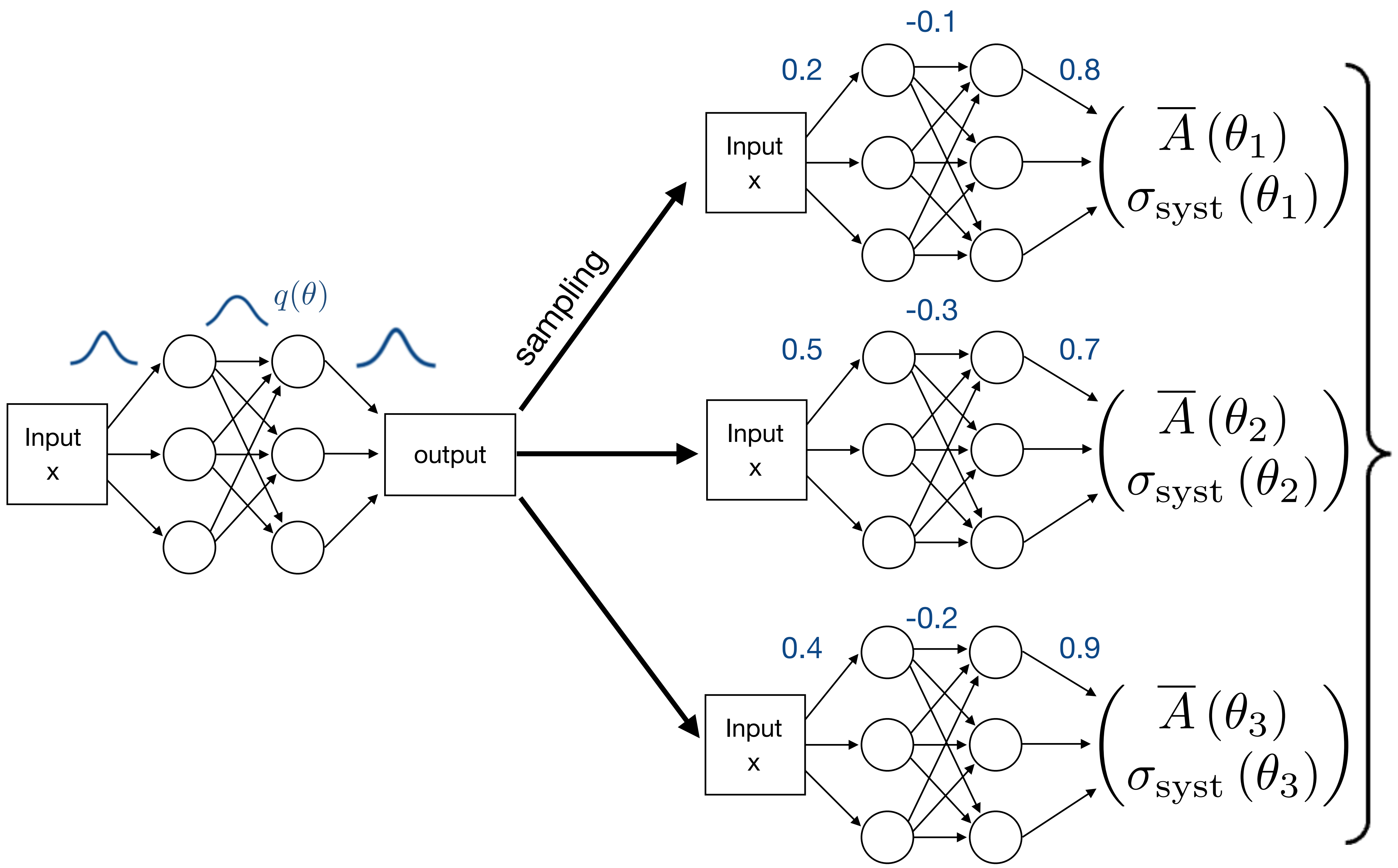
Bayesian neural networks (BNNs)

BNN **Ensemble of networks** **Output**



$$\langle A \rangle = \frac{1}{N} \sum_i^N \overline{A}(\theta_i)$$

$$\sigma^2_{\text{syst}} = \frac{1}{N} \sum_i^N \sigma^2_{\text{syst}}(\theta_i)$$

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$$\mathcal{L}_{\text{BNN}} = \sum_x \Big[\text{KL}[q(\theta), p(\theta)] - \big\langle \log p(D_{\text{train}}|\theta) \big\rangle_{\theta \sim q(\theta)} \Big]$$

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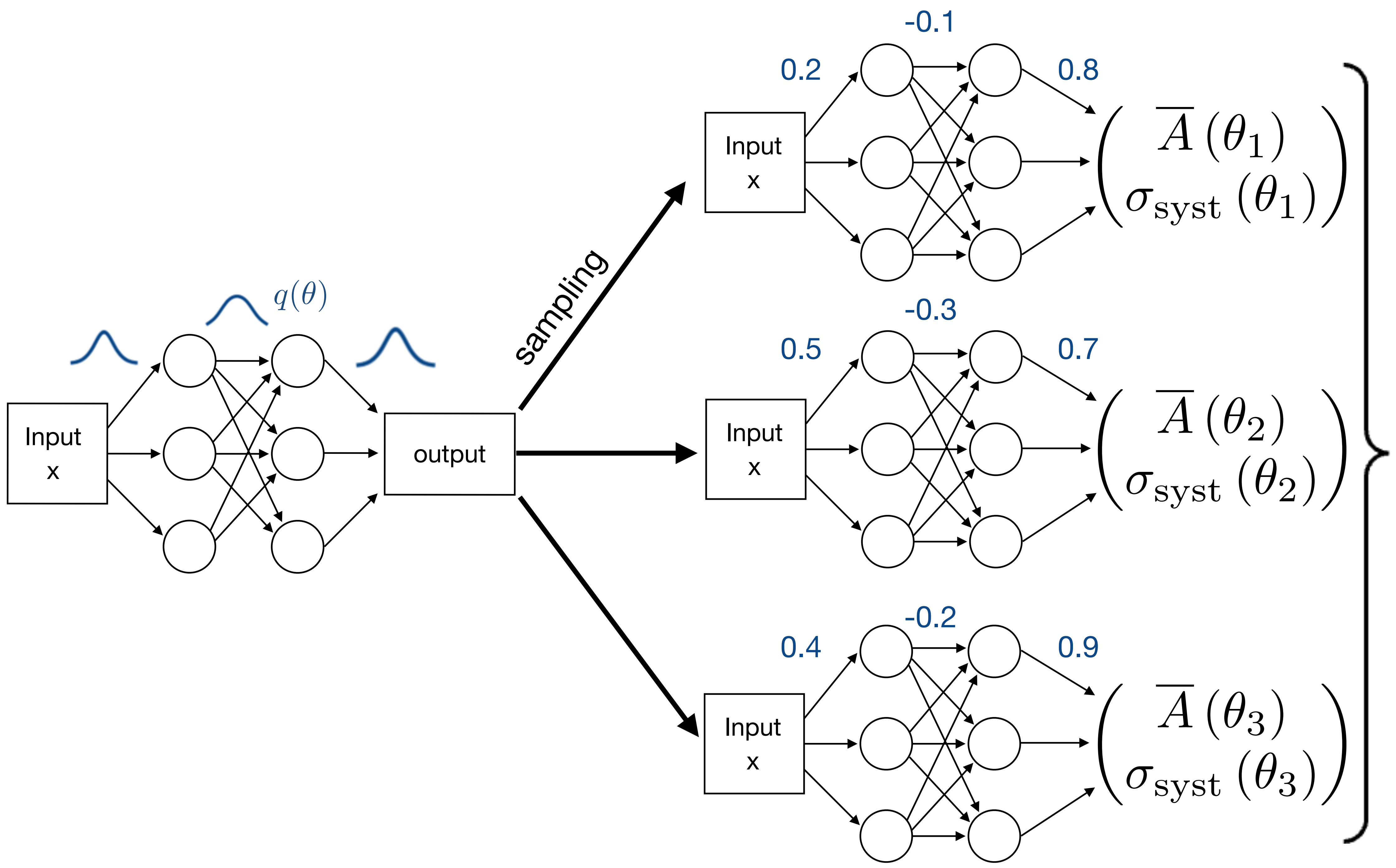

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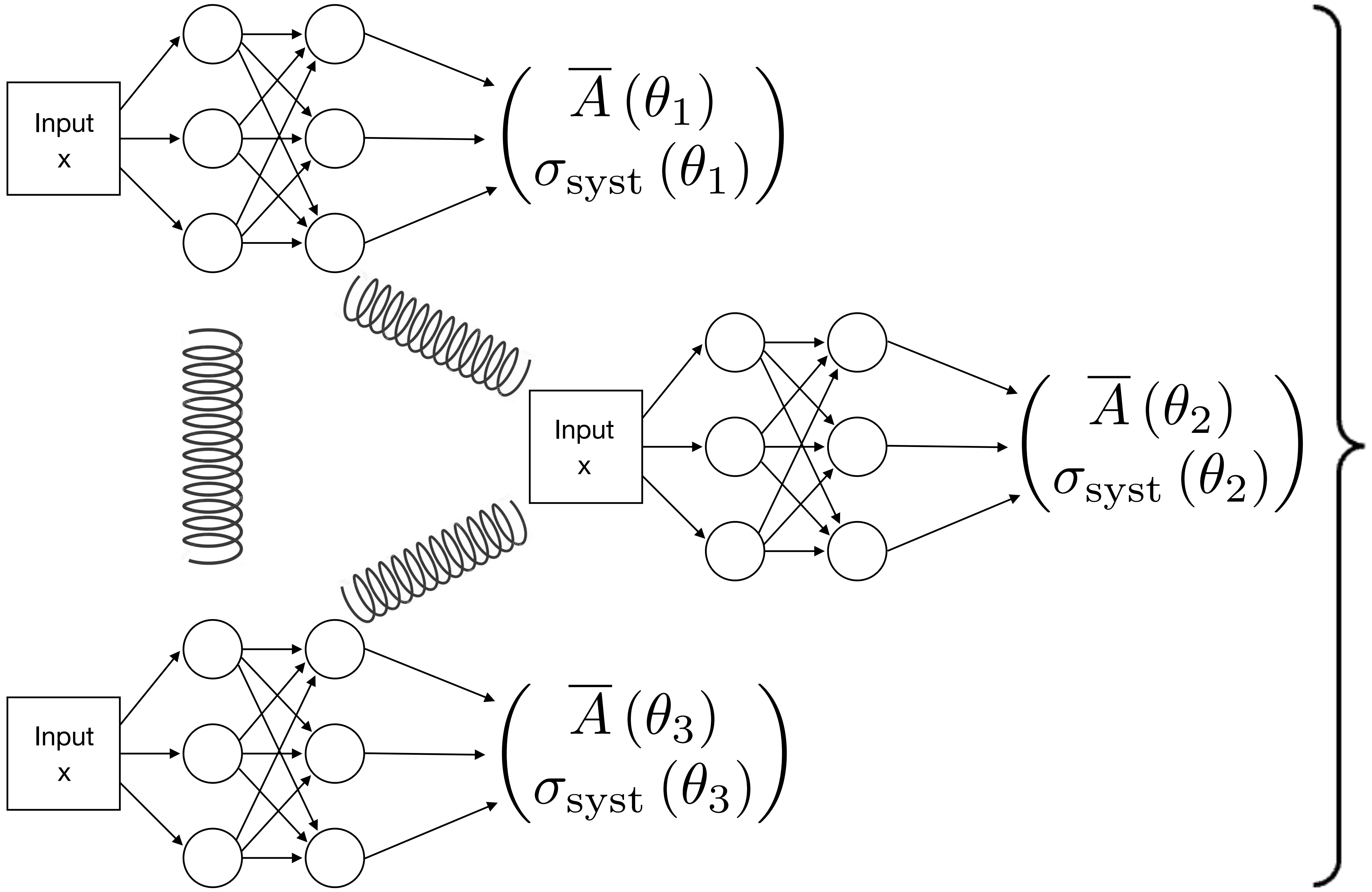
- Parameters: **Network weights $q(\theta)$**
- $q(\theta)$ params of a Gaussian distribution
- Ensemble: Sample from weight distribution

Repulsive ensembles (REs)

Ensemble of networks

Output



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$$\mathcal{L}_{\text{RE}} = \sum_{i=1}^{n}\left[-\frac{1}{B}\sum_{b=1}^{B}\log p(x_b|\theta_i) + \frac{\beta}{N}\frac{\sum_{j=1}^{n} k(A_{\theta_i}(x), \overline{A_{\theta_j}(x)})}{\sum_{j=1}^{n} k(\overline{A_{\theta_i}(x)}, \overline{A_{\theta_j}(x)})} + \frac{\theta_i^2}{2N\sigma^2}\right]$$

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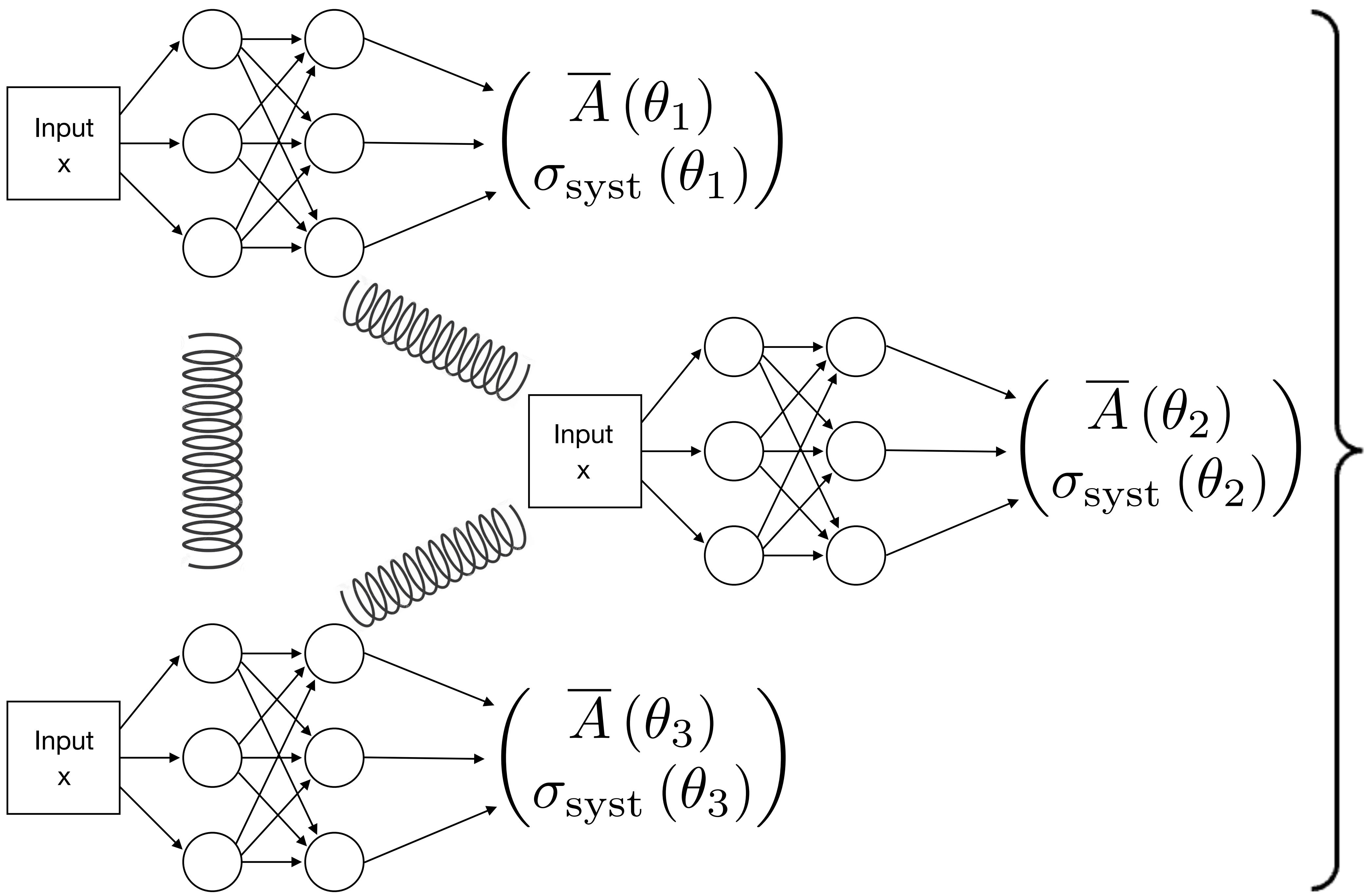

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- Repulsive term: Cover full posterior distribution
- Ensemble members **trained simultaneously**

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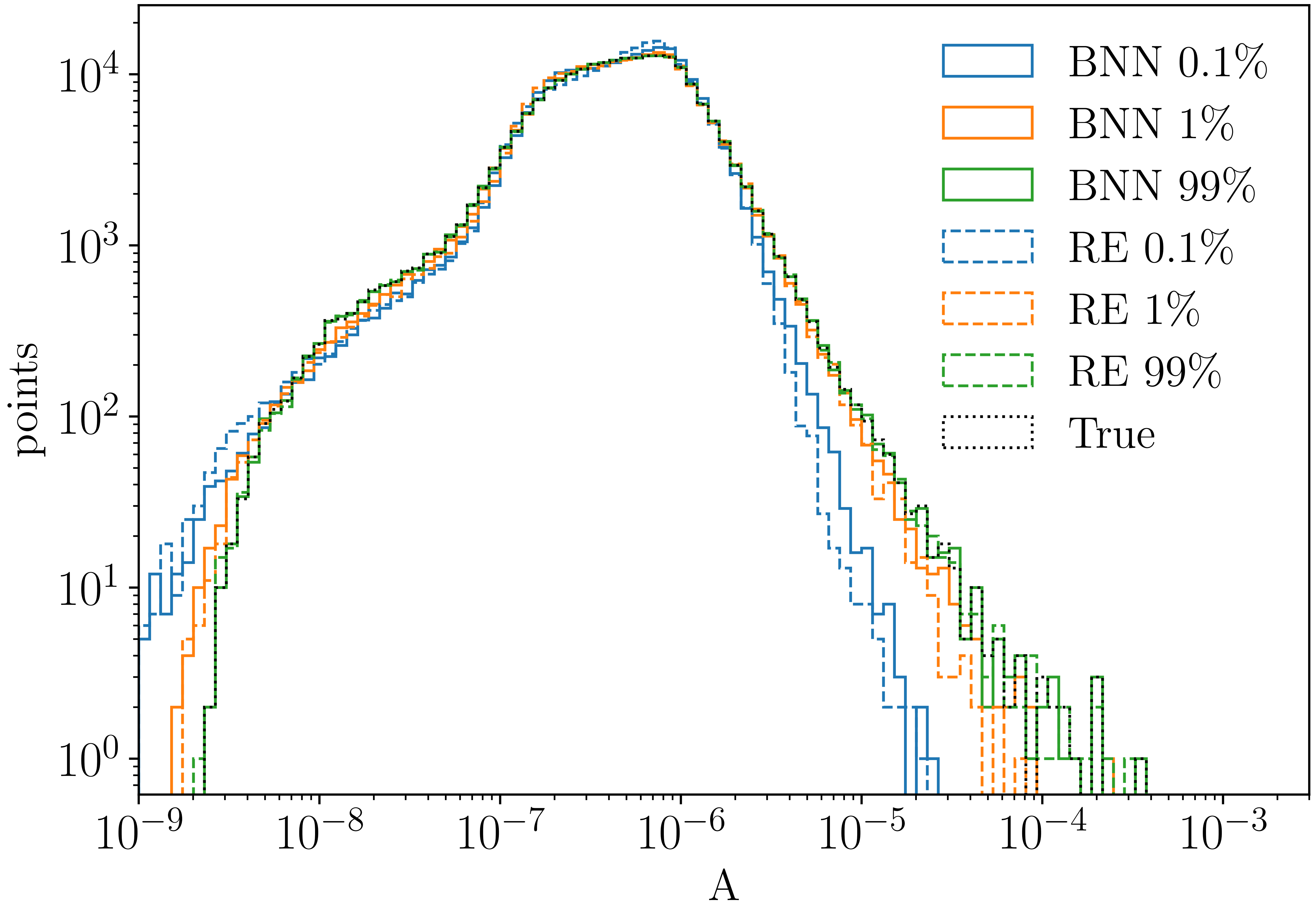
training with different amounts of data



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Adding Gaussian noise

$$\sigma^2_{\text{tot}} = \sigma^2_{\text{syst},0} + \sigma^2_{\text{noise}} + \sigma^2_{\text{stat}}$$

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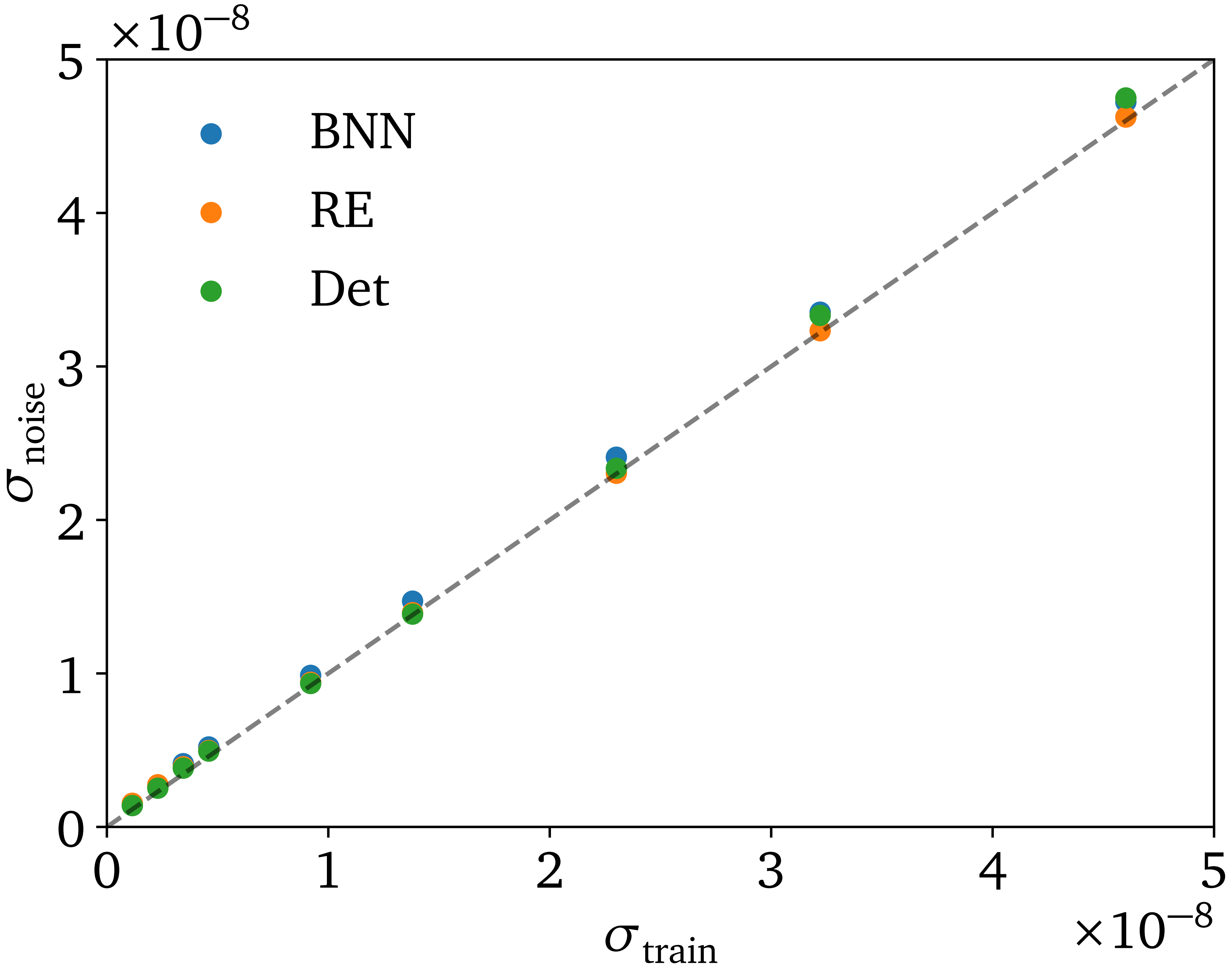

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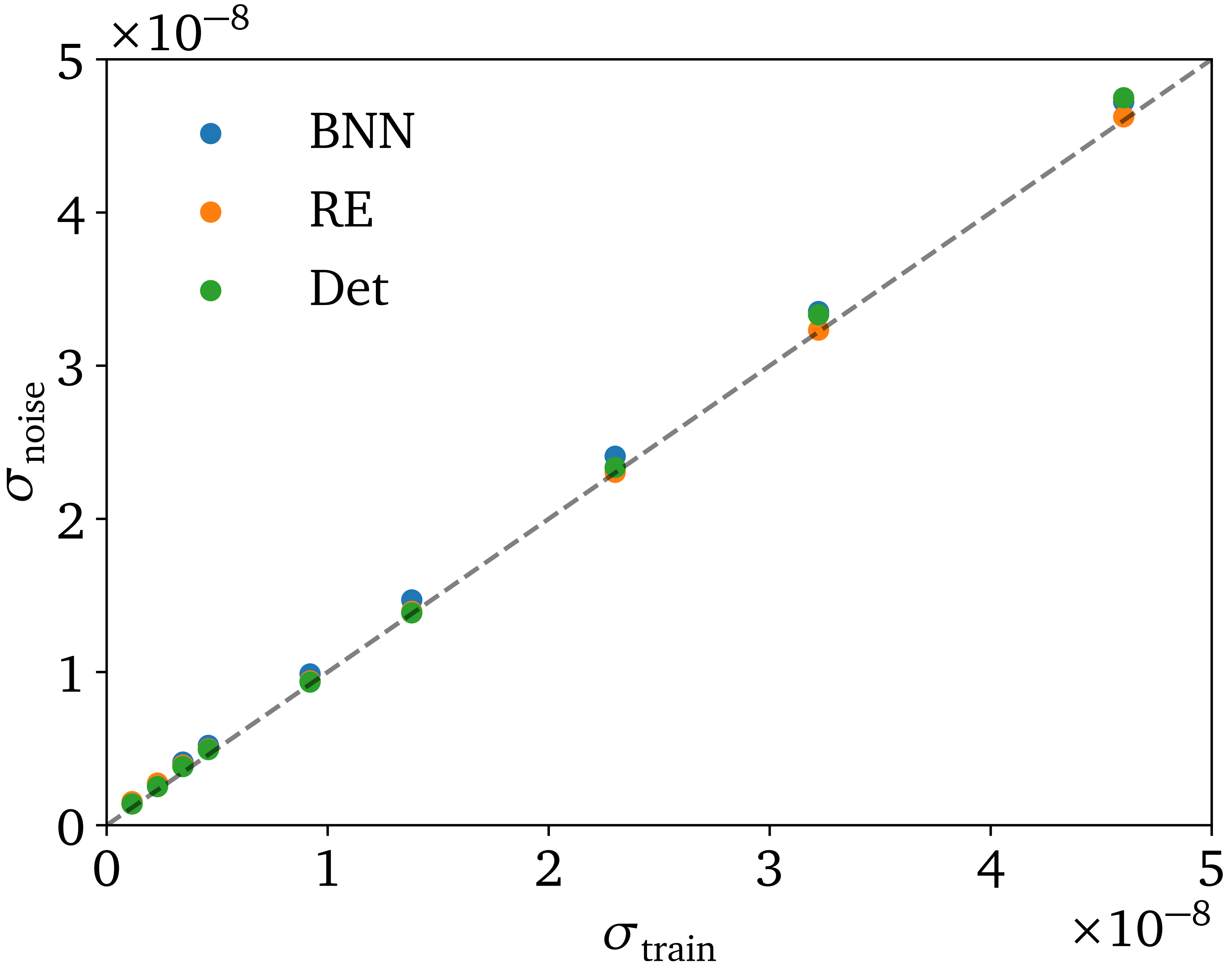

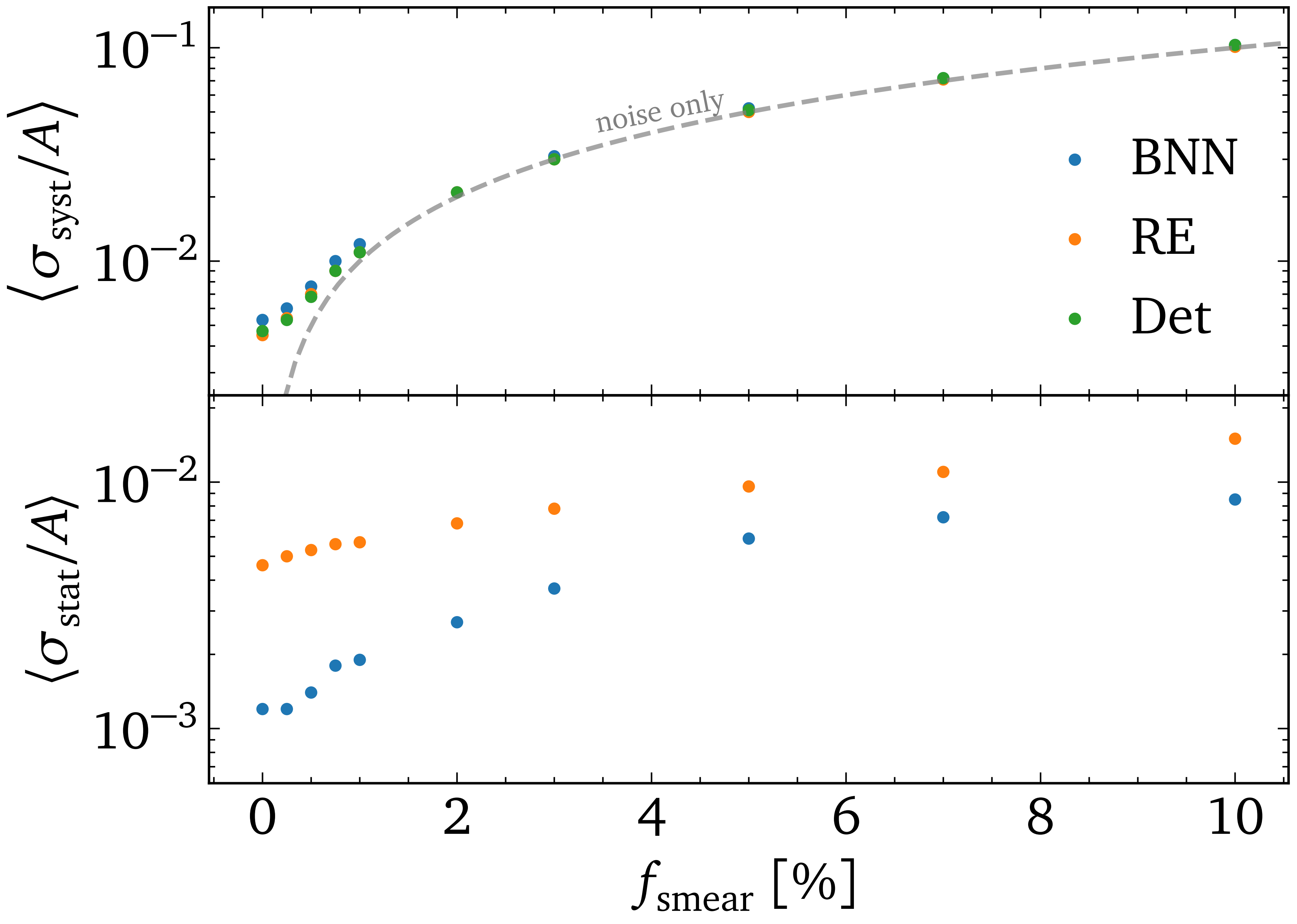

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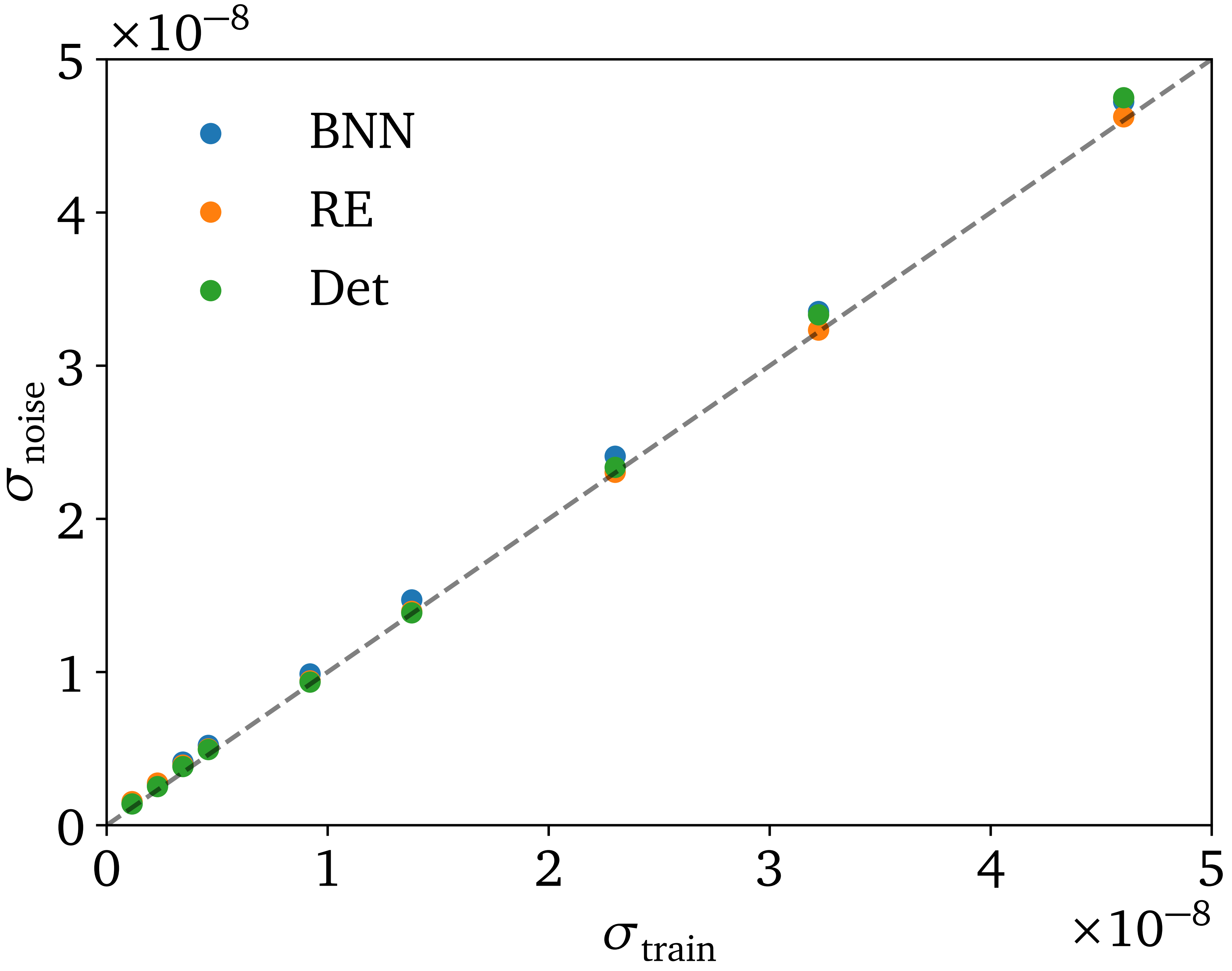
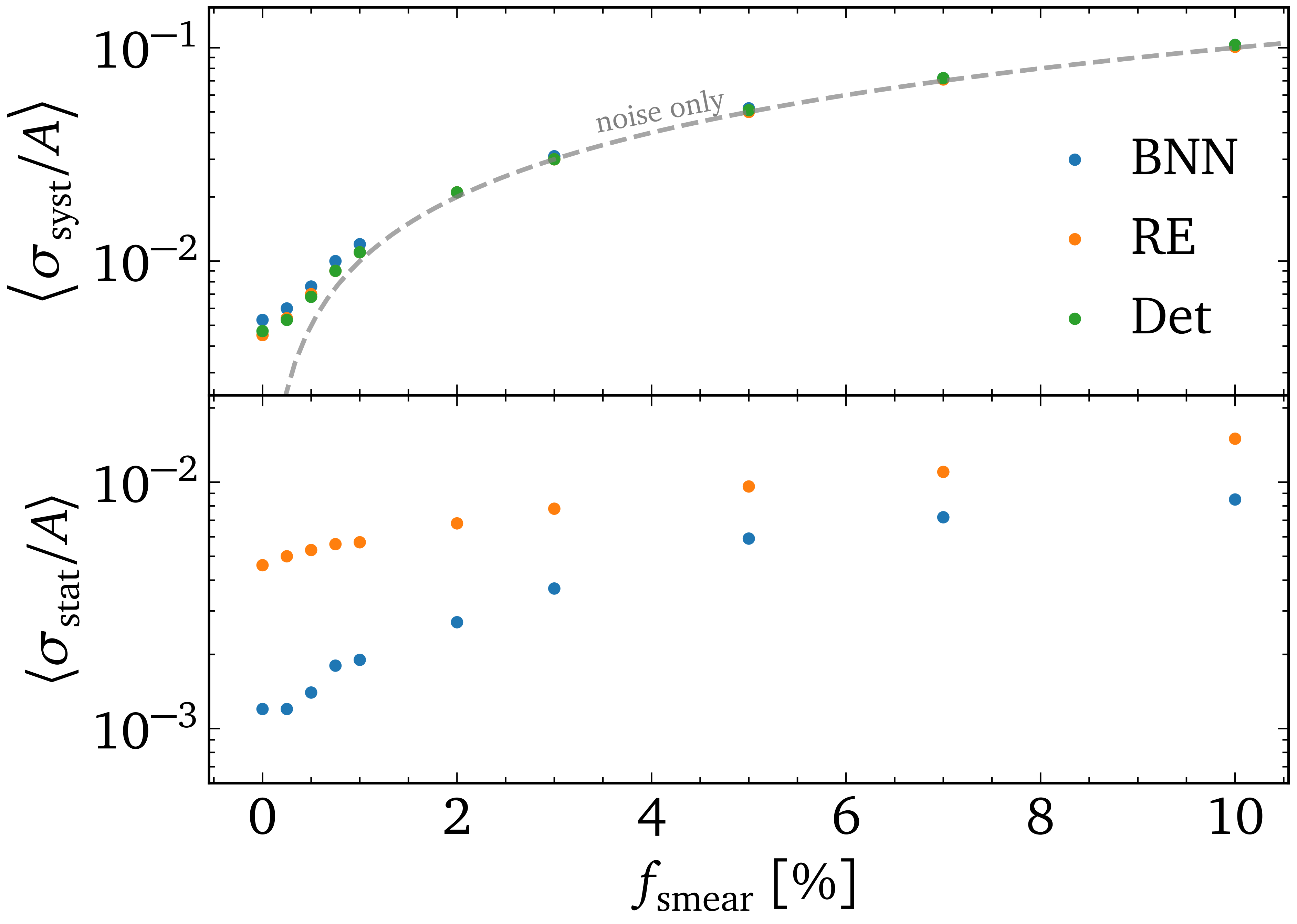
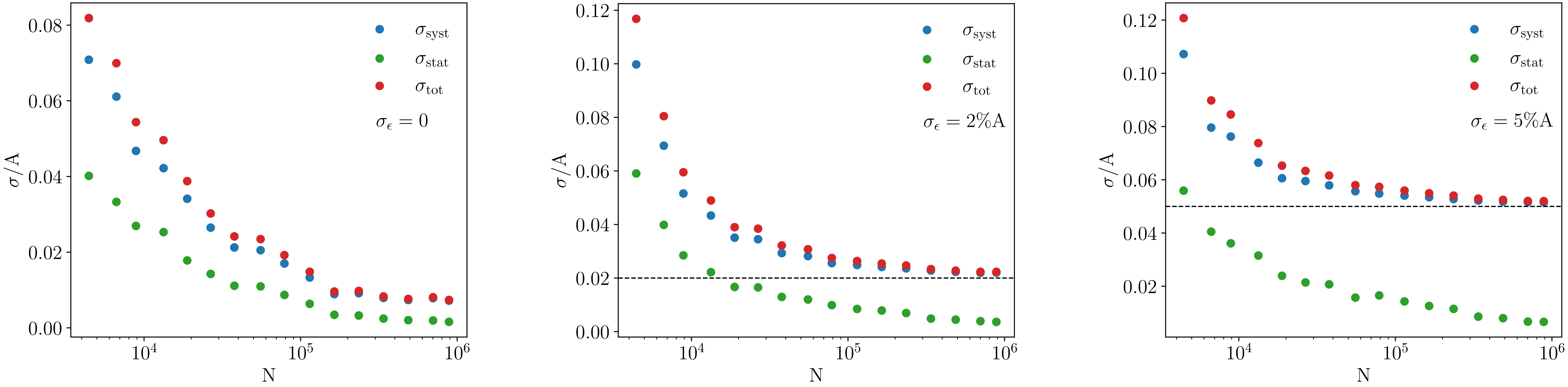




➡ Networks learn noise as **systematic** uncertainties

Uncertainty behavior



BNN only

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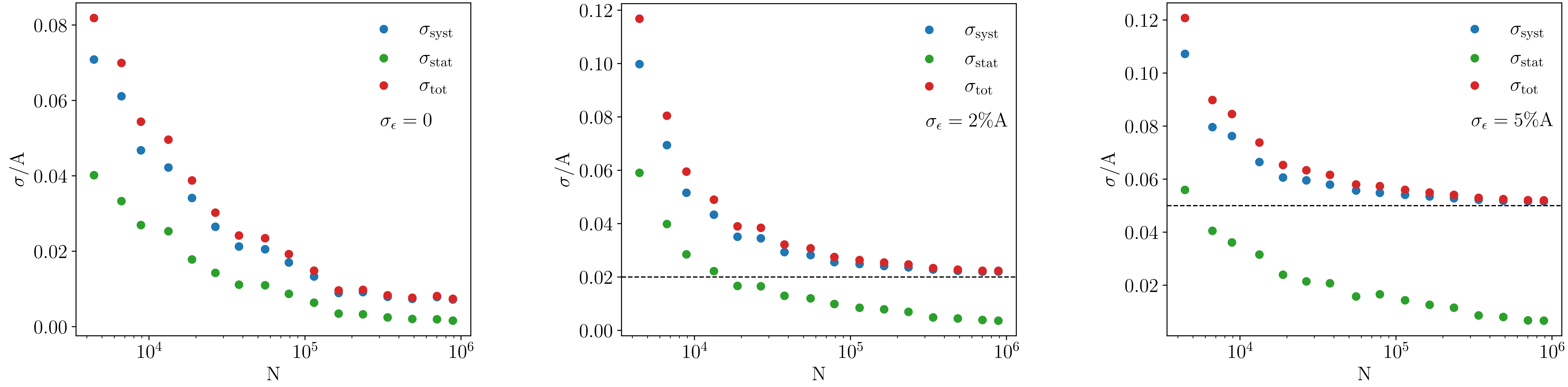

BNN only

1. Statistical uncertainty **independent** of noise

2. Systematic uncertainty **plateaus** on noise level

Calibration of the results

Bias calibration

Uncertainty calibration

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$$\Delta(x) = \frac{A_{\mathrm{NN}}(x) - A_{\mathrm{true}}(x)}{A_{\mathrm{true}}(x)}$$

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Uncertainty calibration

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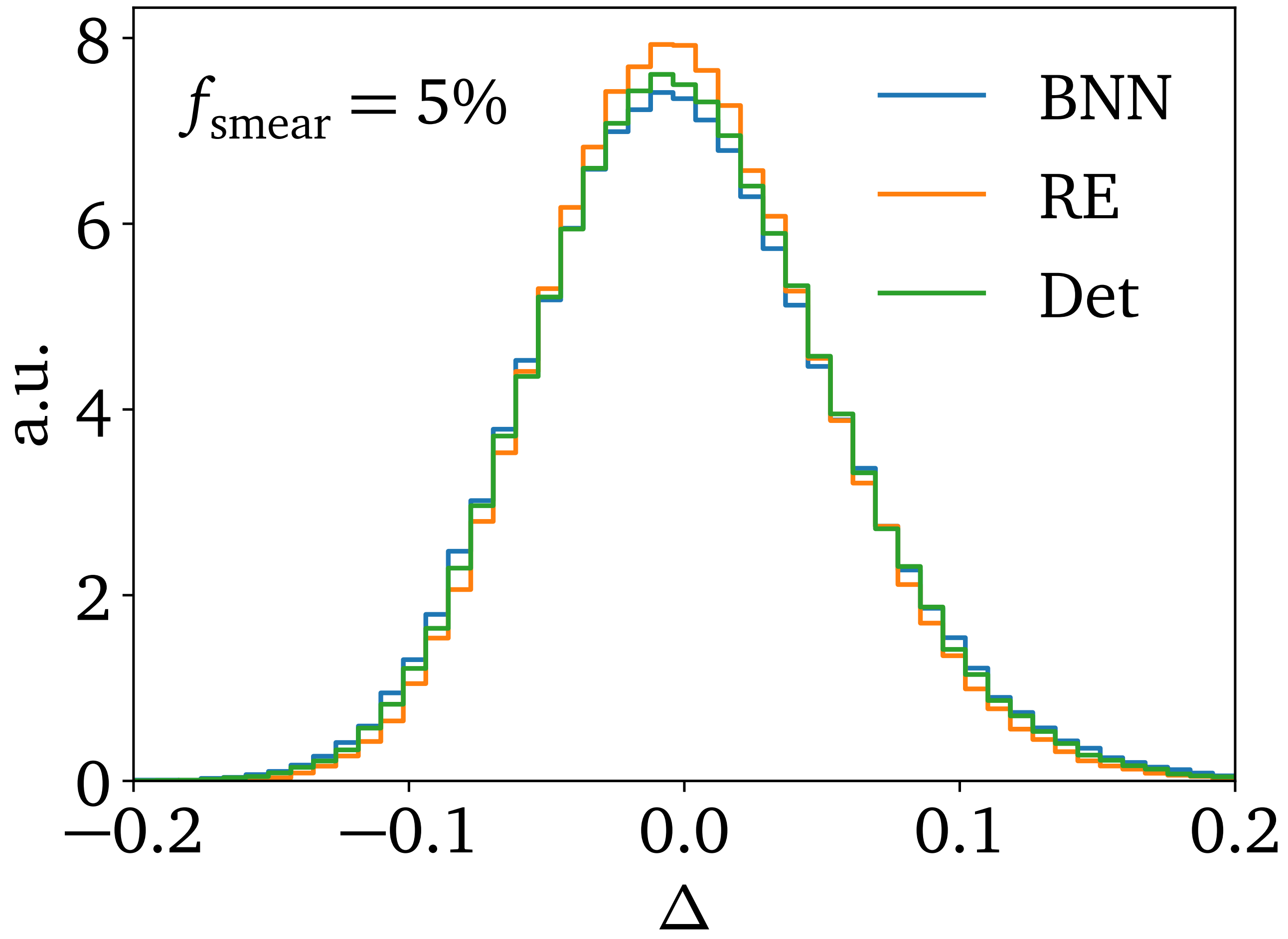
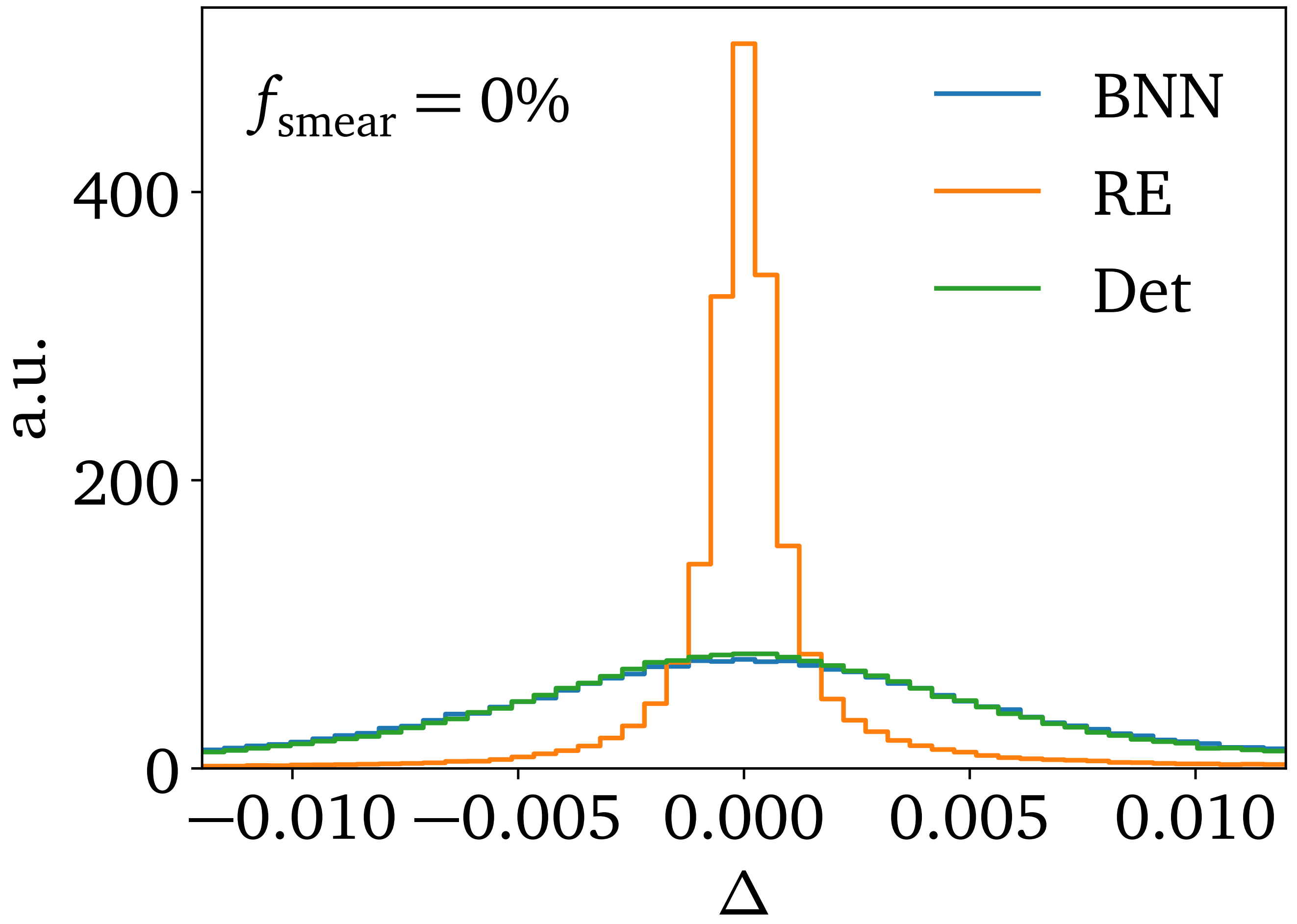
Correctly learned: follow Gaussian

Systematic pull - Results





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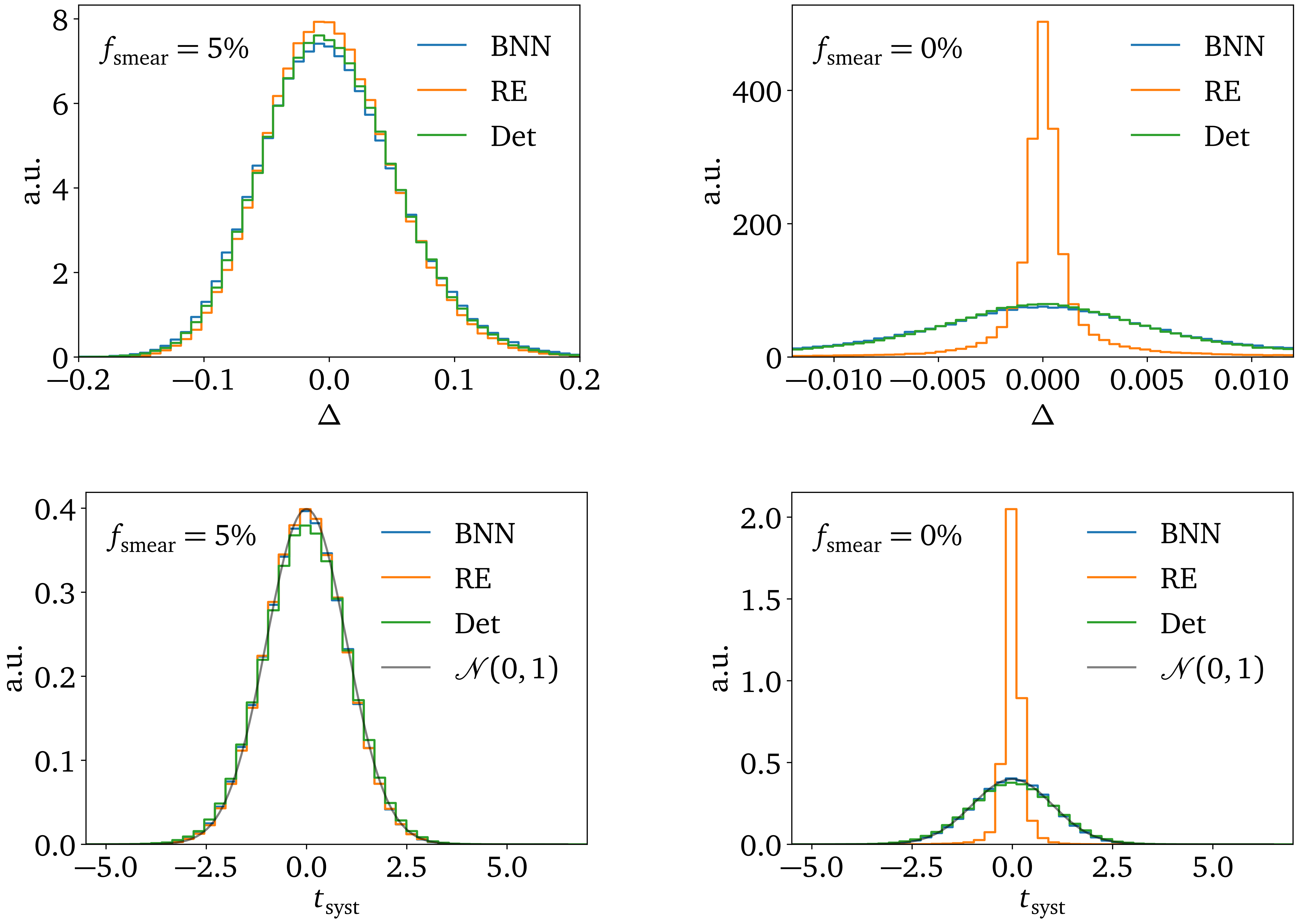

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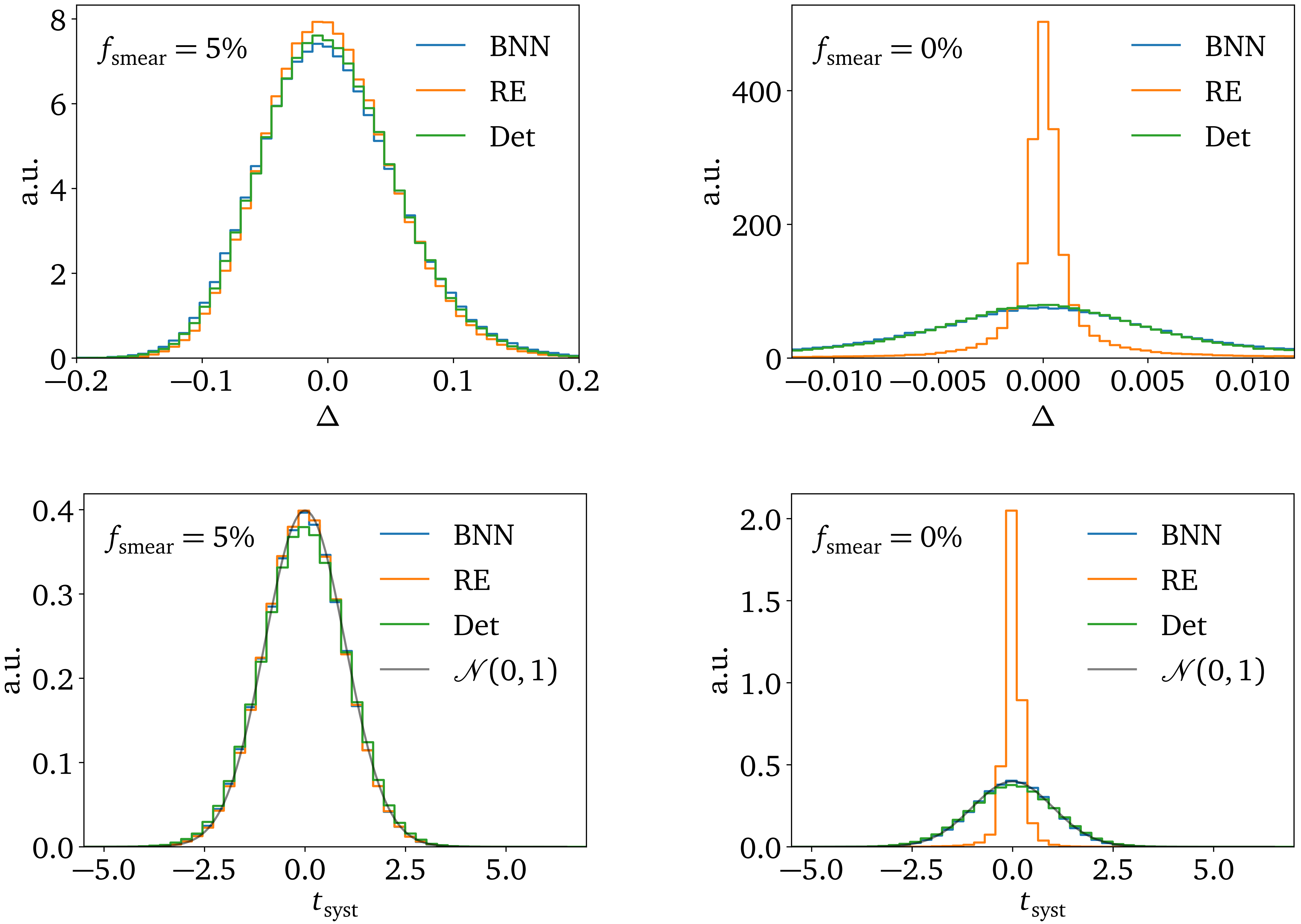

➡ BNN advantage for systematic uncertainties

Systematic pull of REs

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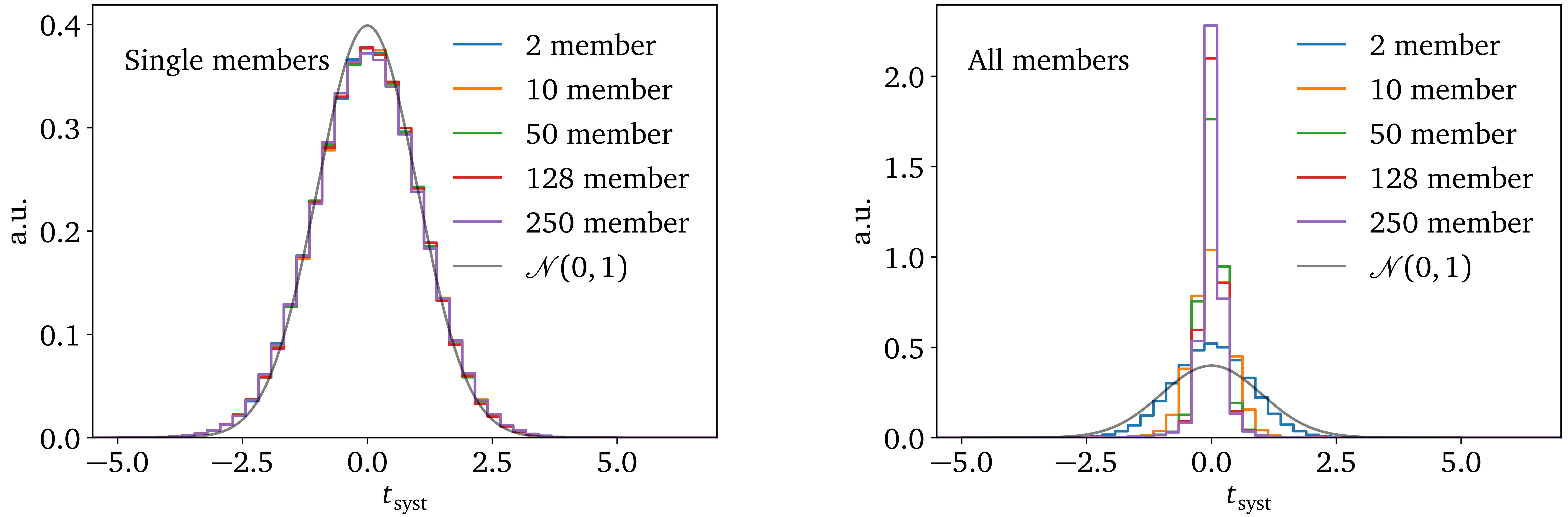

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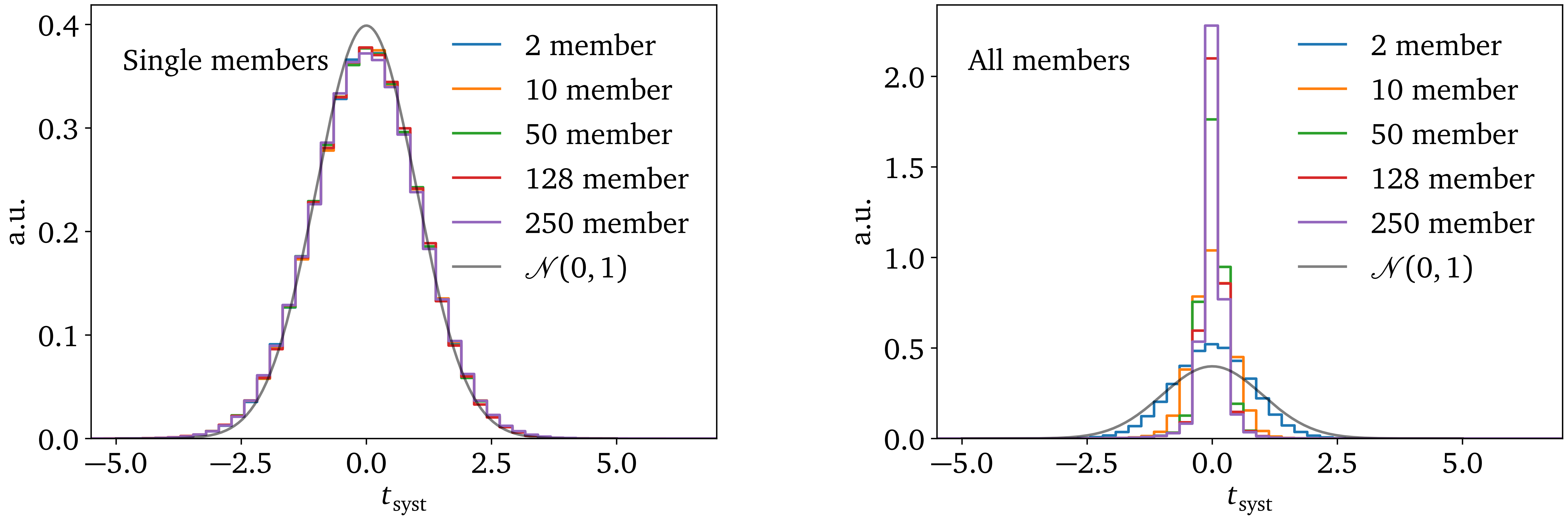
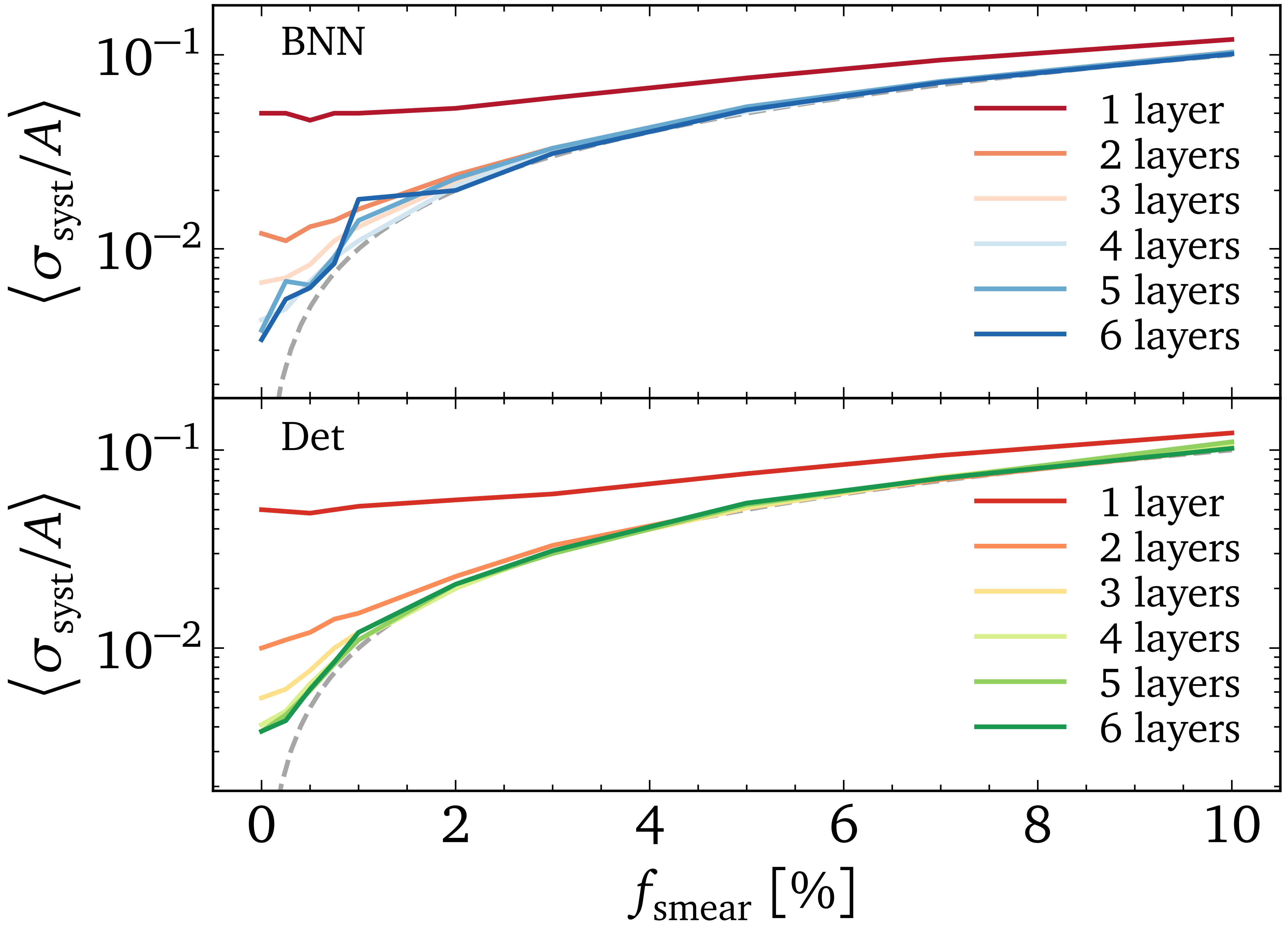


➡Prediction benefits from ensemble nature but not σ_{syst}

Systematics from network expressivity



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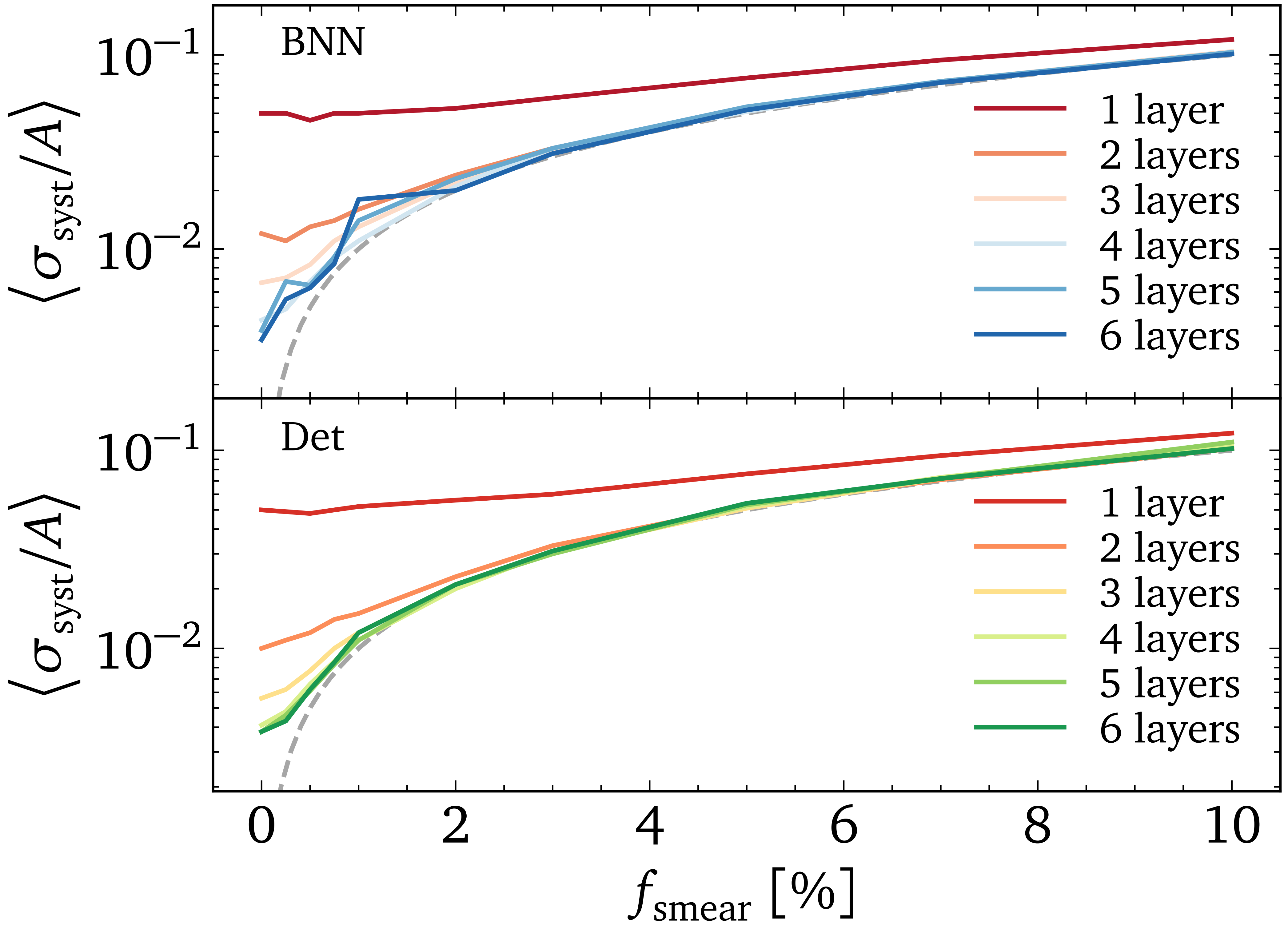
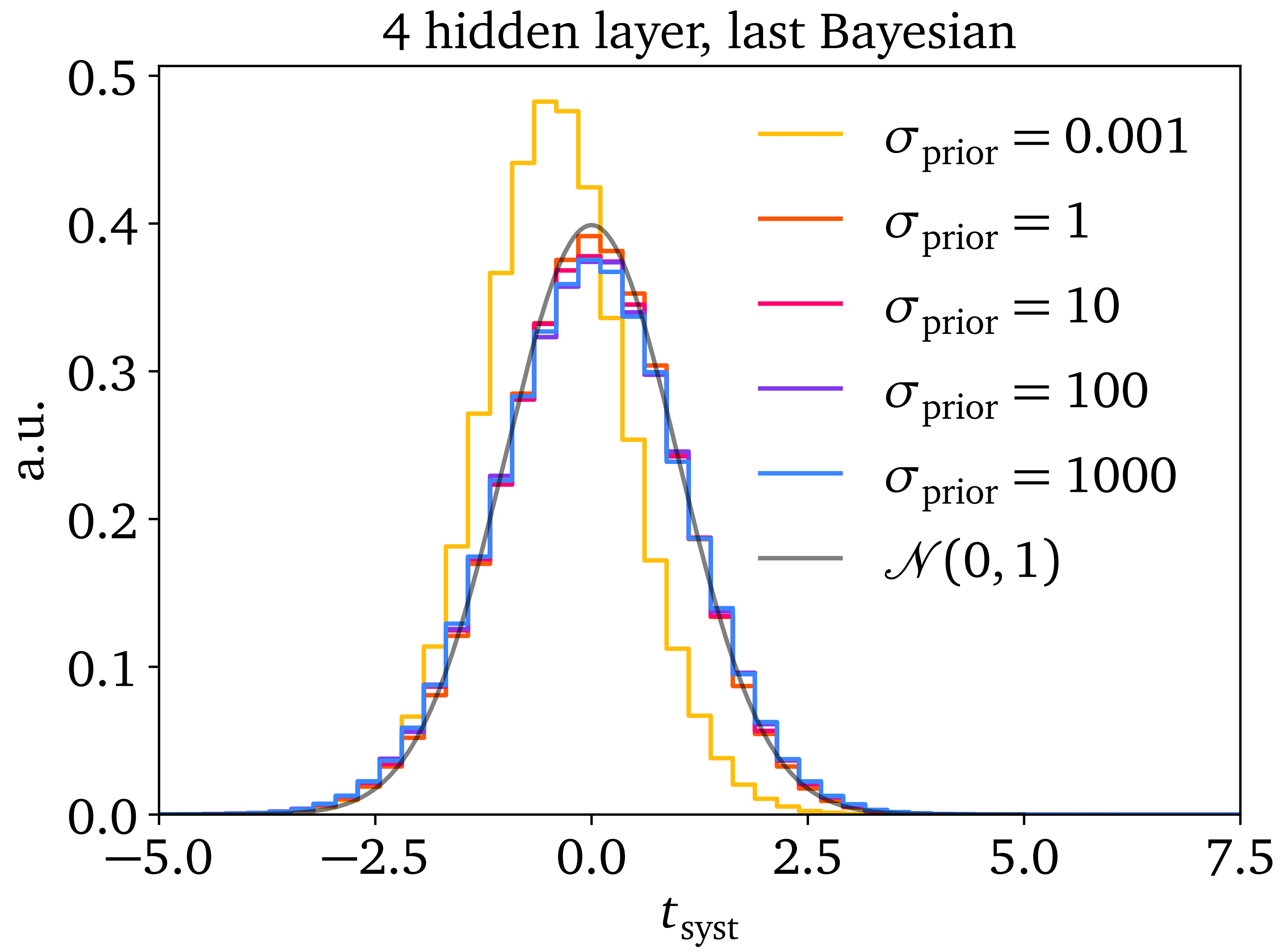
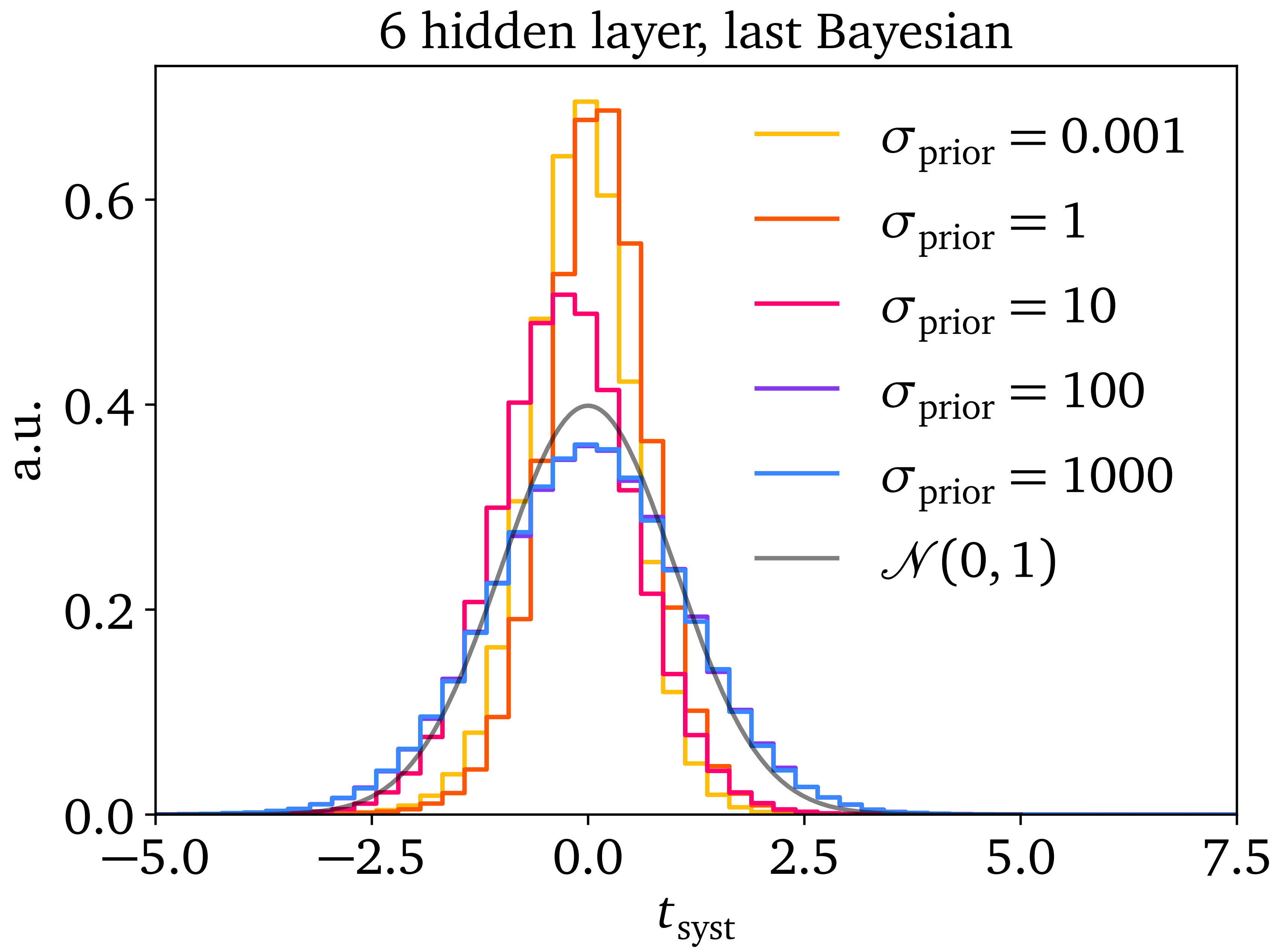


- Need at least three layers
- BNN: only last layer Bayesian
- Six layer: network gets too large

➡ More expressivity and better sensitivity for small noise with more layers

Prior influence in the BNN





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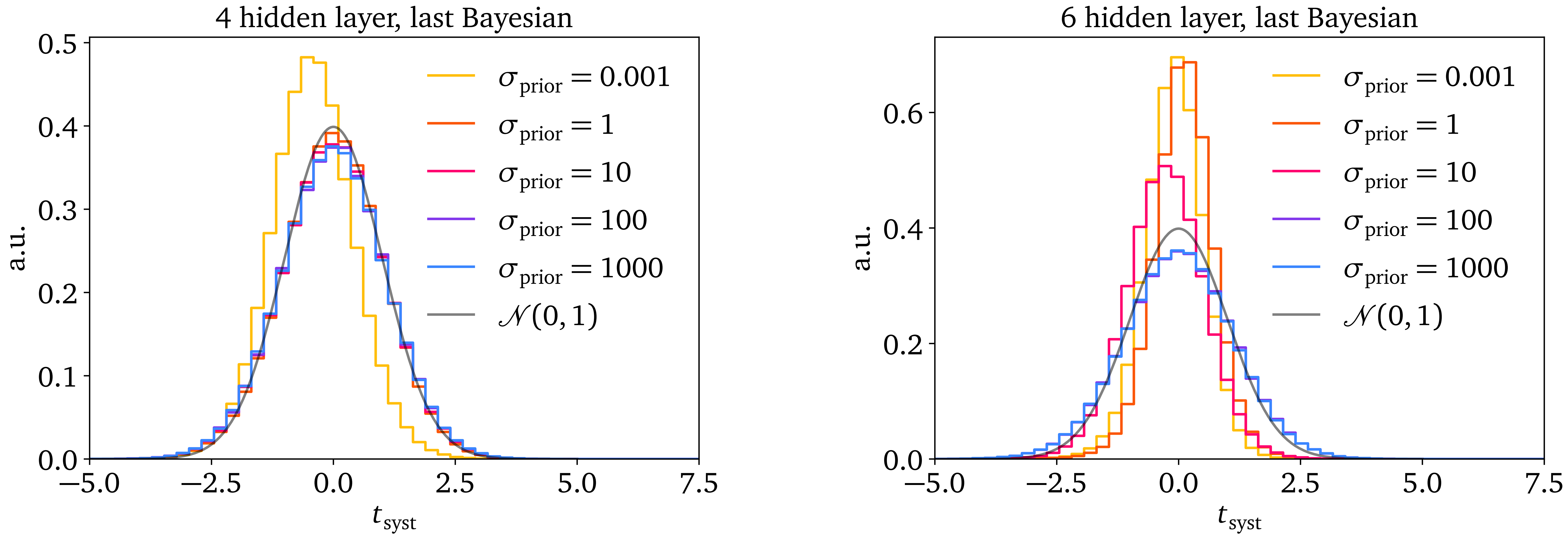


➡Results don't depend on prior

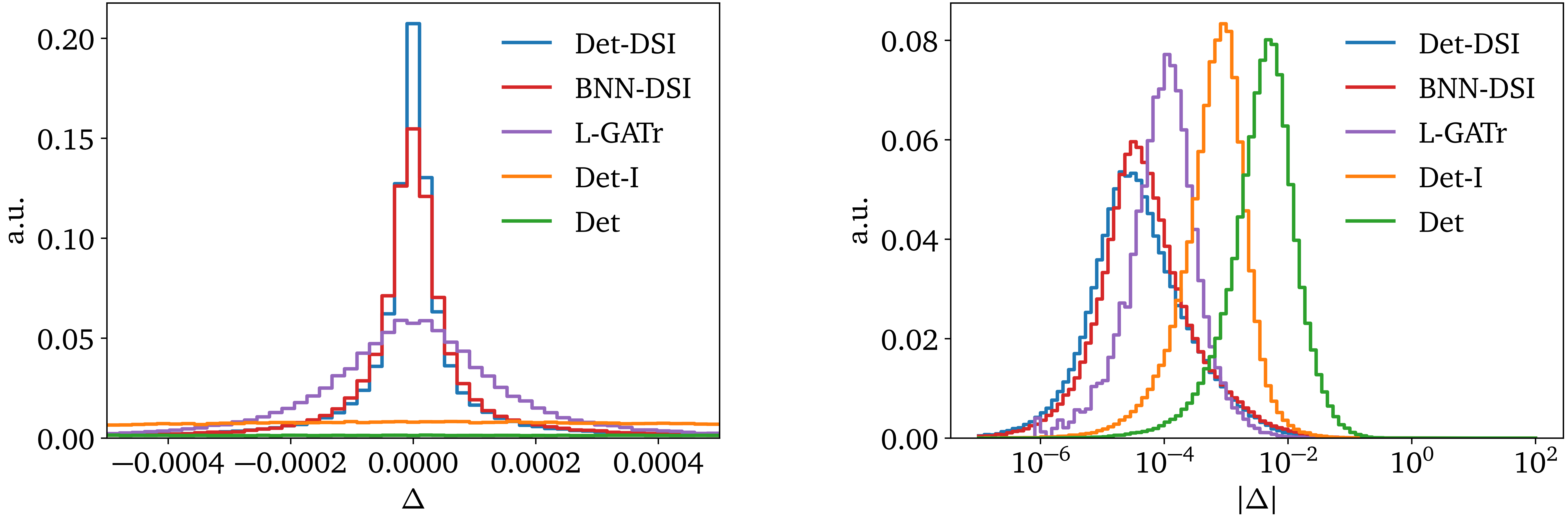
➡For more layers a larger prior is needed

Improving by using advanced architectures

- Enhance standard networks through representation learning:

1. **Deep Sets** (DS): learns embedding for each particle type
2. **Deep Sets Invariants** (DSI): DS with Lorentz invariance added as input
3. **L-GATr**: fully Lorentz equivariant network architecture [2411.00446]

Accuracy for advanced architectures



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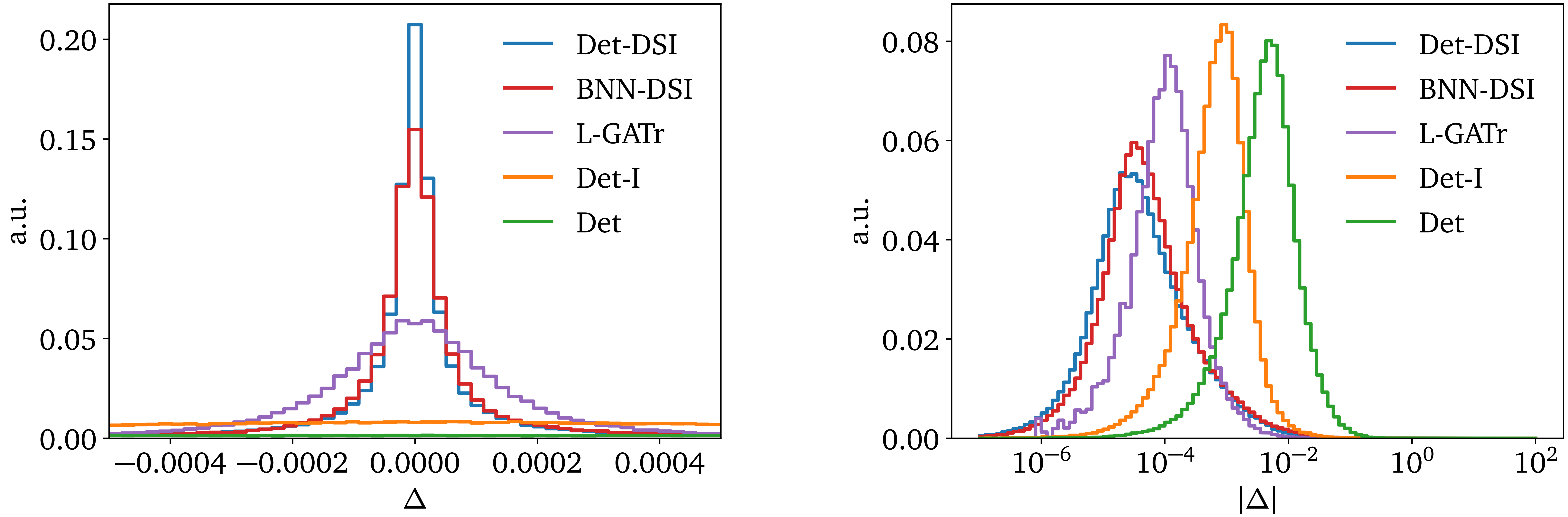
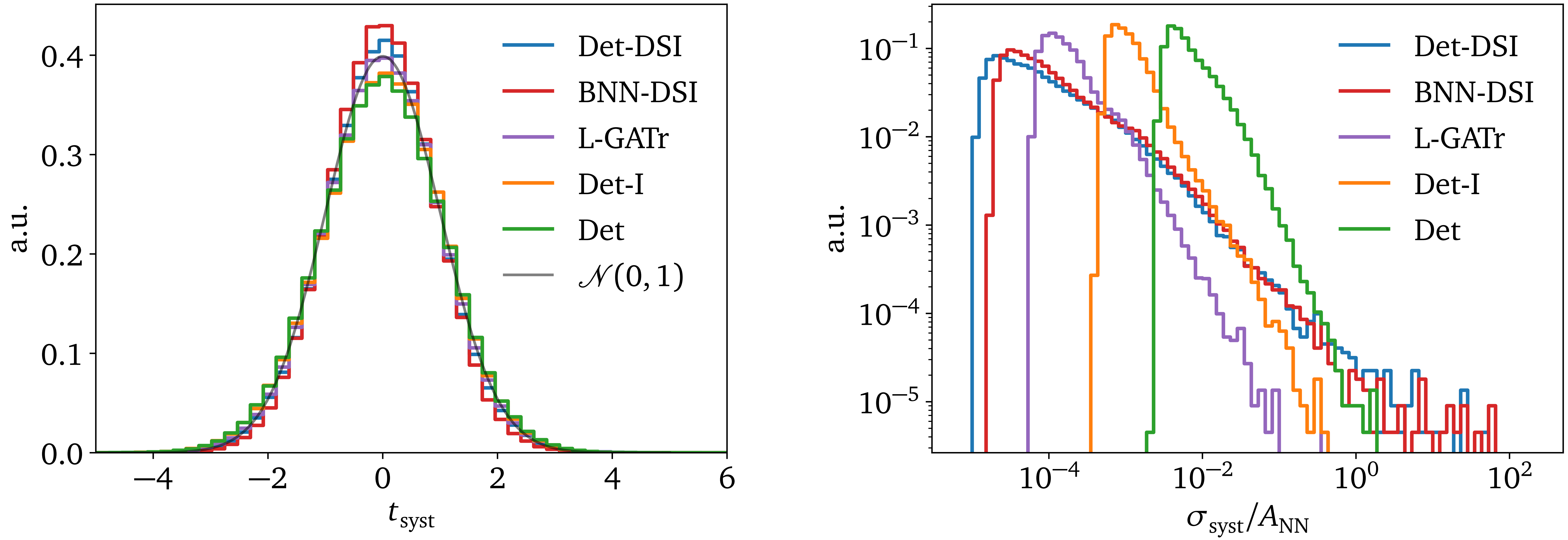


➡ **Controlled accuracy** to 10^{-5} level

Uncertainties from advanced architectures



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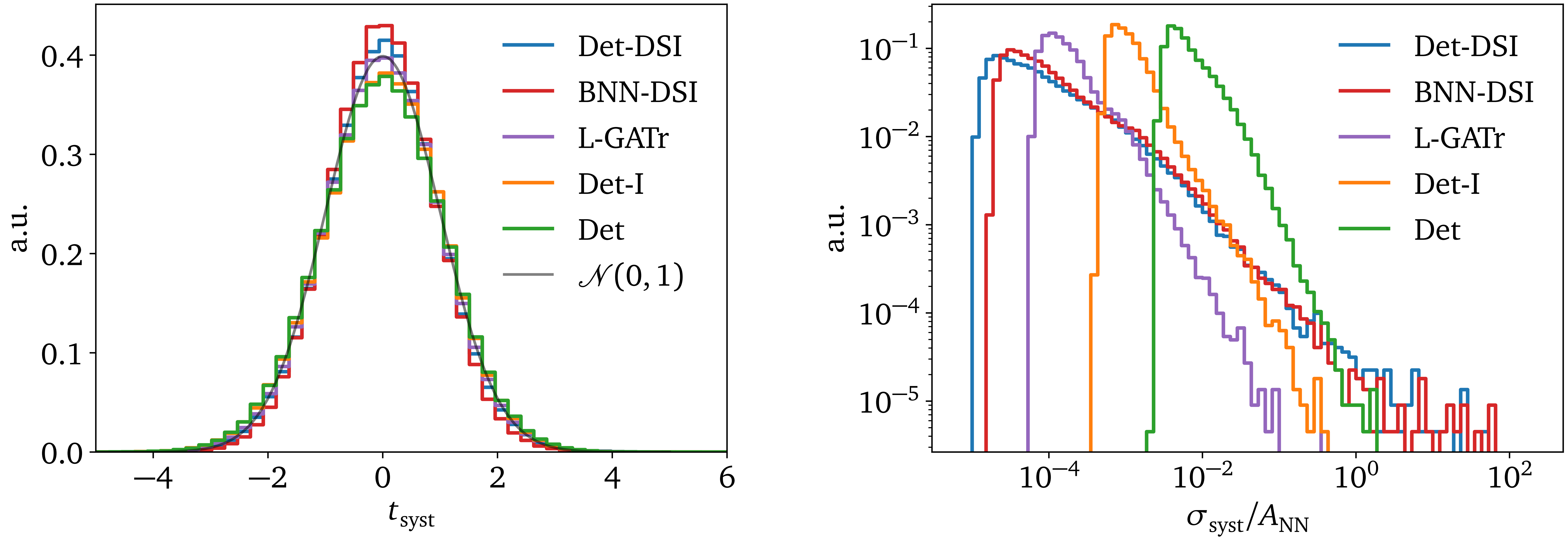

➡**Calibrated uncertainty** with **precision** on 10^{-5} level

➡**Data preprocessing** gain improvement in intrinsic uncertainties

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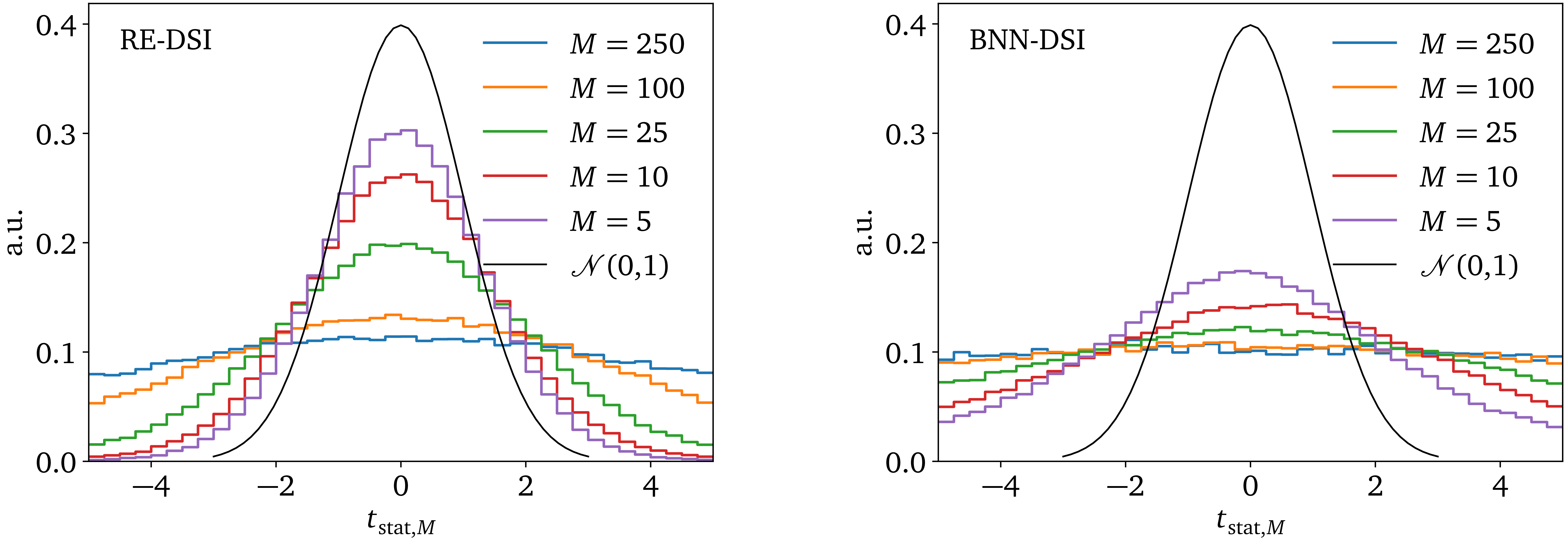
Part III: **Statistical uncertainties**

Scaled statistical pull



- Use N=512 samples for BNN and RE
- Evaluate scaled pull for subset M
- M→N: correlation increases, $\sigma_{\mathrm{stat,M}} \to \sigma_{\mathrm{stat}}$

Reducing the training size

- Systematic uncertainty dominant over statsitical
- Training on 700000 phase space points: $\sigma_{\mathrm{tot}}(x) \approx \sigma_{\mathrm{syst}}(x) \gg \sigma_{\mathrm{stat}}(x)$
- Reducing training data to 100000 phase space points

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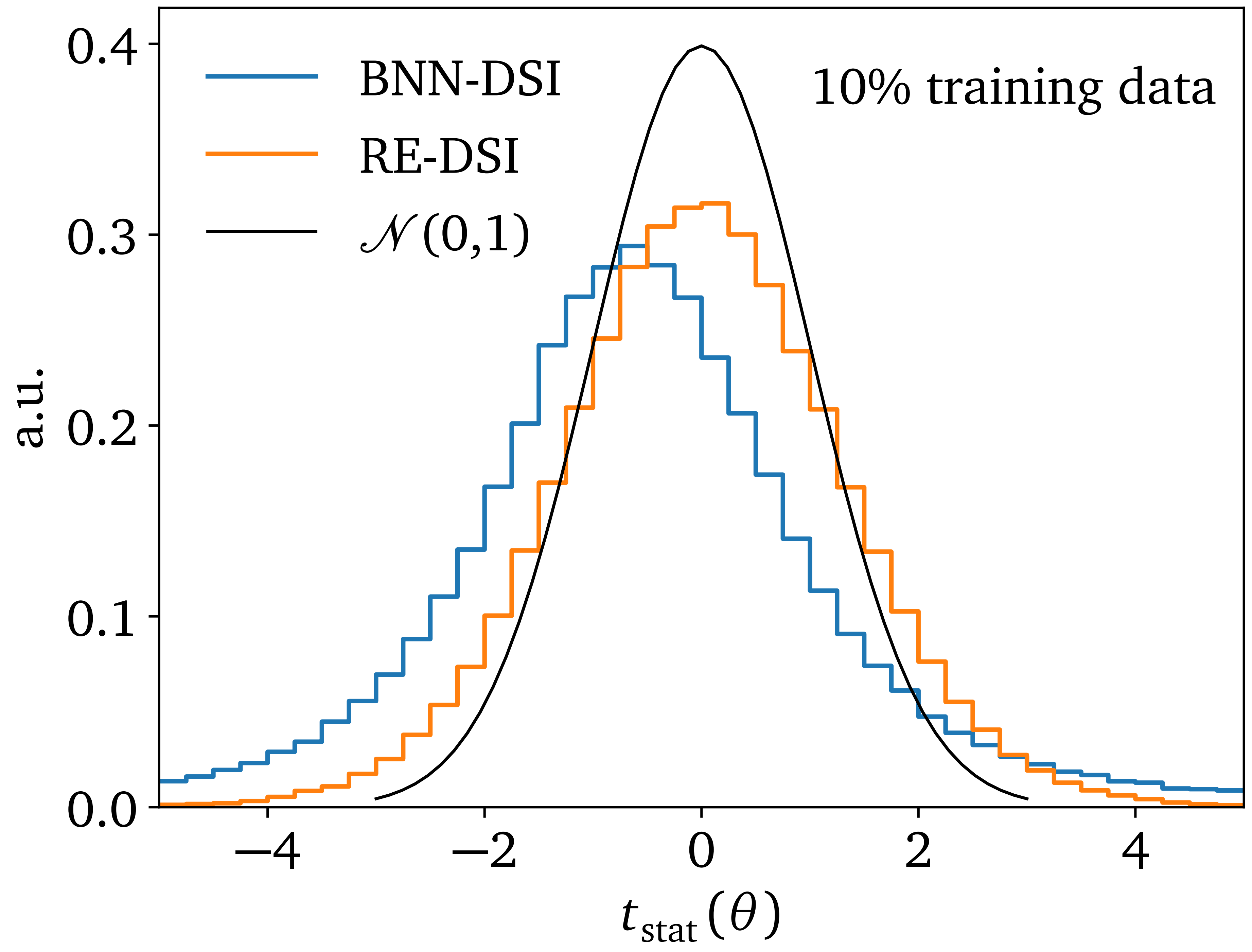
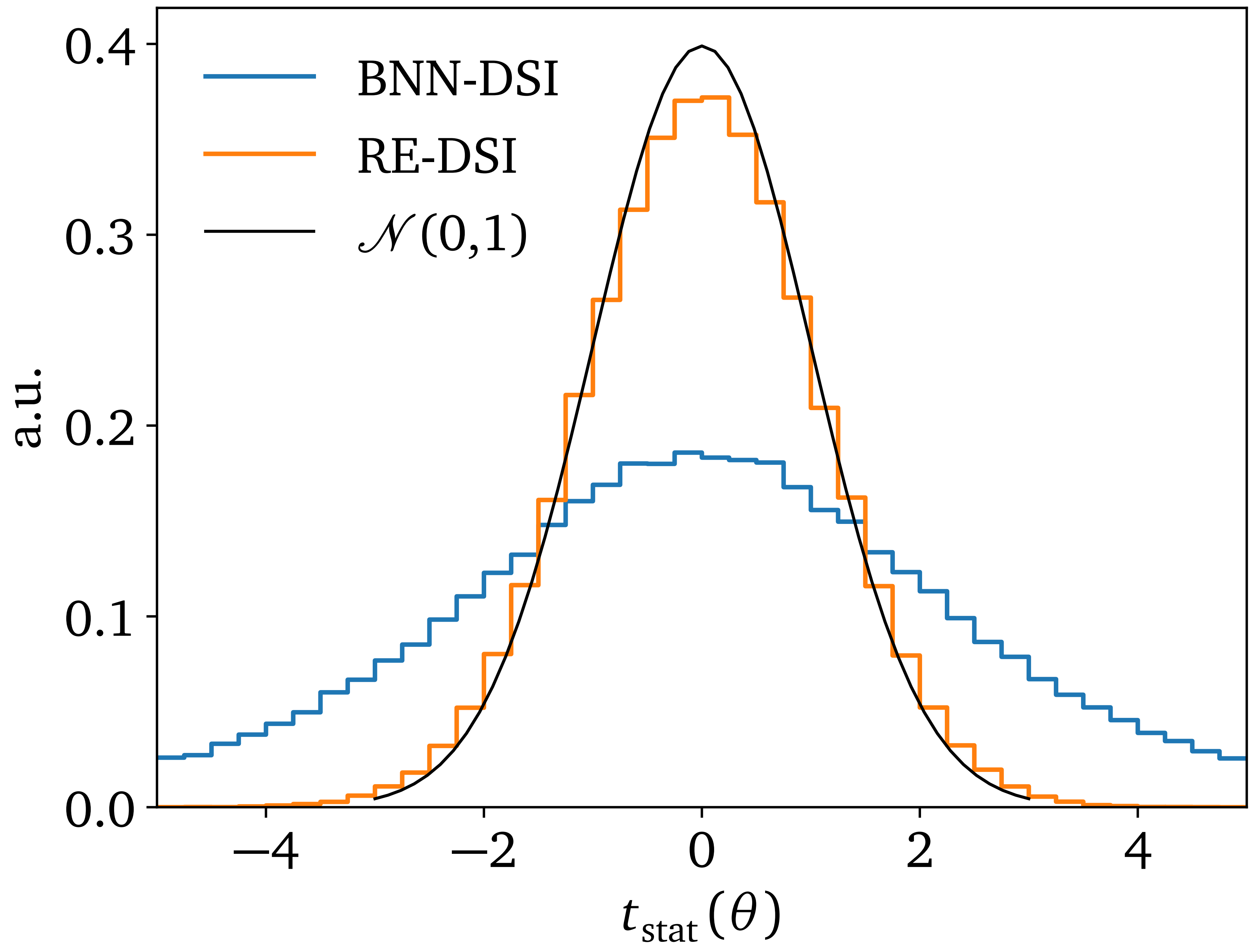
	70%	10%
$\langle \sigma_{\text{syst, BNN-DSI}}/A \rangle$	$8.7 \cdot 10^{-5}$	$2.5 \cdot 10^{-4}$
$\langle \sigma_{\text{stat, BNN-DSI}}/A \rangle$	$3.6 \cdot 10^{-5}$	$1.5 \cdot 10^{-4}$
$\langle \sigma_{\text{syst, RE-DSI}}/A \rangle$	$5.1 \cdot 10^{-5}$	$2.9 \cdot 10^{-4}$
$\langle \sigma_{\text{stat, RE-DSI}}/A \rangle$	$4.8 \cdot 10^{-5}$	$2.2 \cdot 10^{-4}$

Dependence on training size





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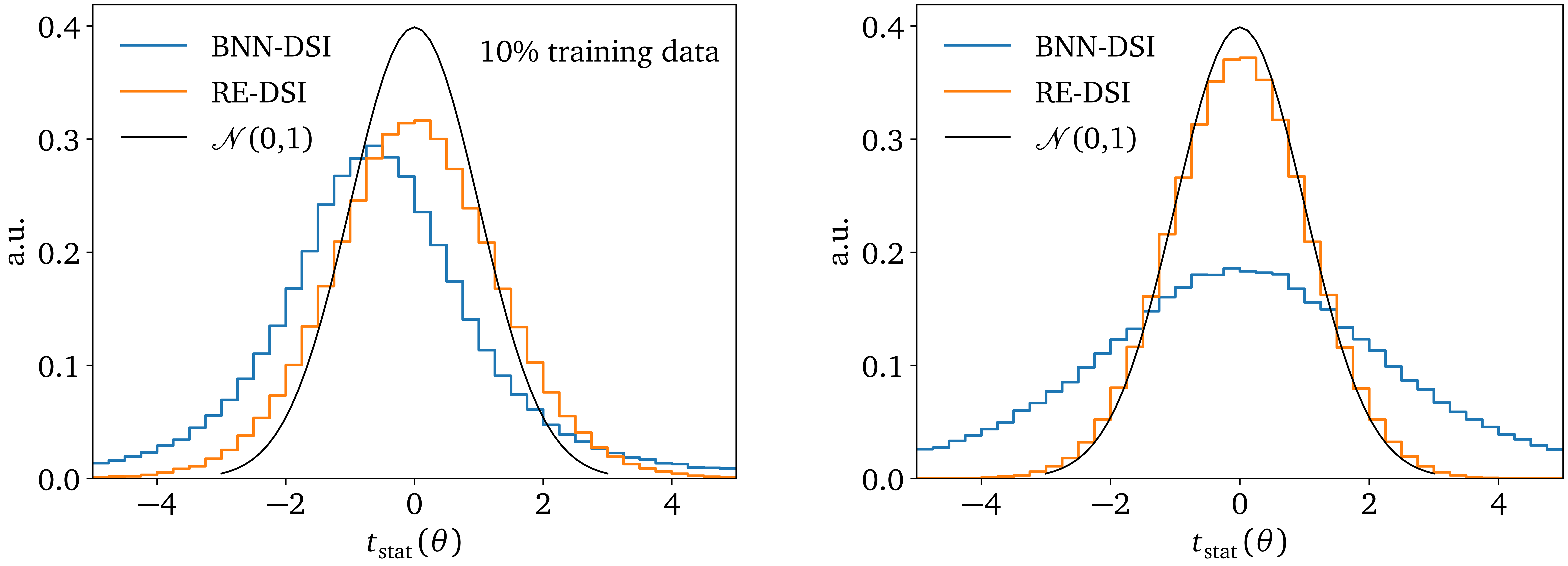
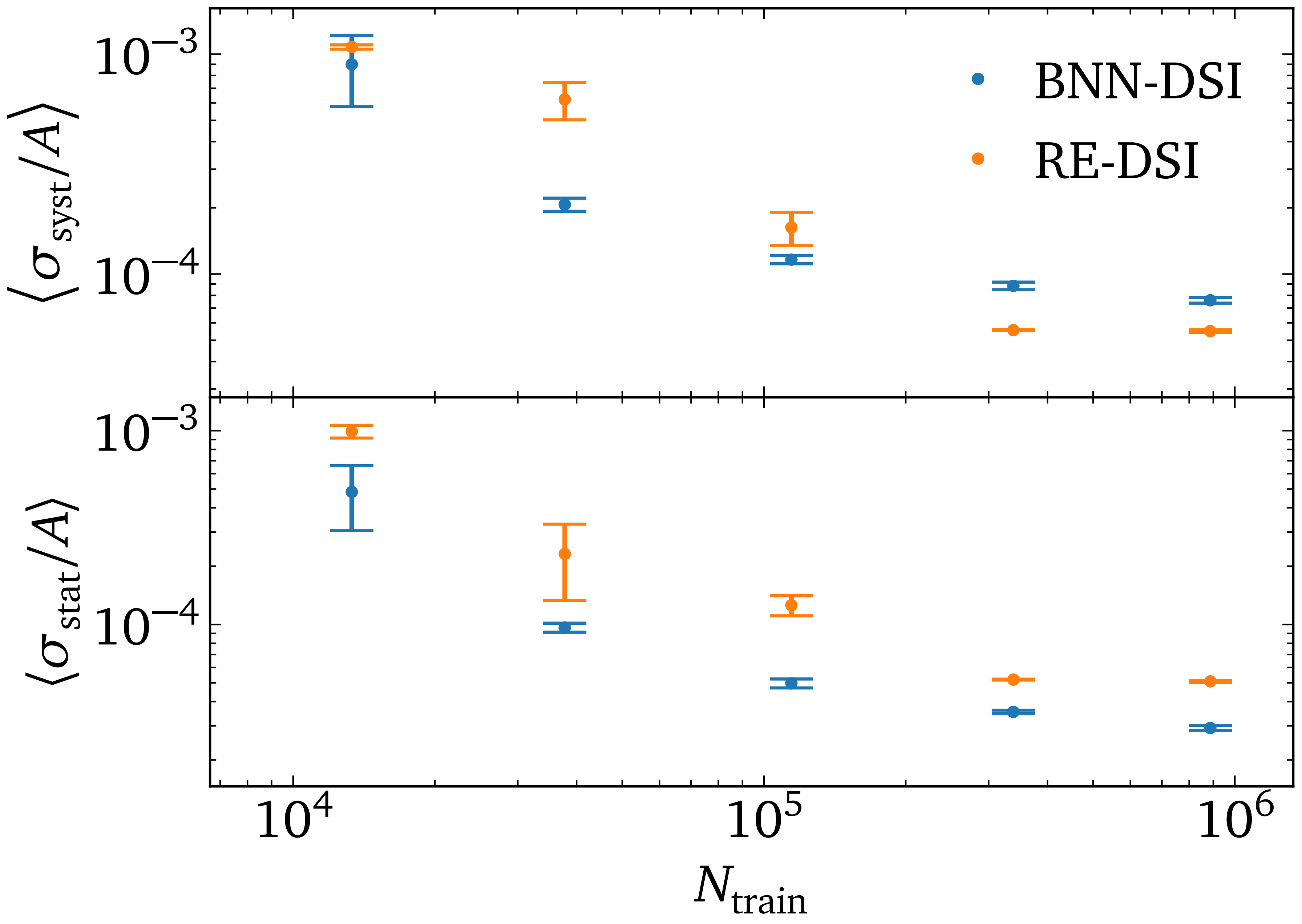


- Repulsive ensemble advantage in statistical uncertainty

Relative uncertainty vs training size



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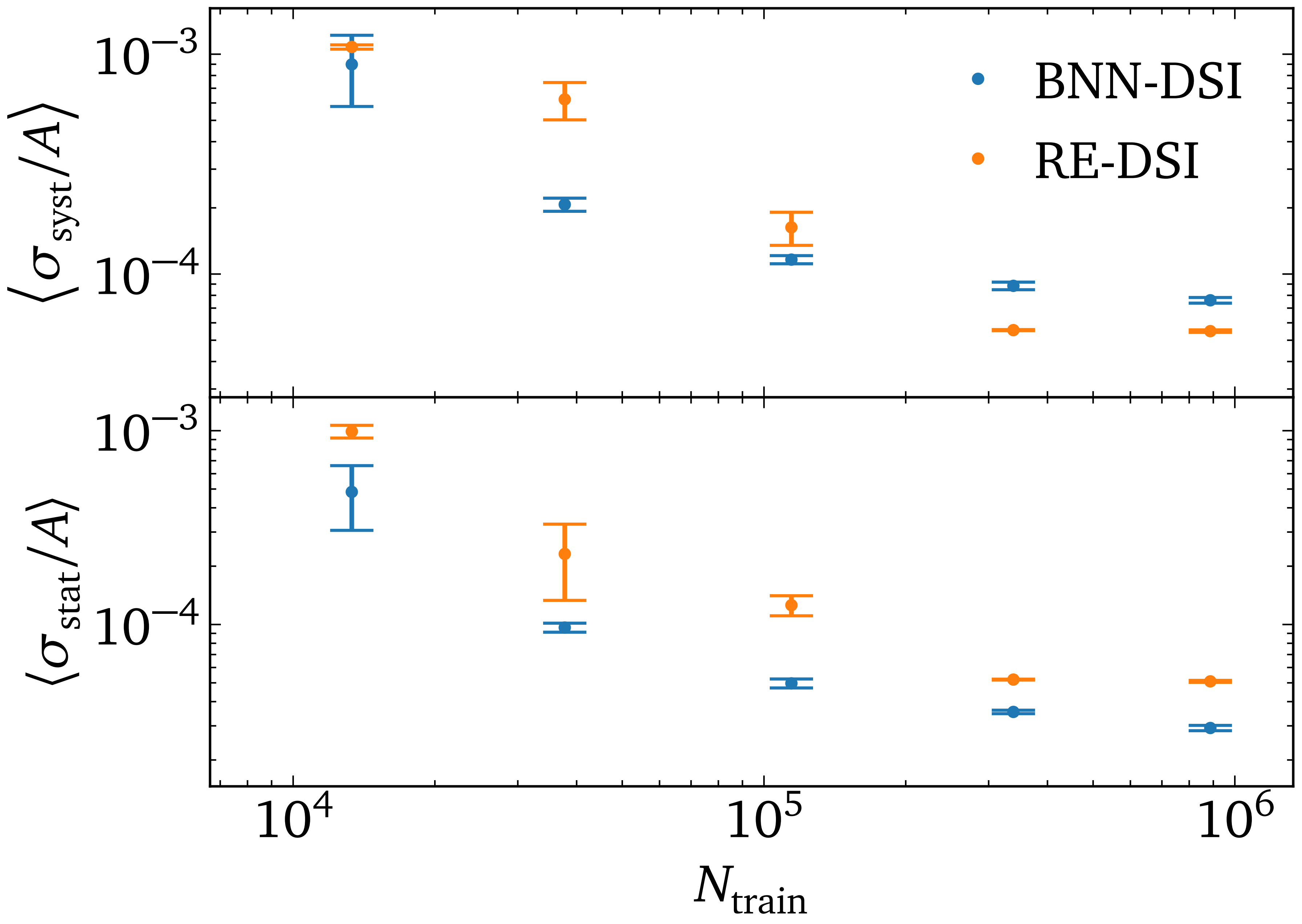
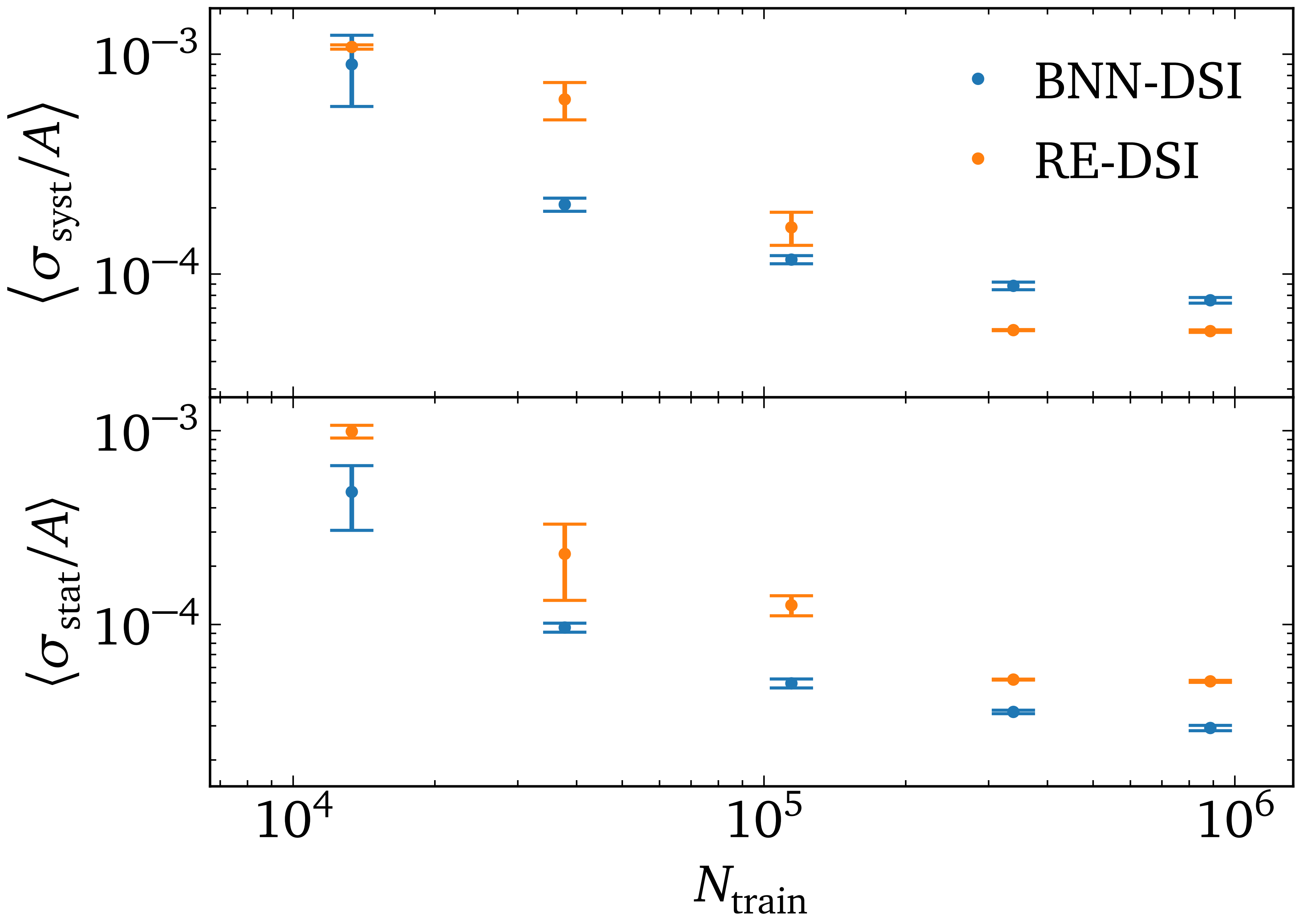
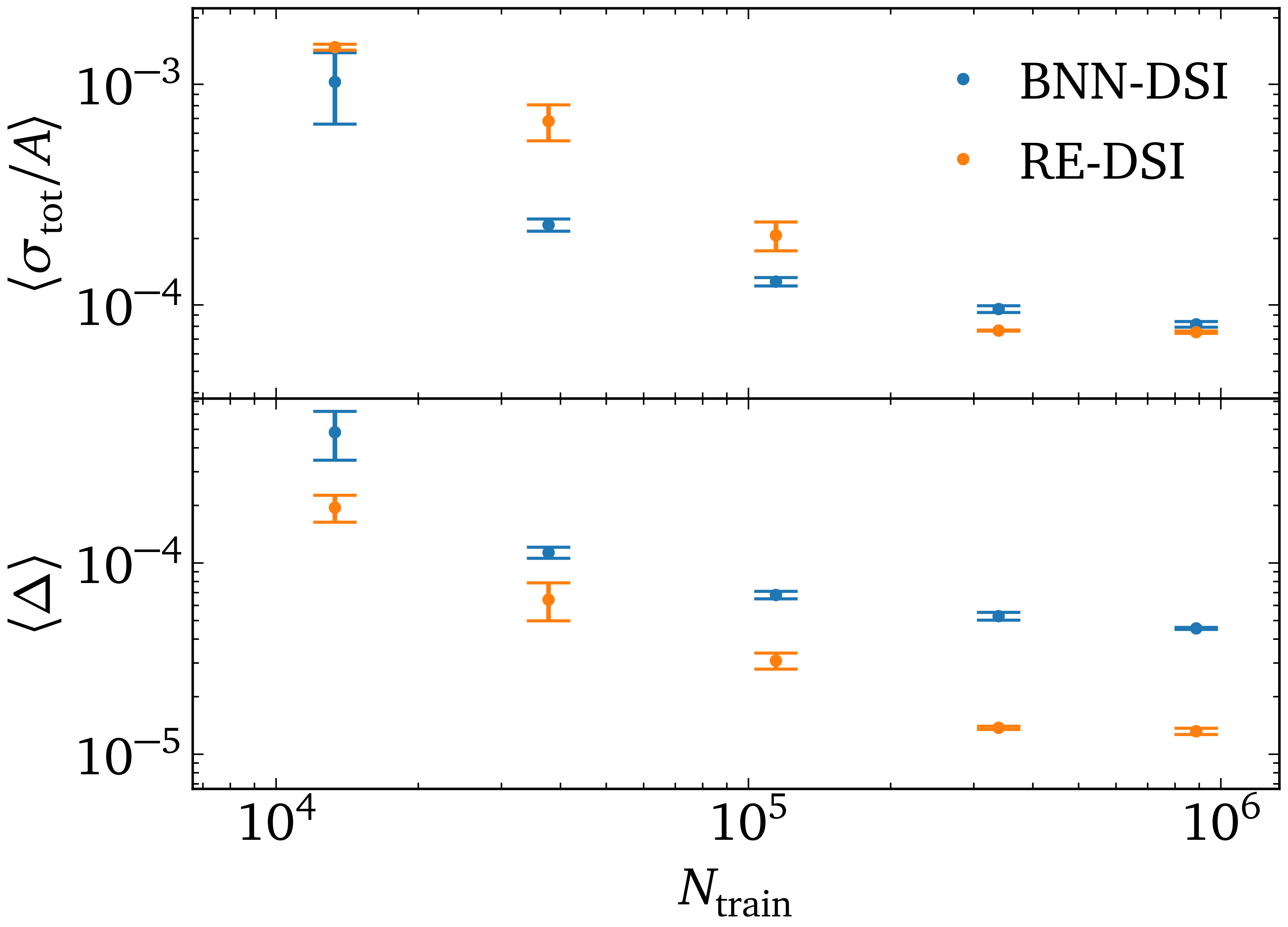


➡σ_{syst} always larger

➡σ larger for RE-DSI than BNN-DSI

Relative uncertainty vs training size





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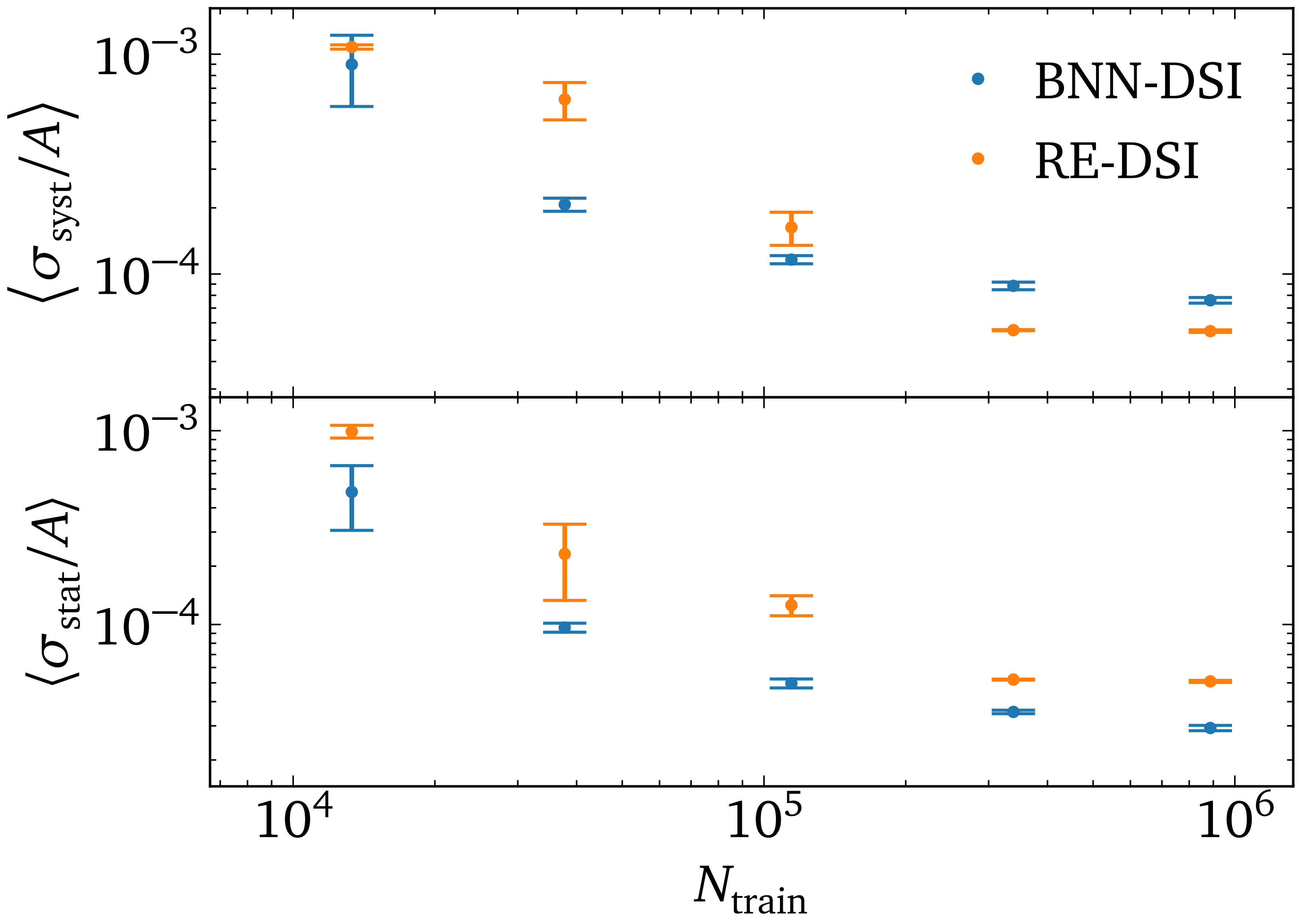

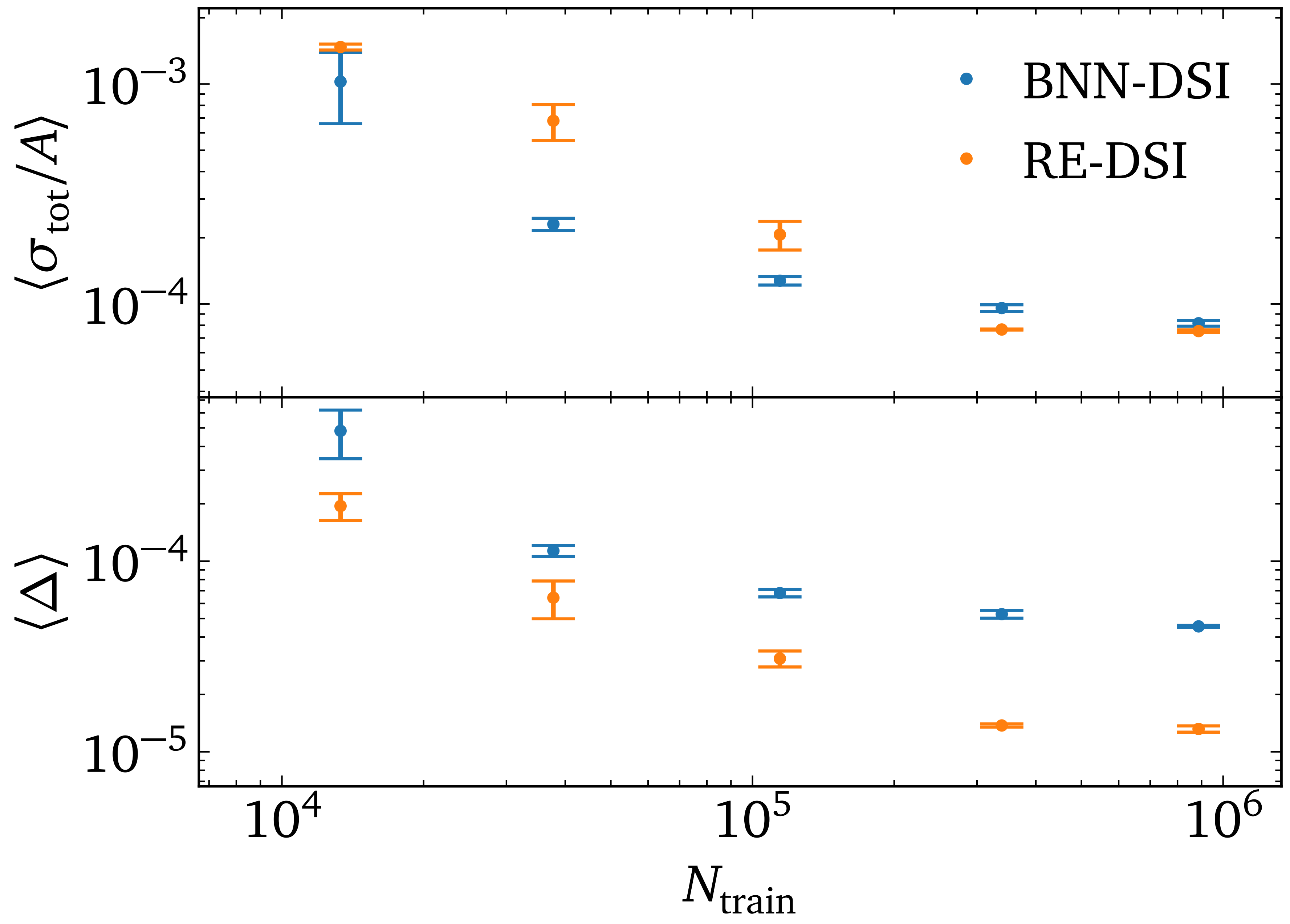

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➡σ larger for RE-DSI than BNN-DSI

➡Difference in σ_{tot} for small data

➡RE-DSI more accurate in prediction

Conclusion

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Thank you for your attention!