Accuracy and uncertainty control for ML-Amplitudes

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

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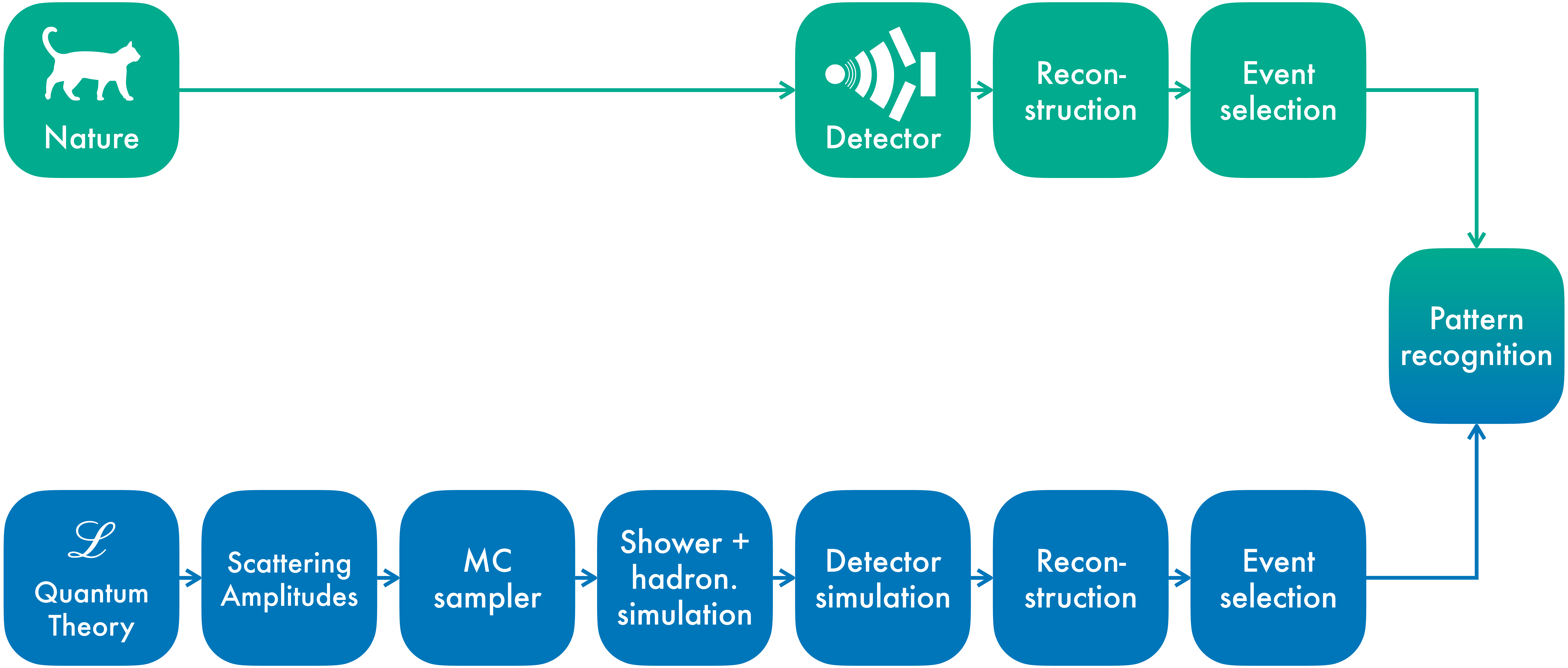
IMPRS
for Precision Tests of Fundamental Symmetries
INTERNATIONAL MAX PLANCK RESEARCH SCHOOL

LHC physics and machine learning



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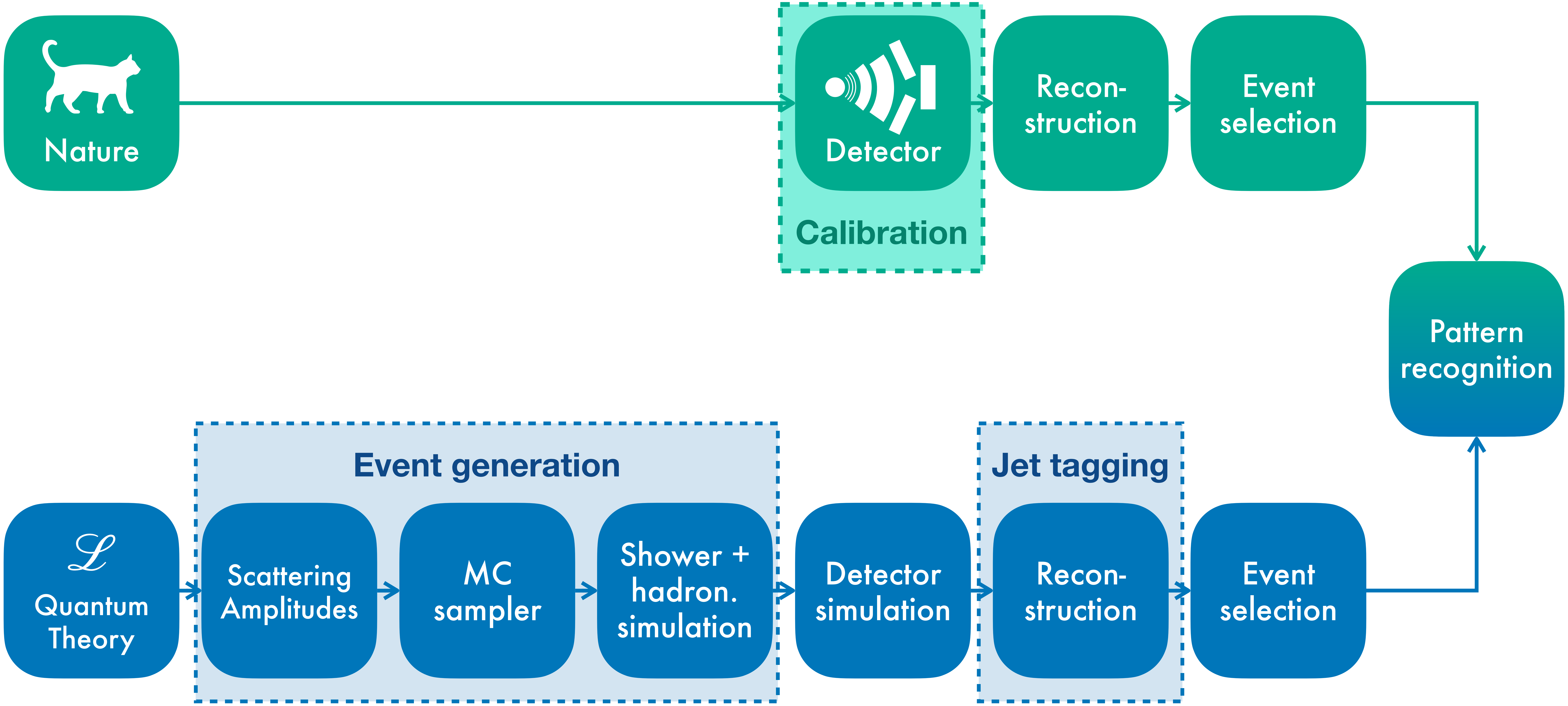

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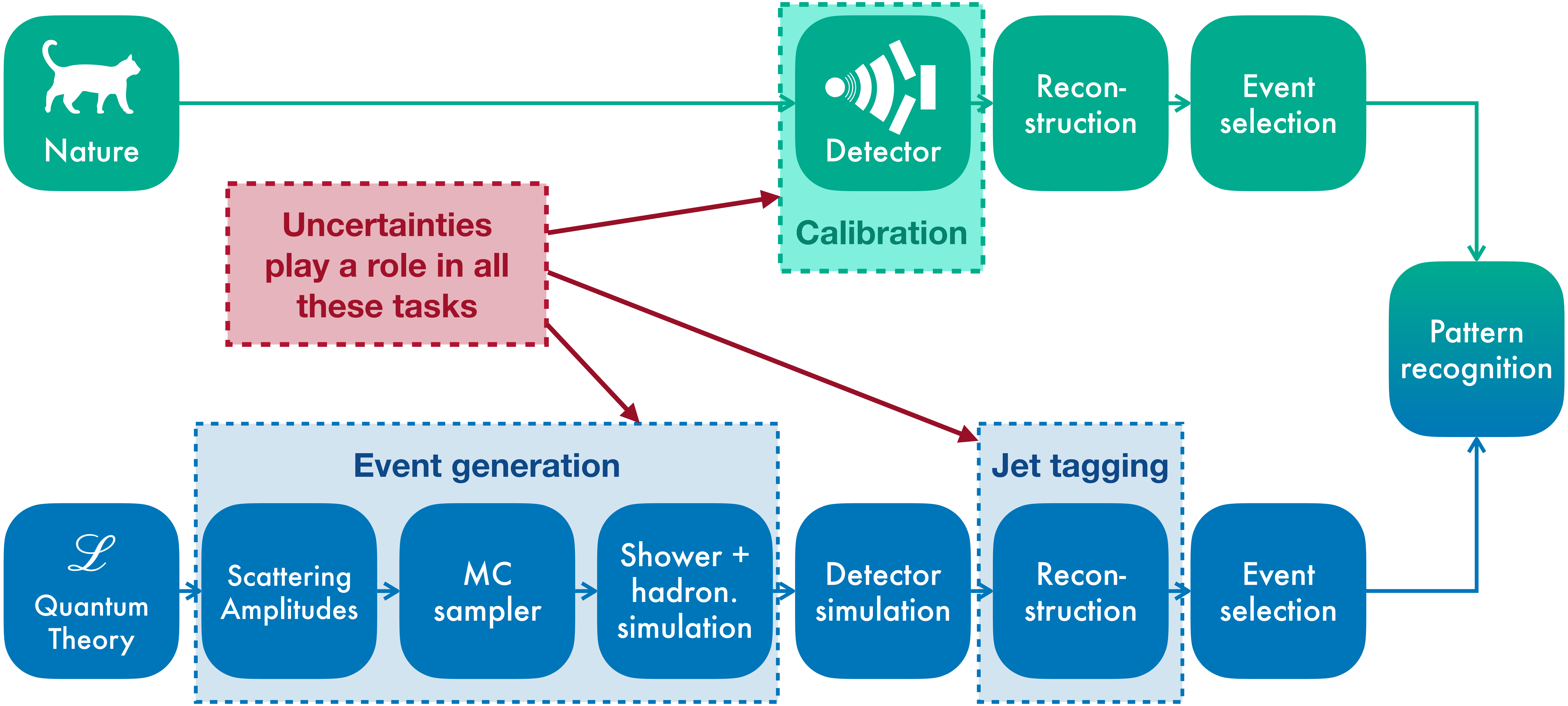

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Motivation

- **Reliable interpolation** of two-loop amplitudes [2412.09534]
  - Scaling up to $Z + 5j$ [2411.00446]
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1. **Faster precision** simulations
2. **Control** through calibrated uncertainties

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- Two types of uncertainties:
  - **Systematic**: Plateaus for perfect training (epistemic uncertainty)
  - **Statistical**: Vanishes for perfect training (aleatoric uncertainty)

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

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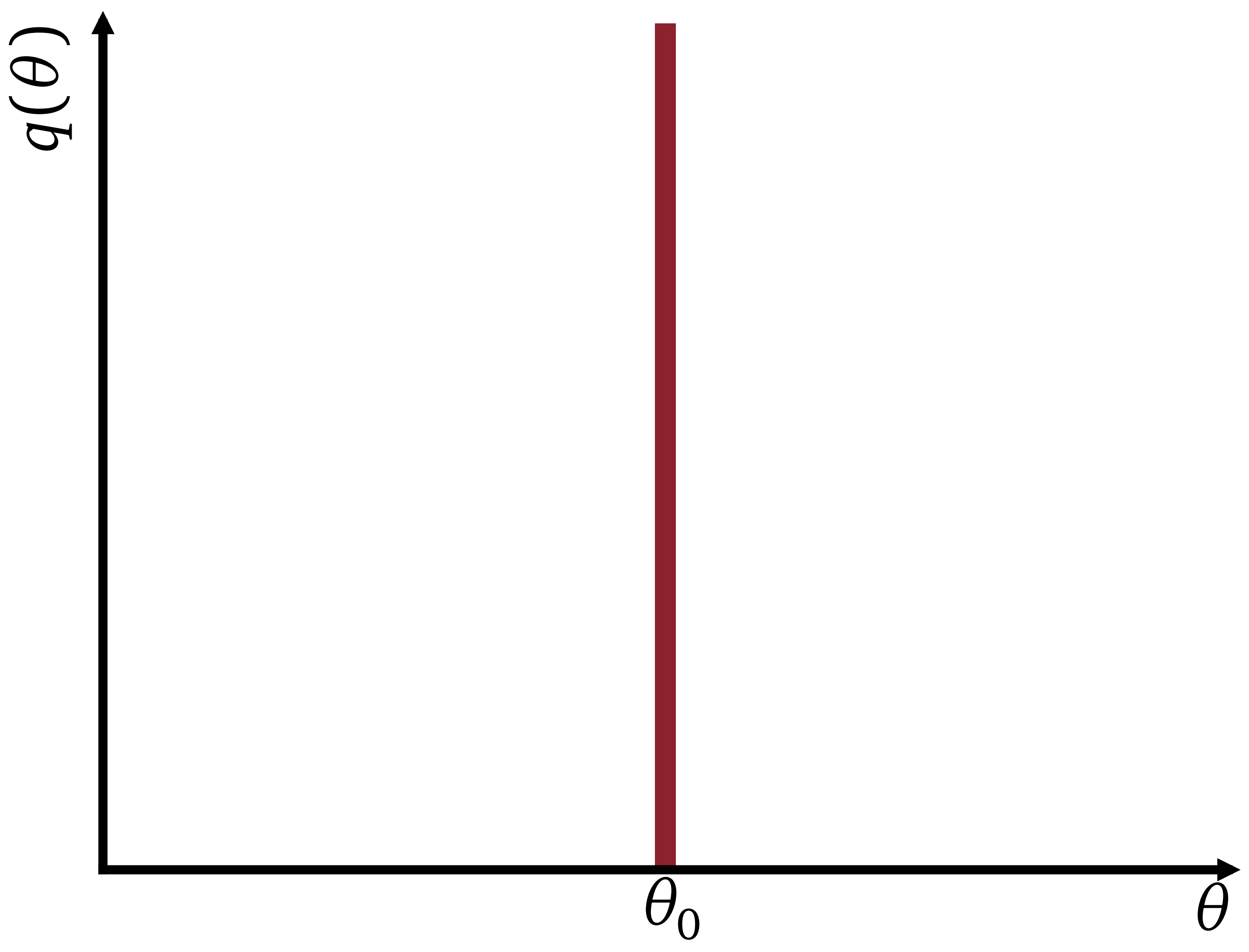
Bayesian neural networks (BNNs)

Neural network



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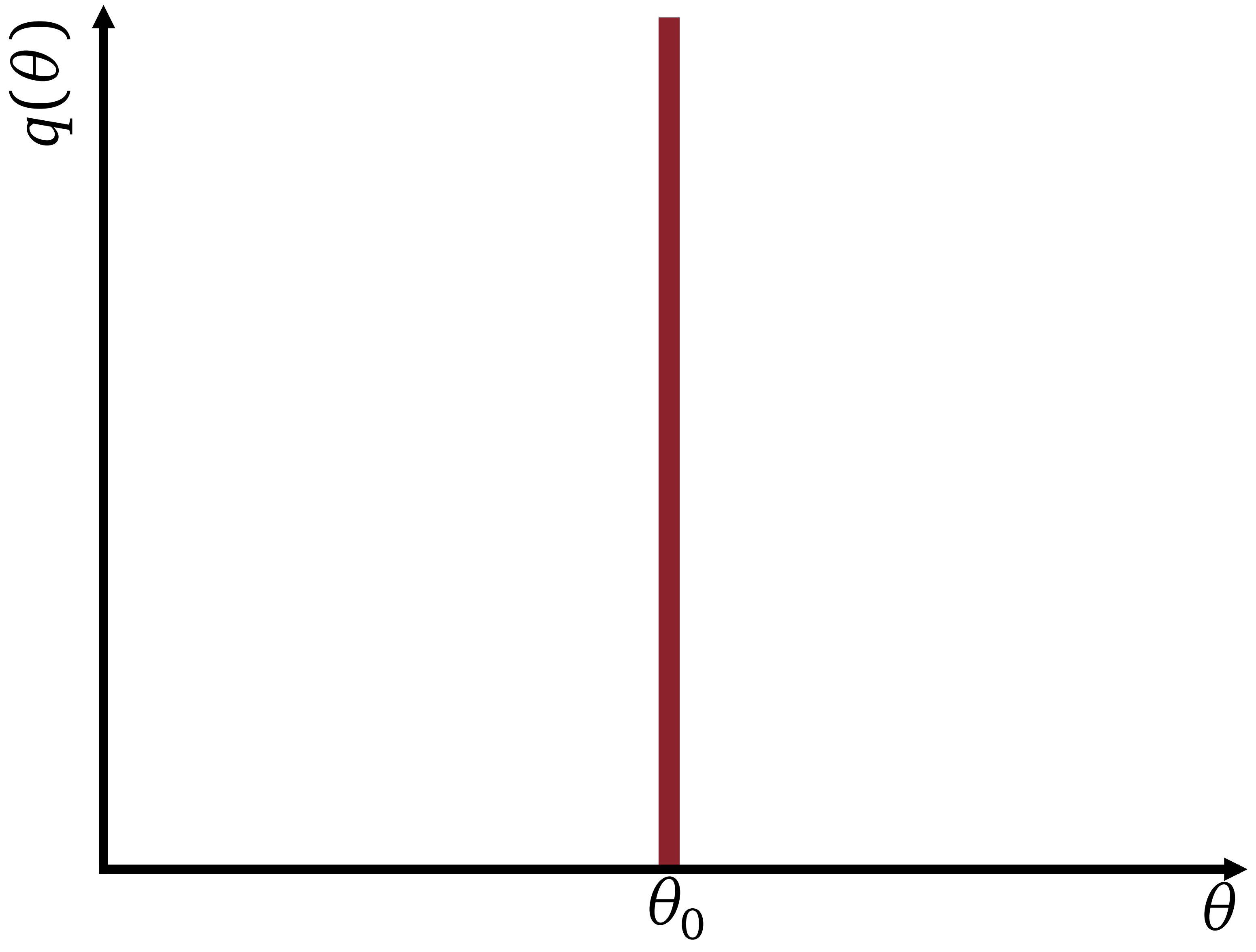

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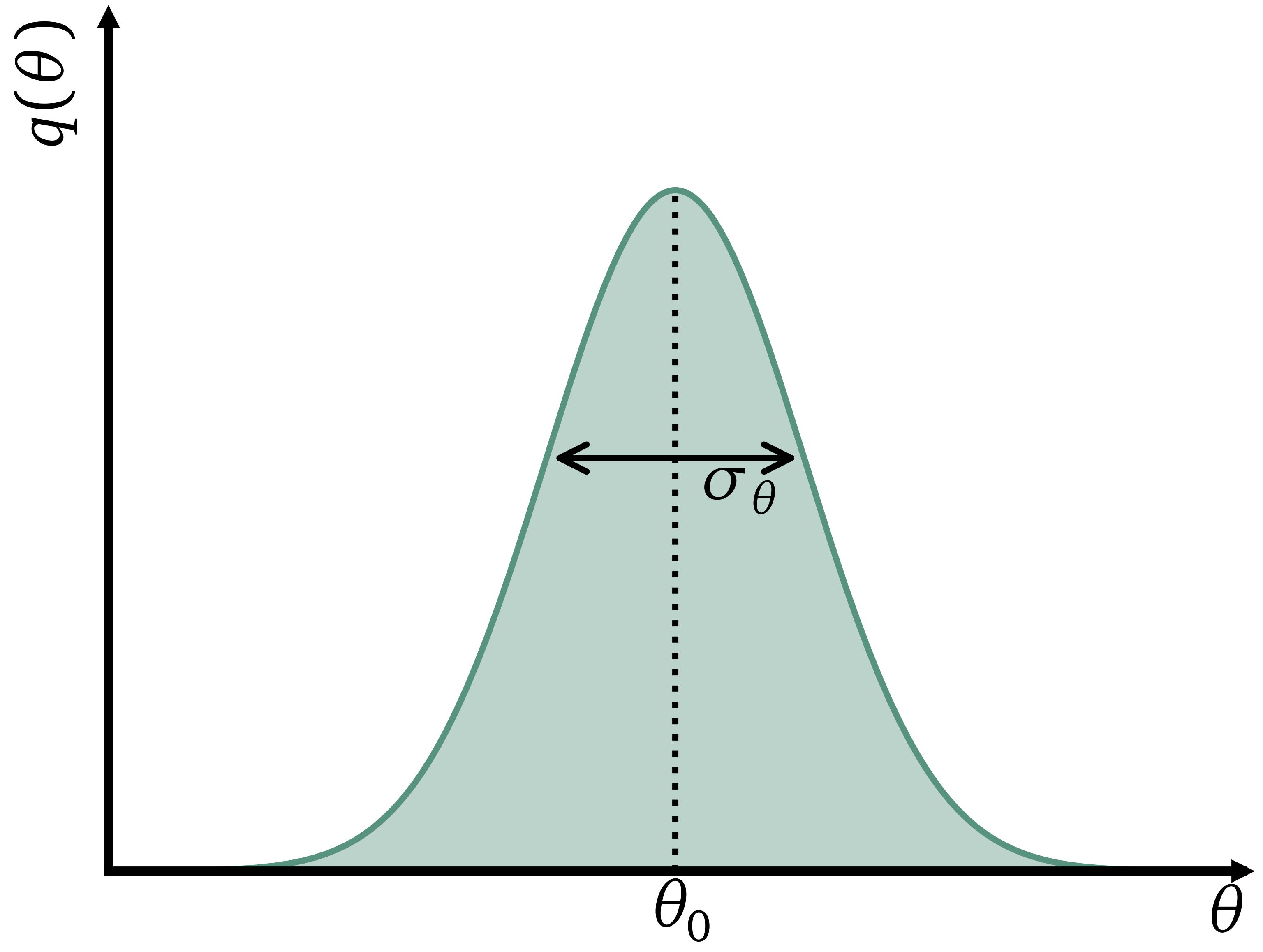
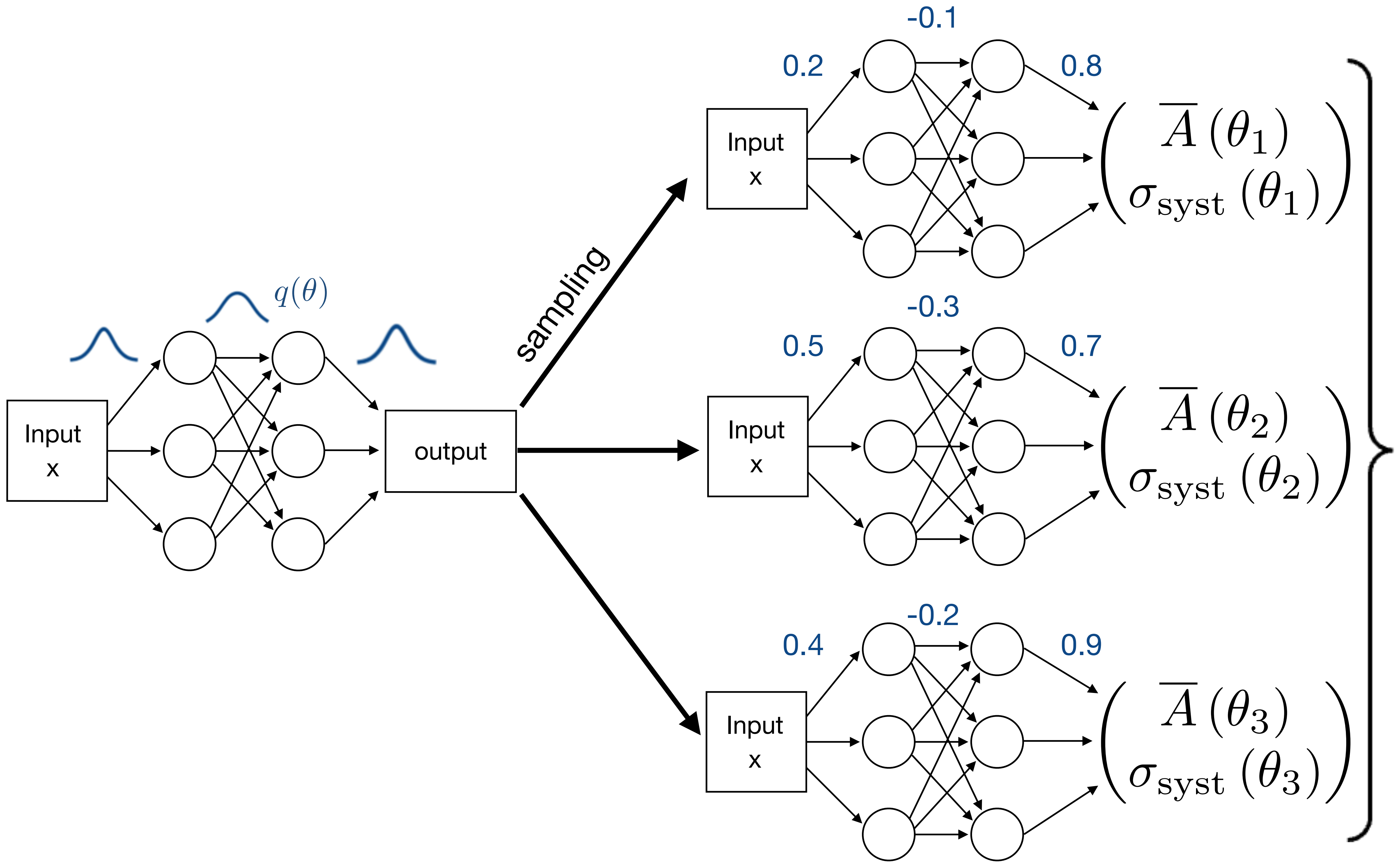


Network weights are drawn from distribution

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

Bayesian neural networks (BNNs)

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



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

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$$\sigma^2_{\text{stat}} = \frac{1}{N} \sum_i^N \left(\langle A \rangle - \overline{A}\,(\theta_i)\right)^2$$

- Parameters: **Network weights** $q(\theta)$
- $q(\theta)$: Params of a Gaussian
- Ensemble: **Sample** $q(\theta)$

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

Repulsive ensembles (REs)

Ensemble of networks

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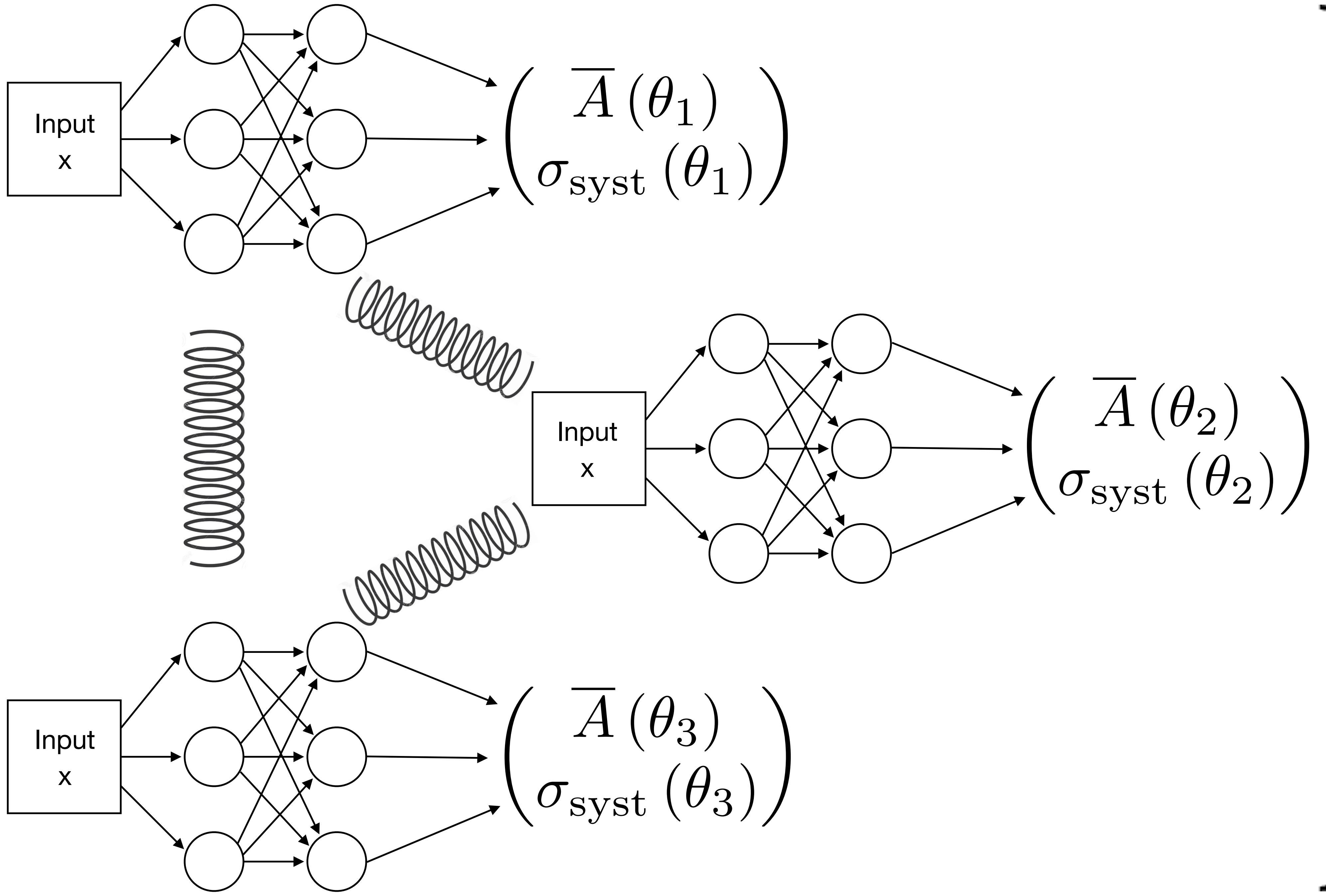

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  Cover **full posterior** distribution
- Members **trained simultaneously**

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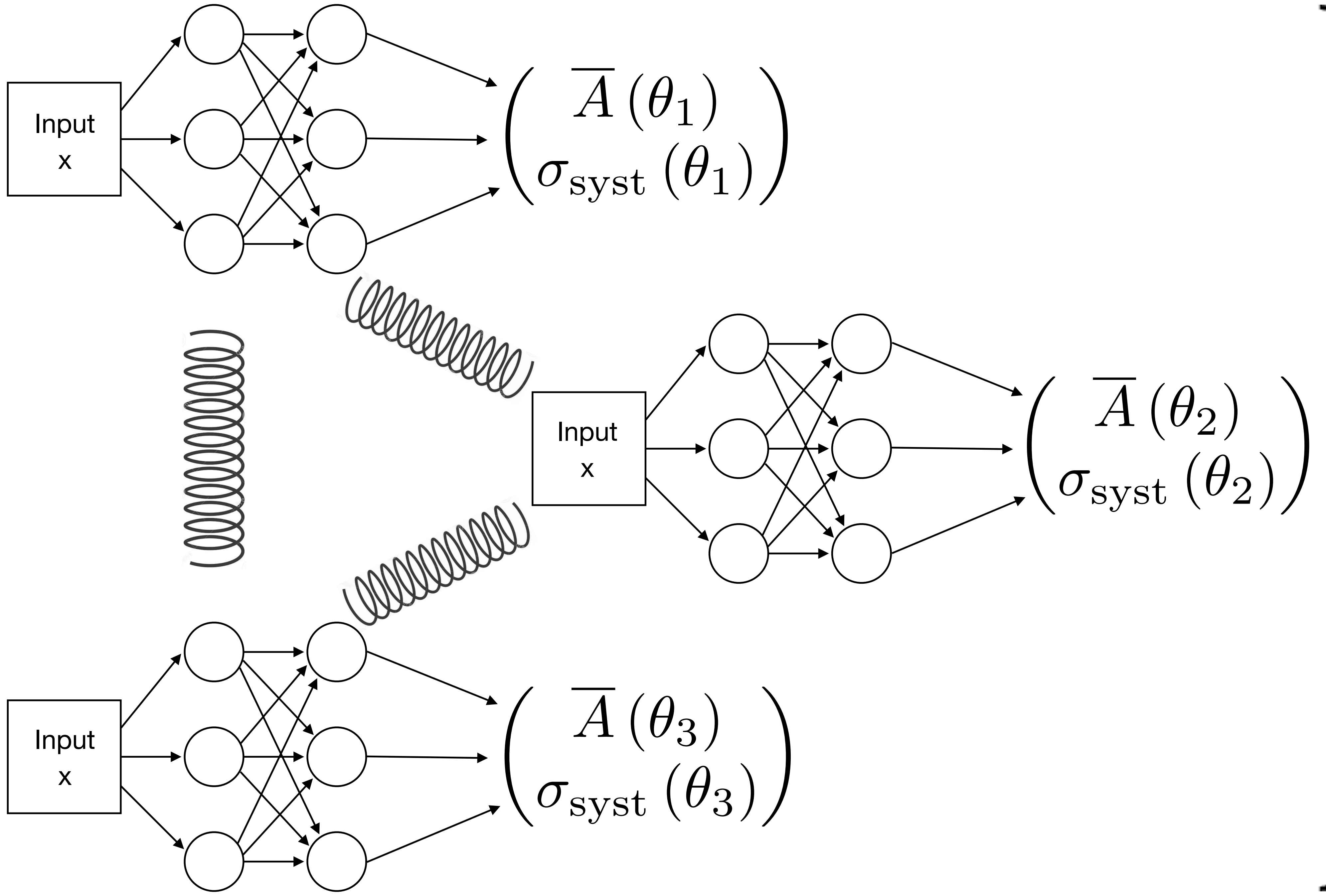

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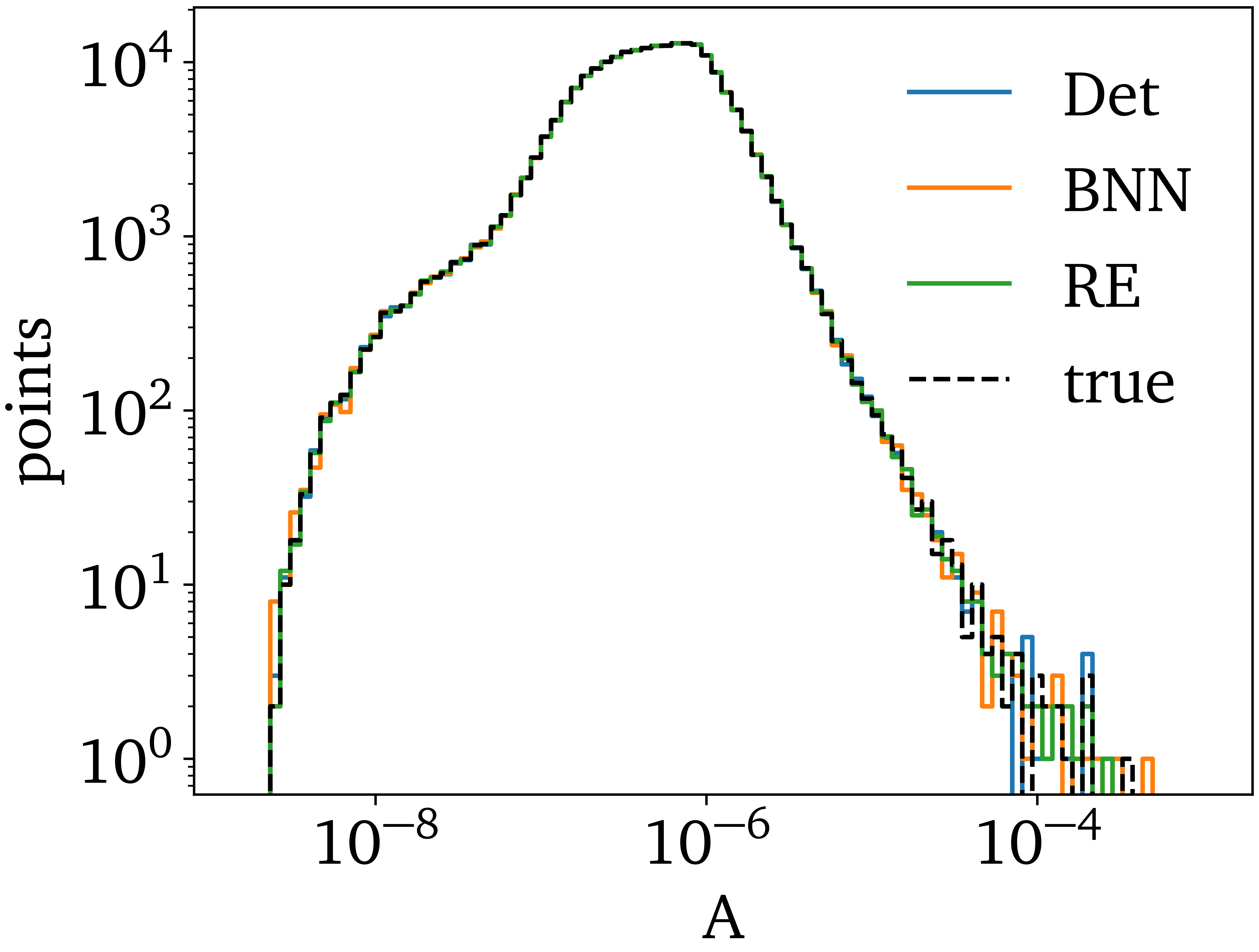

Adding Gaussian noise

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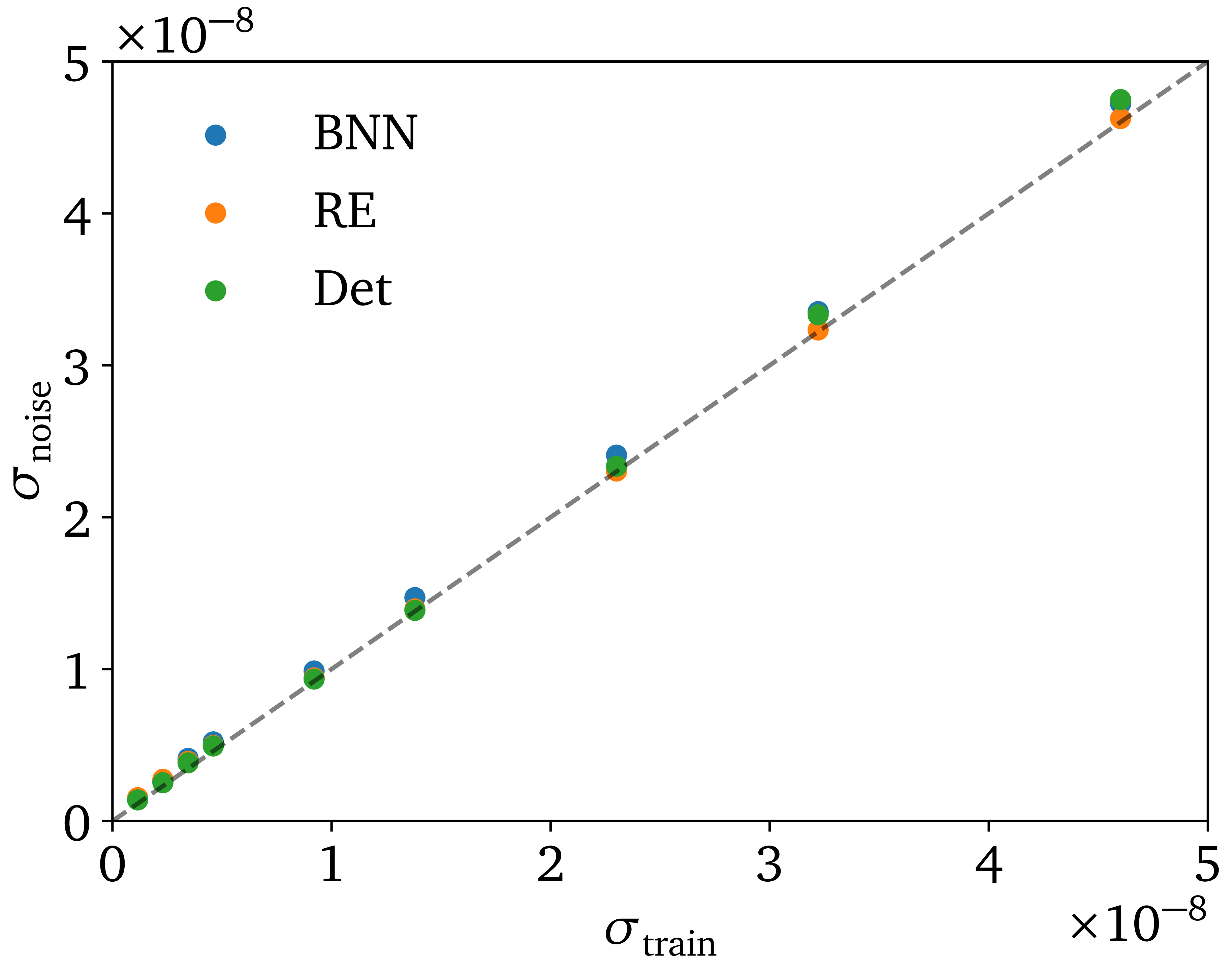

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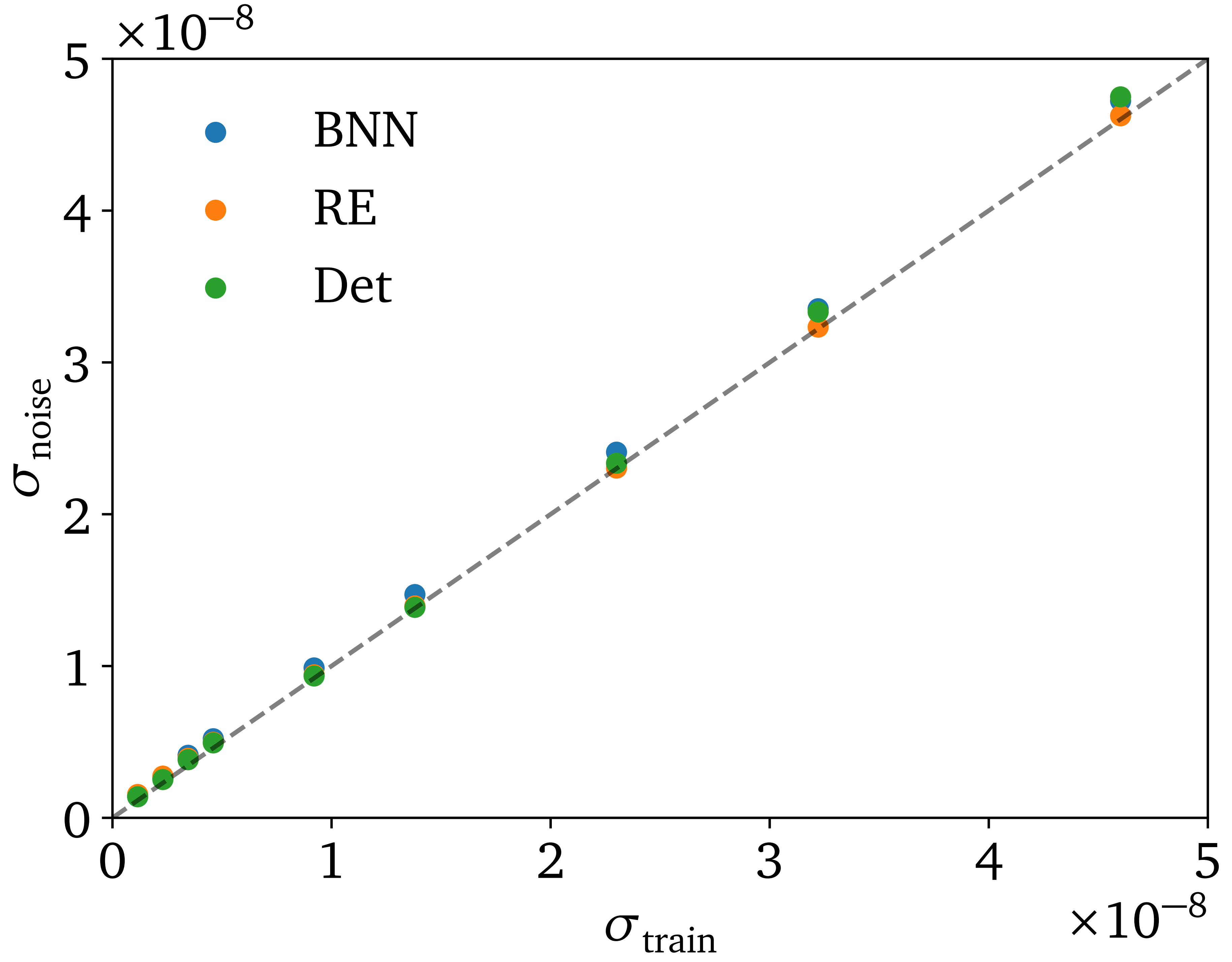

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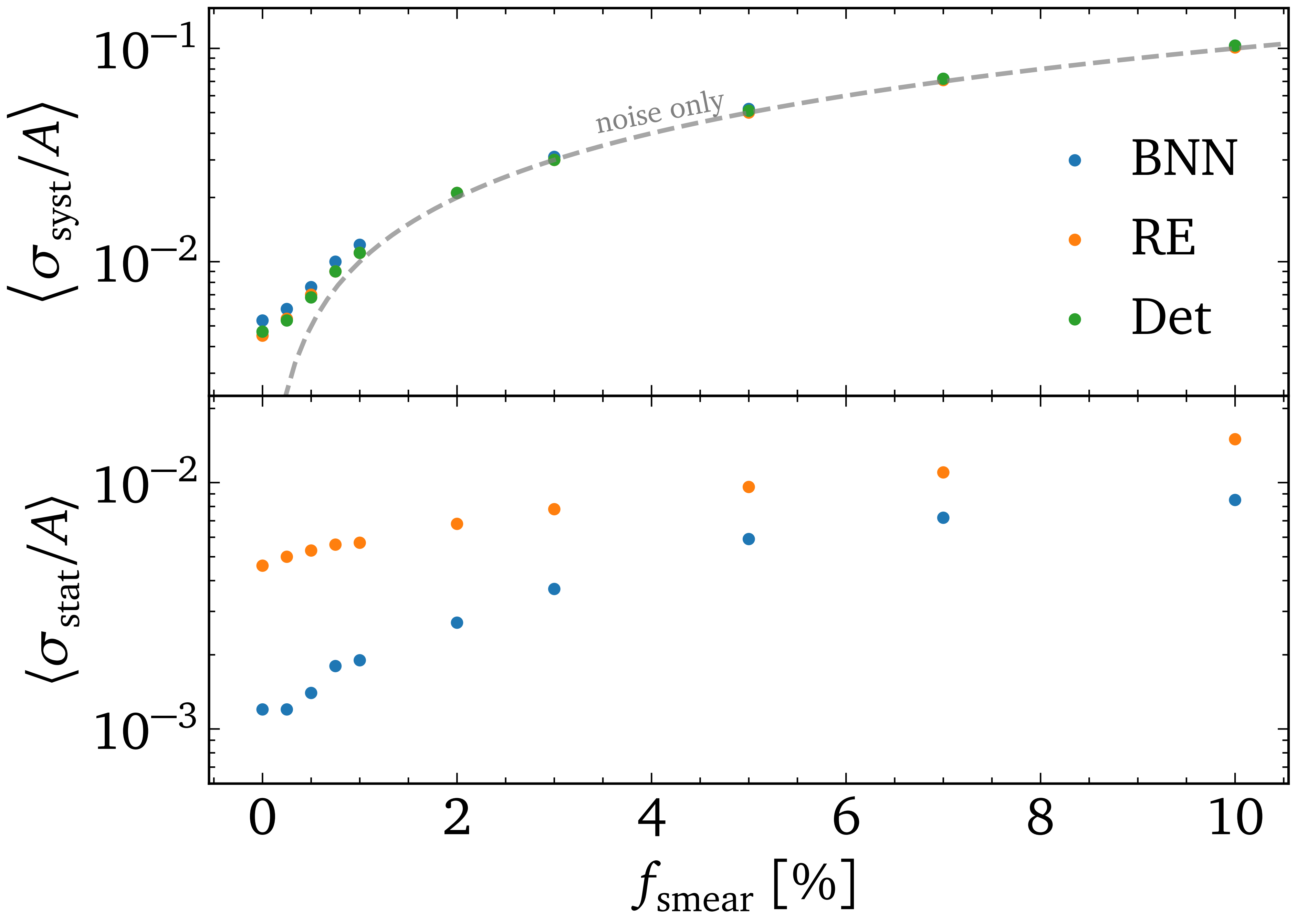

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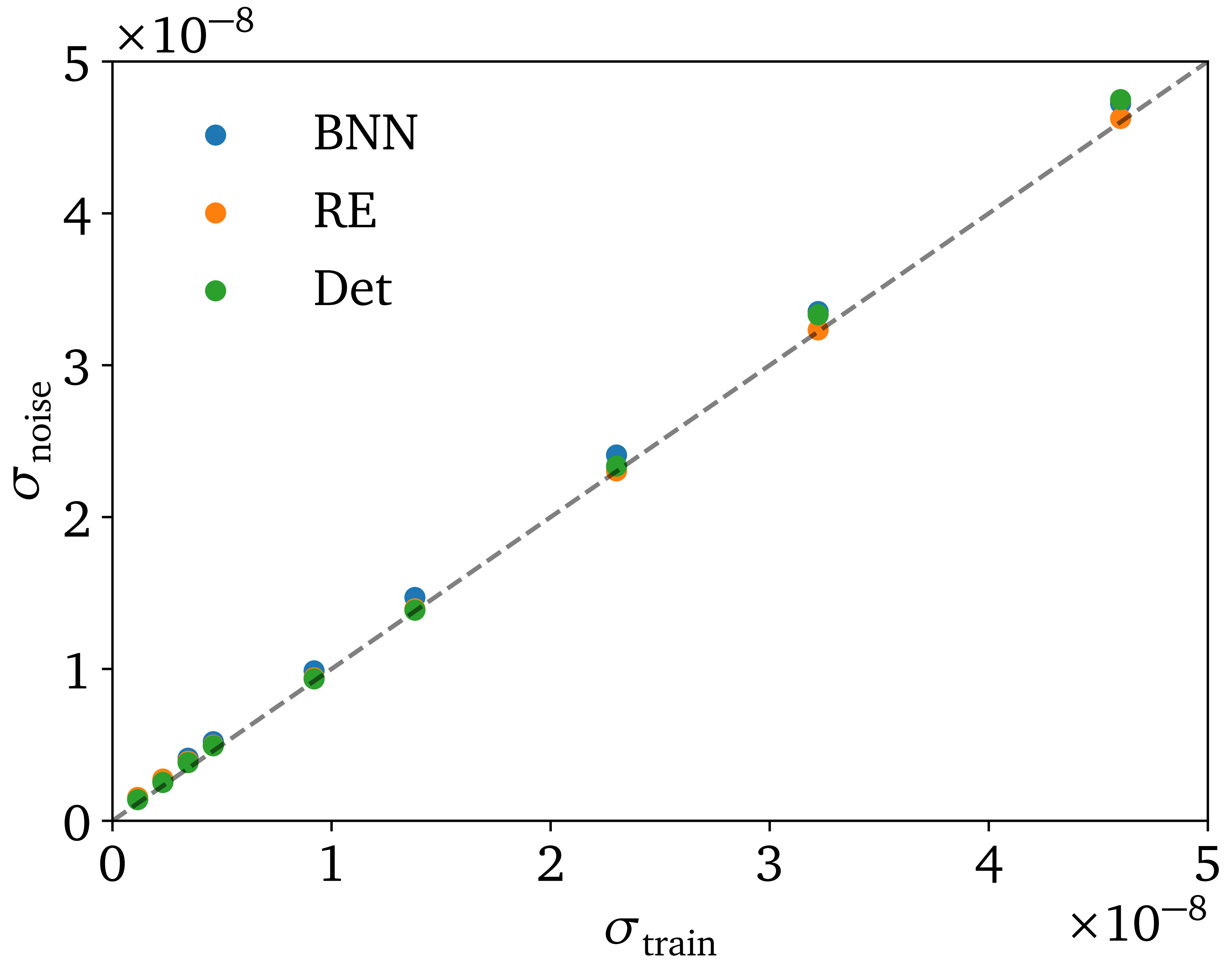
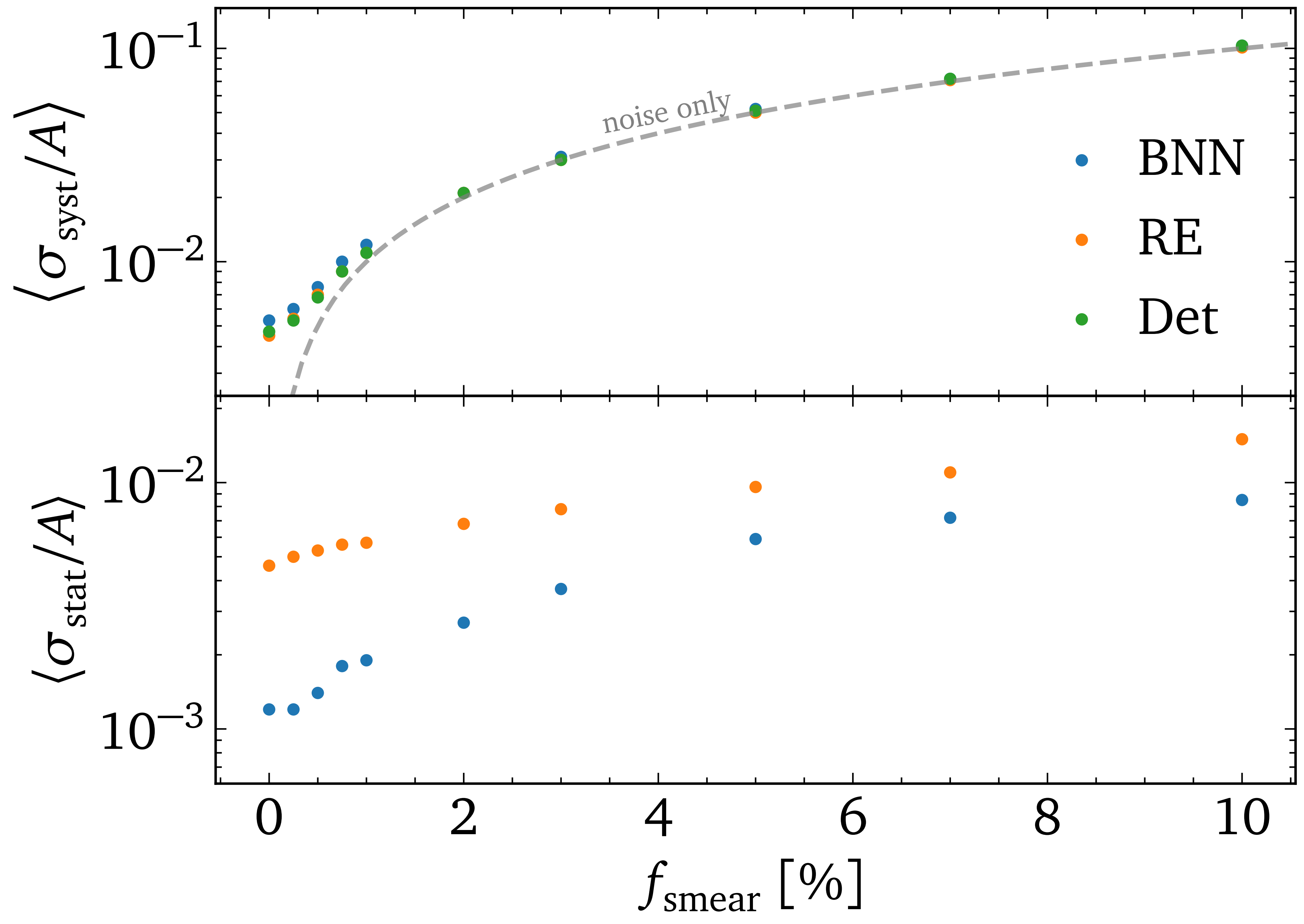
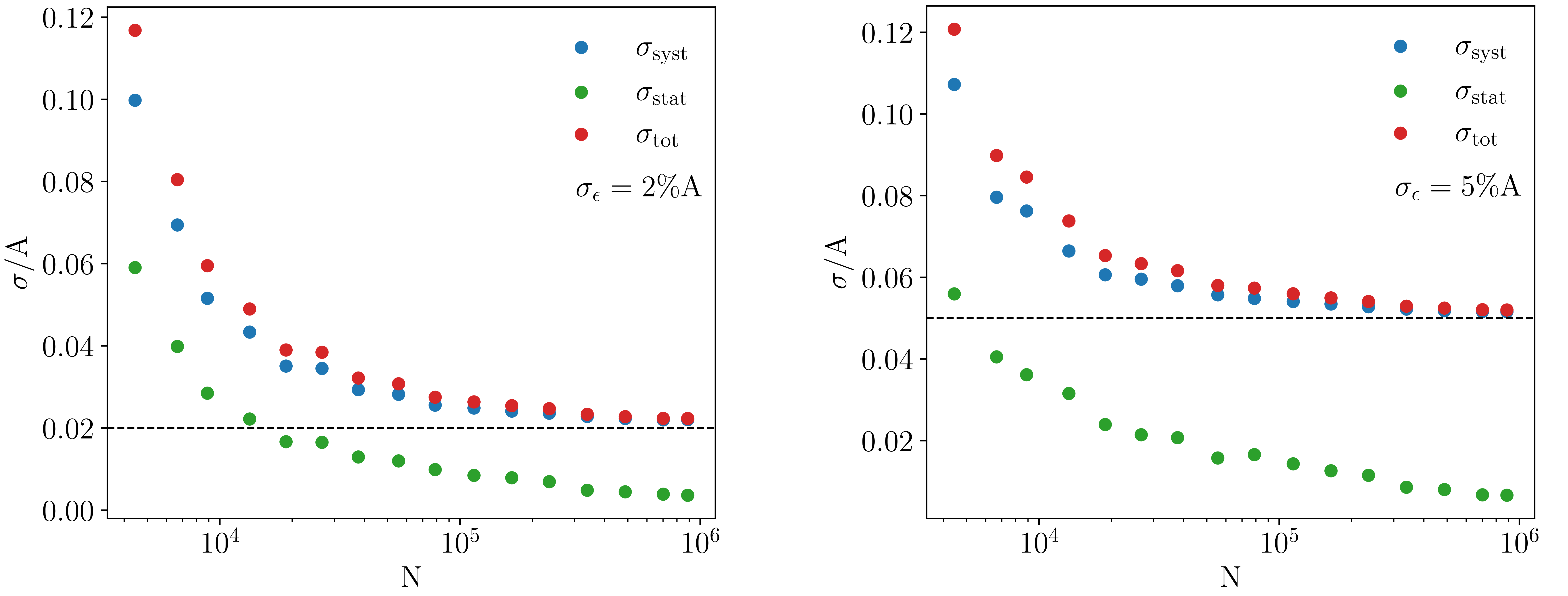




➡ Networks learn noise as **systematic** uncertainty

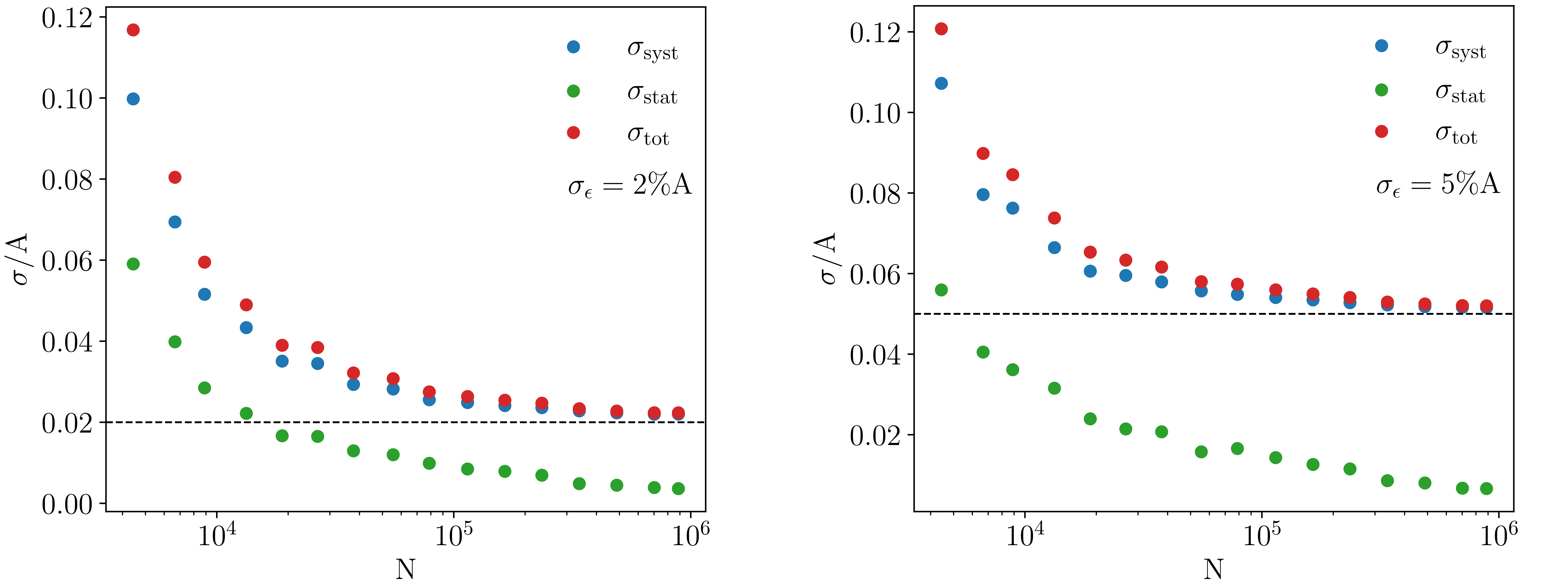
➡**Intrinsic uncertainty** of 0.4%

Uncertainty behavior



BNN only

Uncertainty behavior



BNN only

1. Statistical uncertainty **independent** of noise

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

Calibration of results

Relative deviation

Pull distribution

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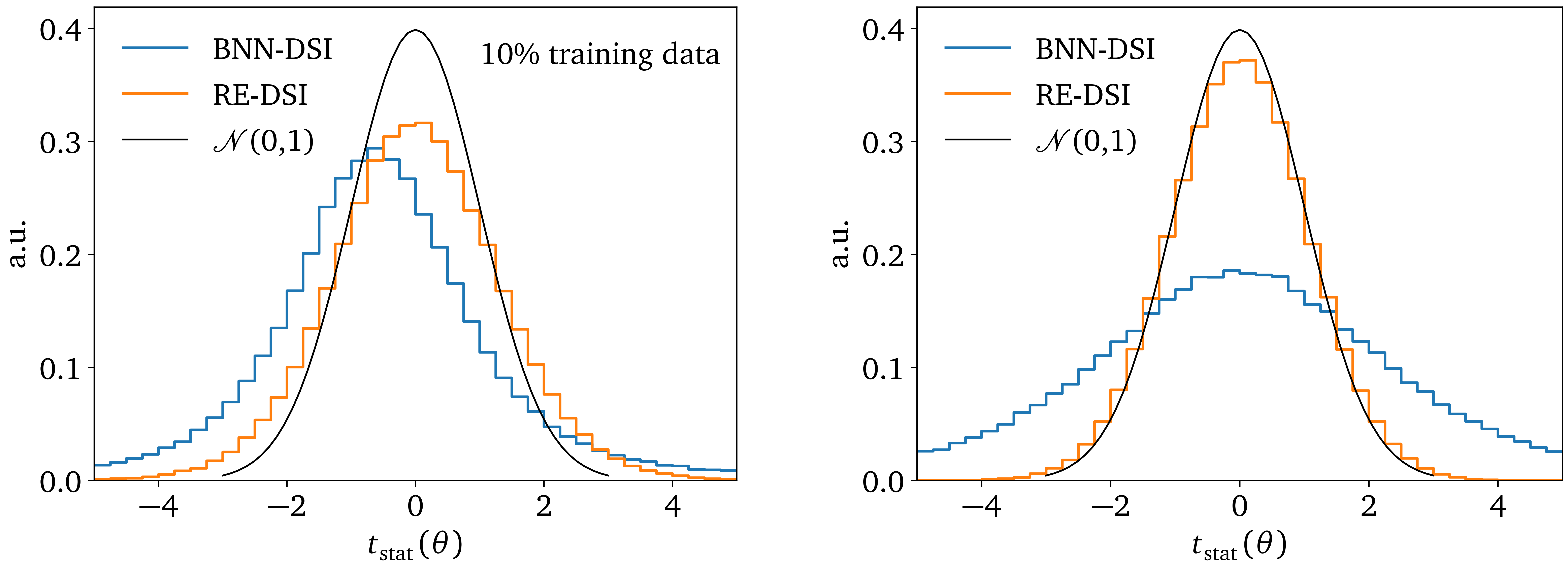
Correctly learned: follow **Gaussian**

Reducing the training size

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

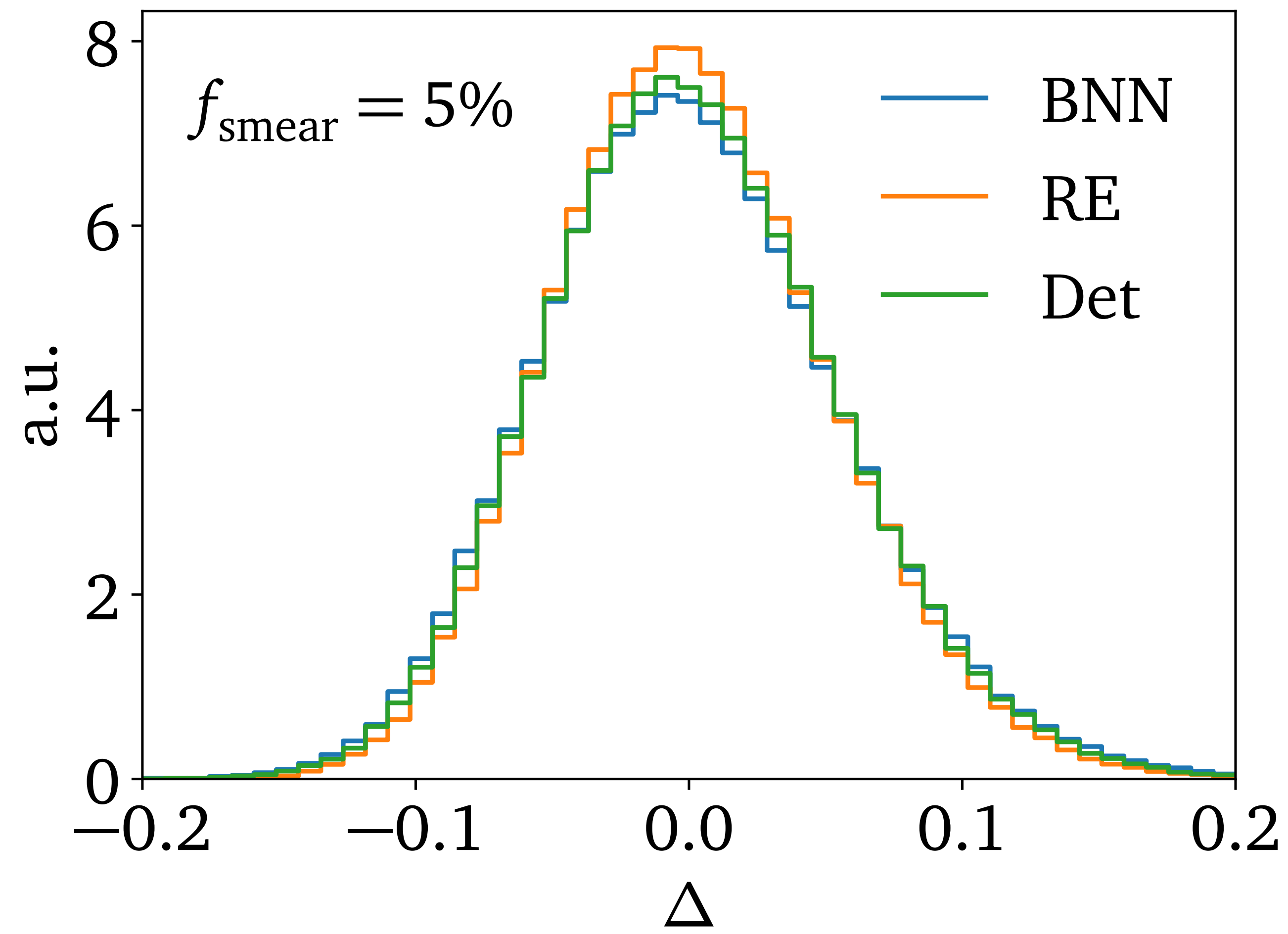
	70%	10%
$\langle \sigma_{\text{syst, BNN-DSI}}/A \rangle$	$8.7 \cdot 10^{-5}$	$2.5 \cdot 10^{-4}$
$\langle \sigma_{\text{stat, BNN-DSI}}/A \rangle$	$3.6 \cdot 10^{-5}$	$1.5 \cdot 10^{-4}$
$\langle \sigma_{\text{syst, RE-DSI}}/A \rangle$	$5.1 \cdot 10^{-5}$	$2.9 \cdot 10^{-4}$
$\langle \sigma_{\text{stat,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

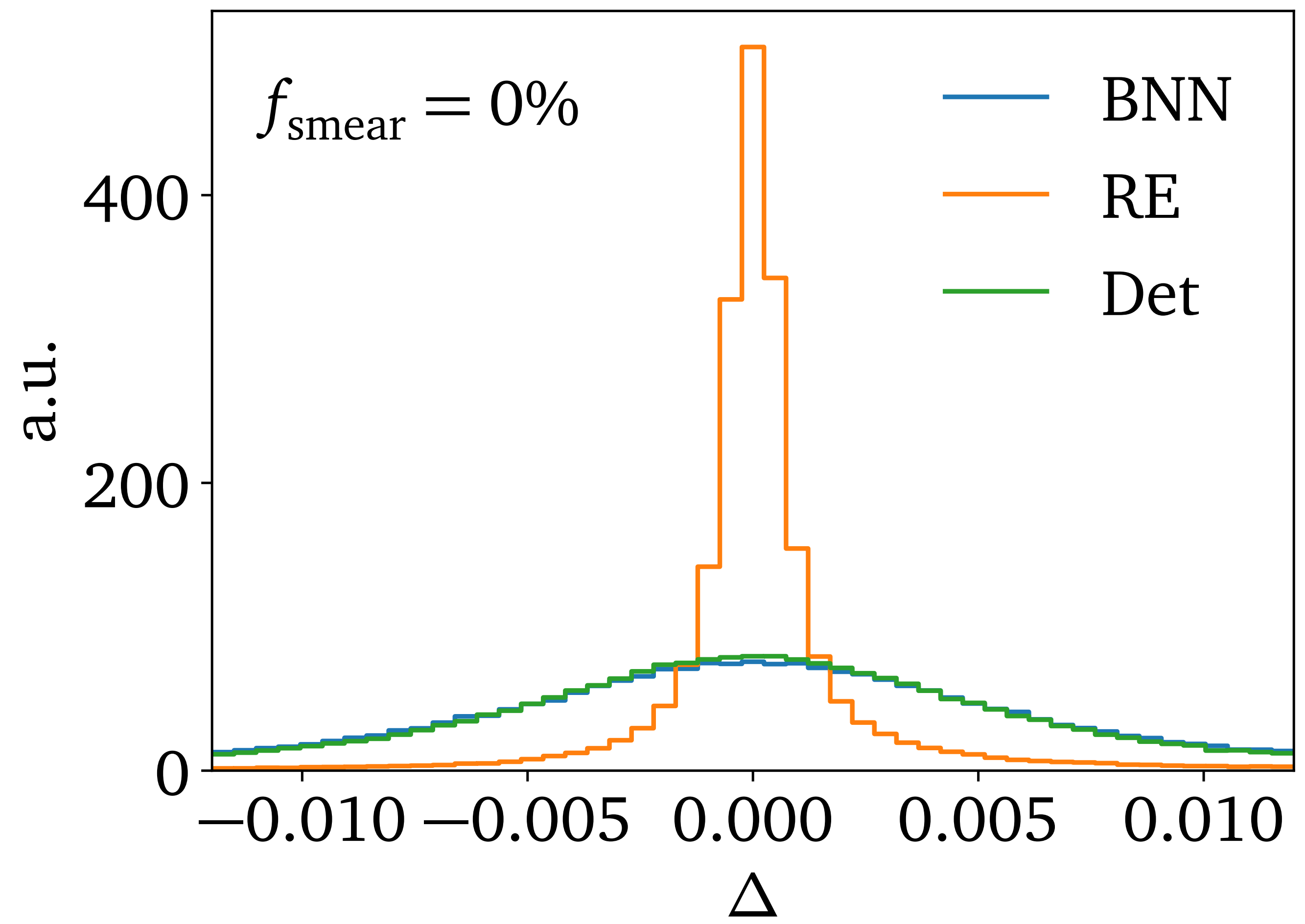
Statistical pull



➡Repulsive ensemble: Advantage for **statistical** uncertainty

Systematic pull and accuracy





➡Calibrated results

➡BNN: Advantage for learning **systematics**

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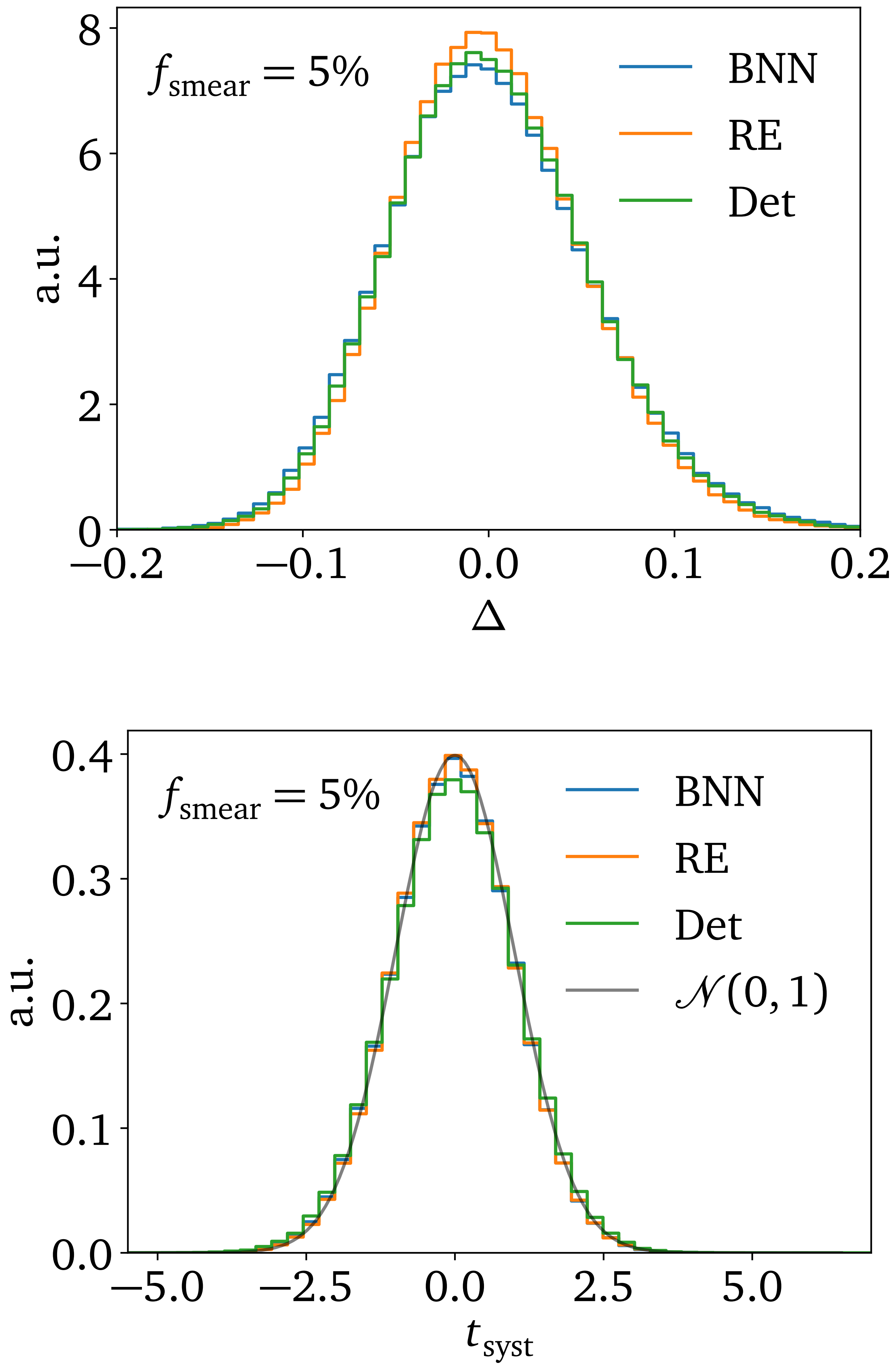

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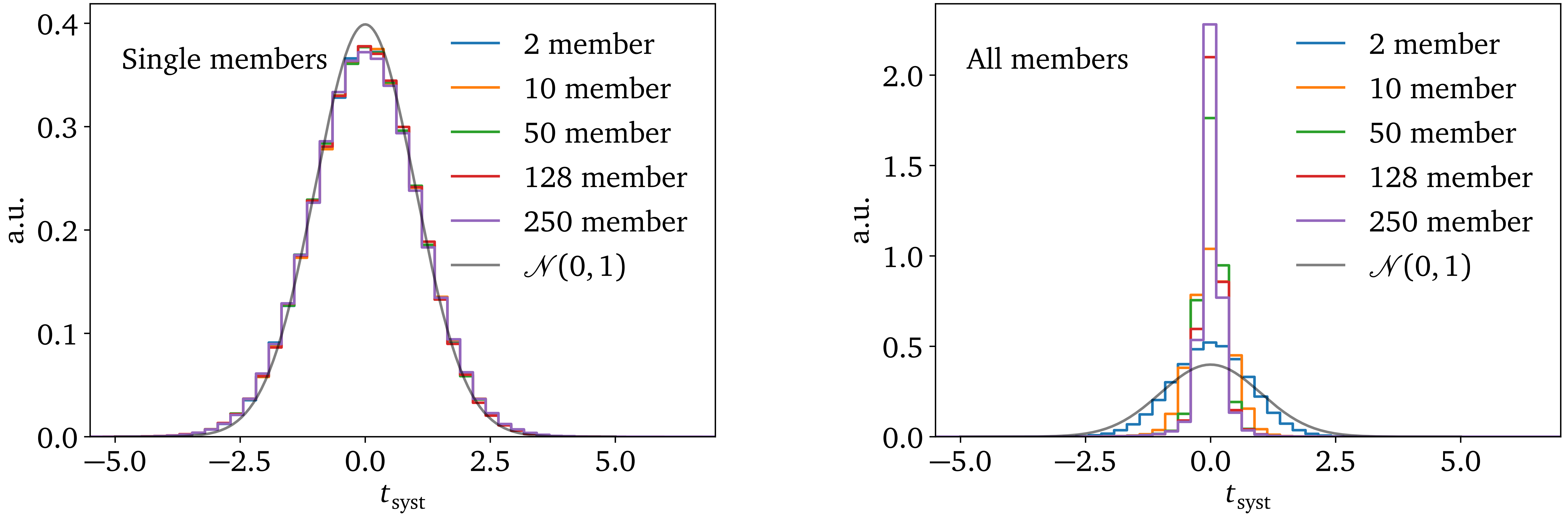
Systematic pull for REs

- Learned $\sigma_{syst}(x)$ too conservative



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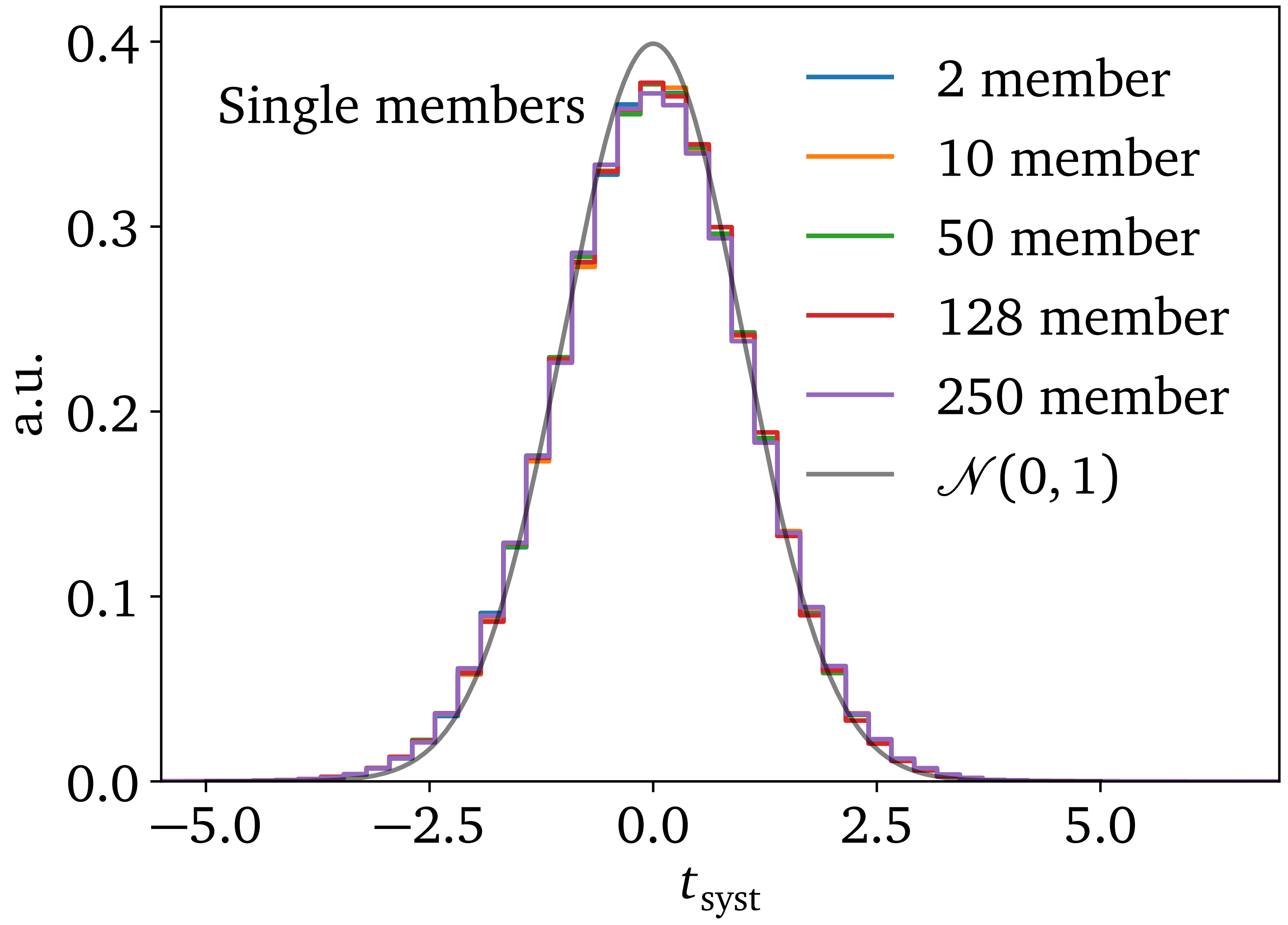
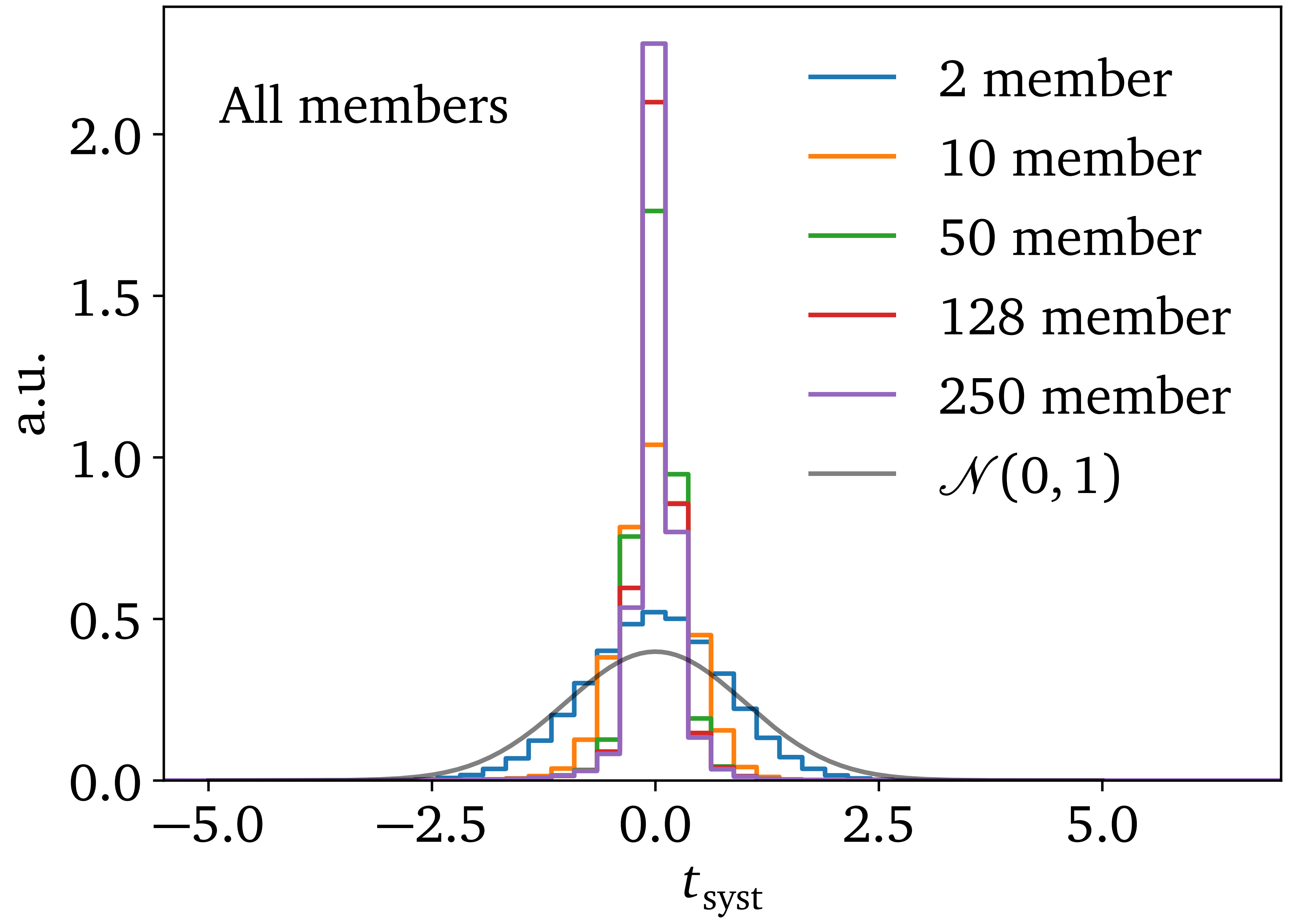
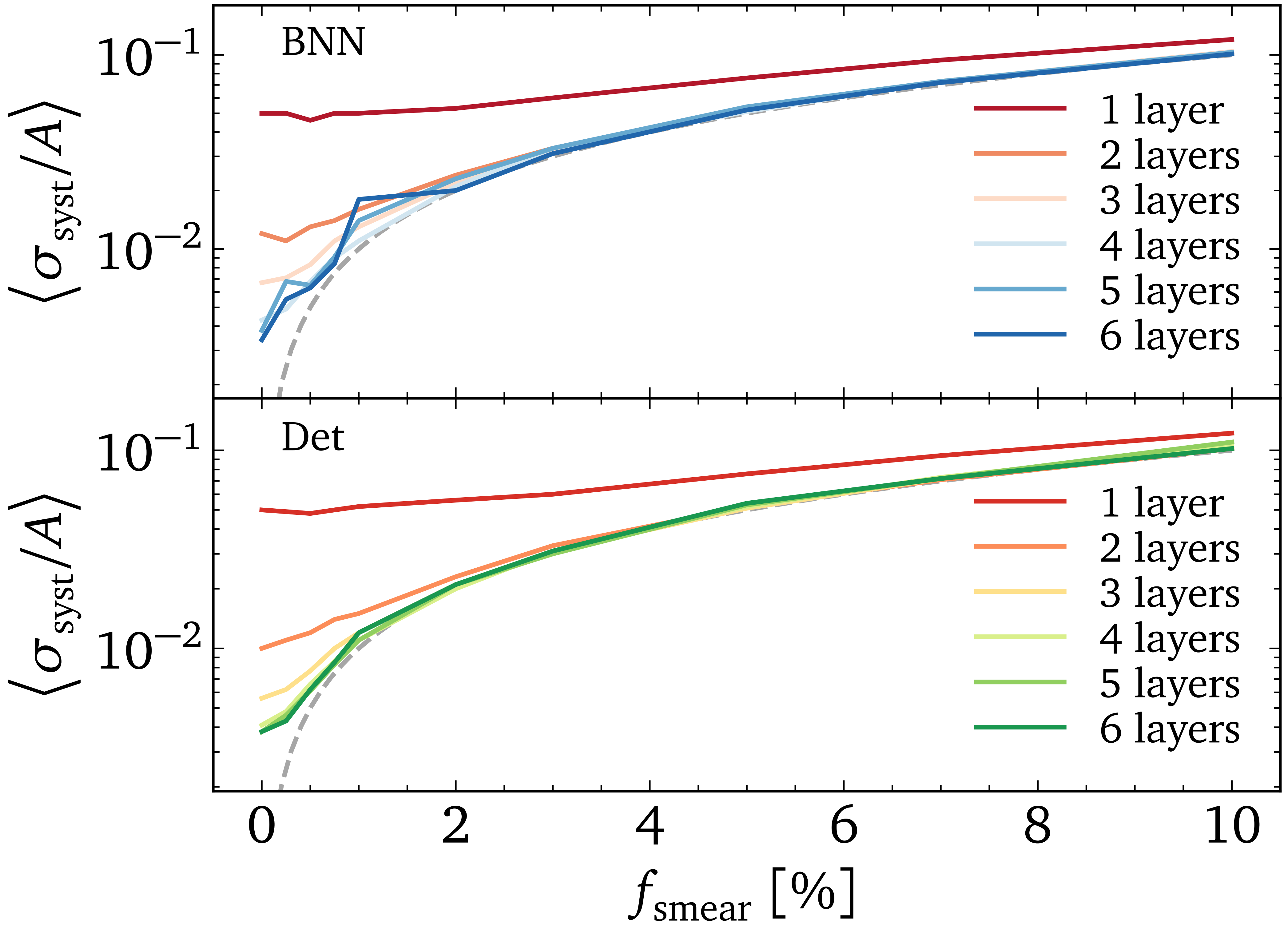




➡ Prediction benefits from ensemble nature but not σ_{syst}

Improve network expressivity



- Source of intrinsic uncertainty?
- BNN: Only last layer Bayesian

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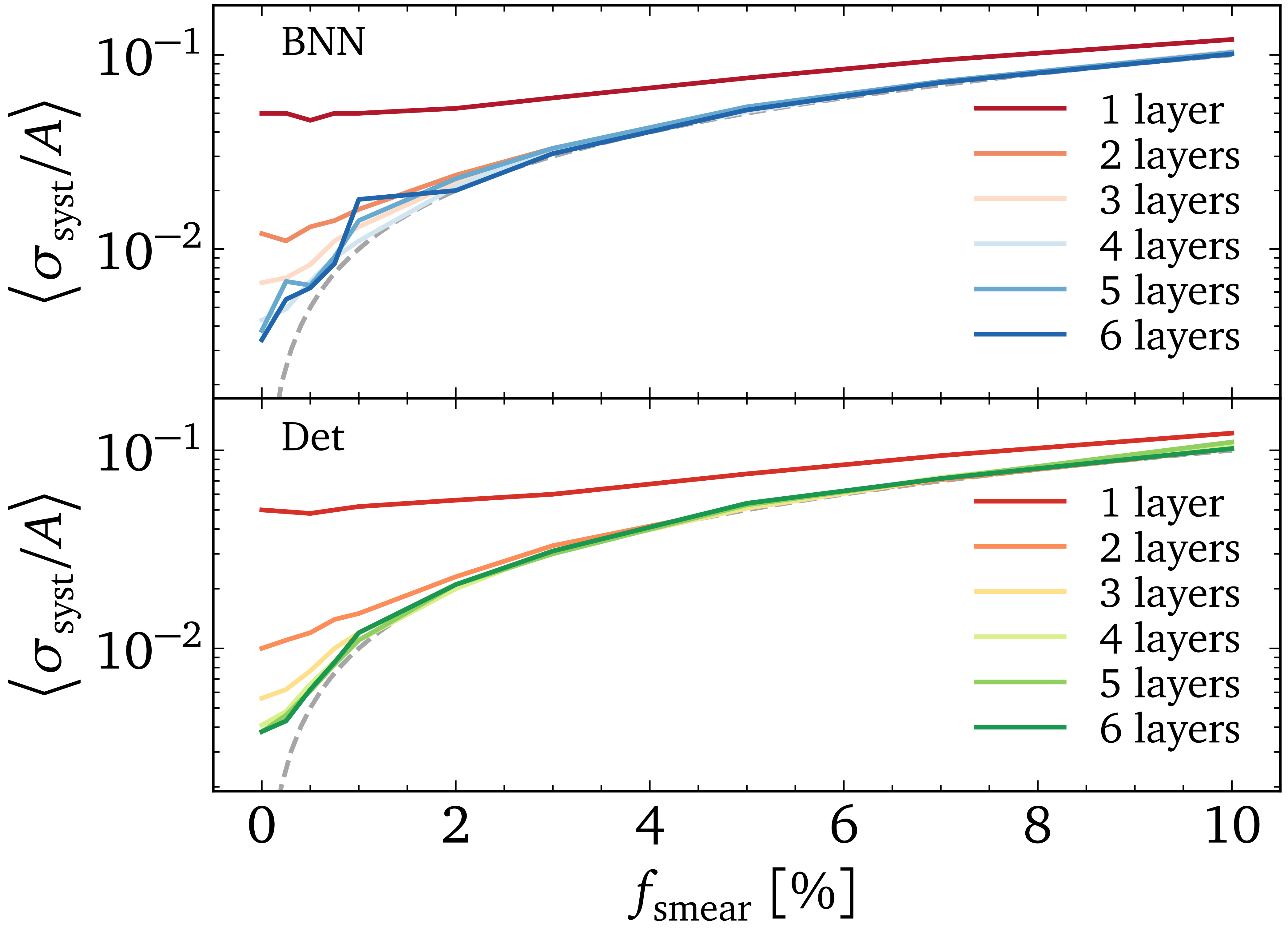

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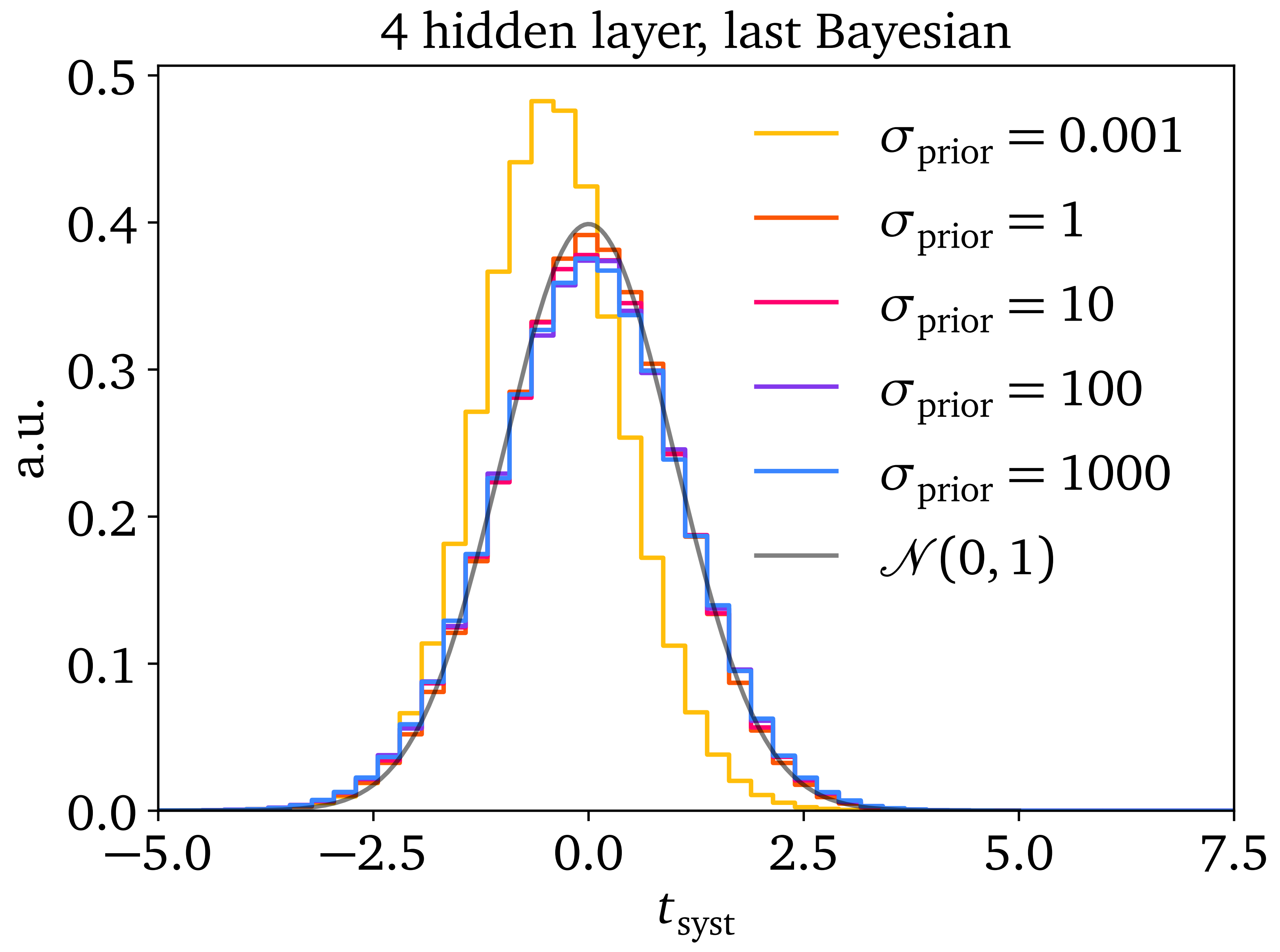
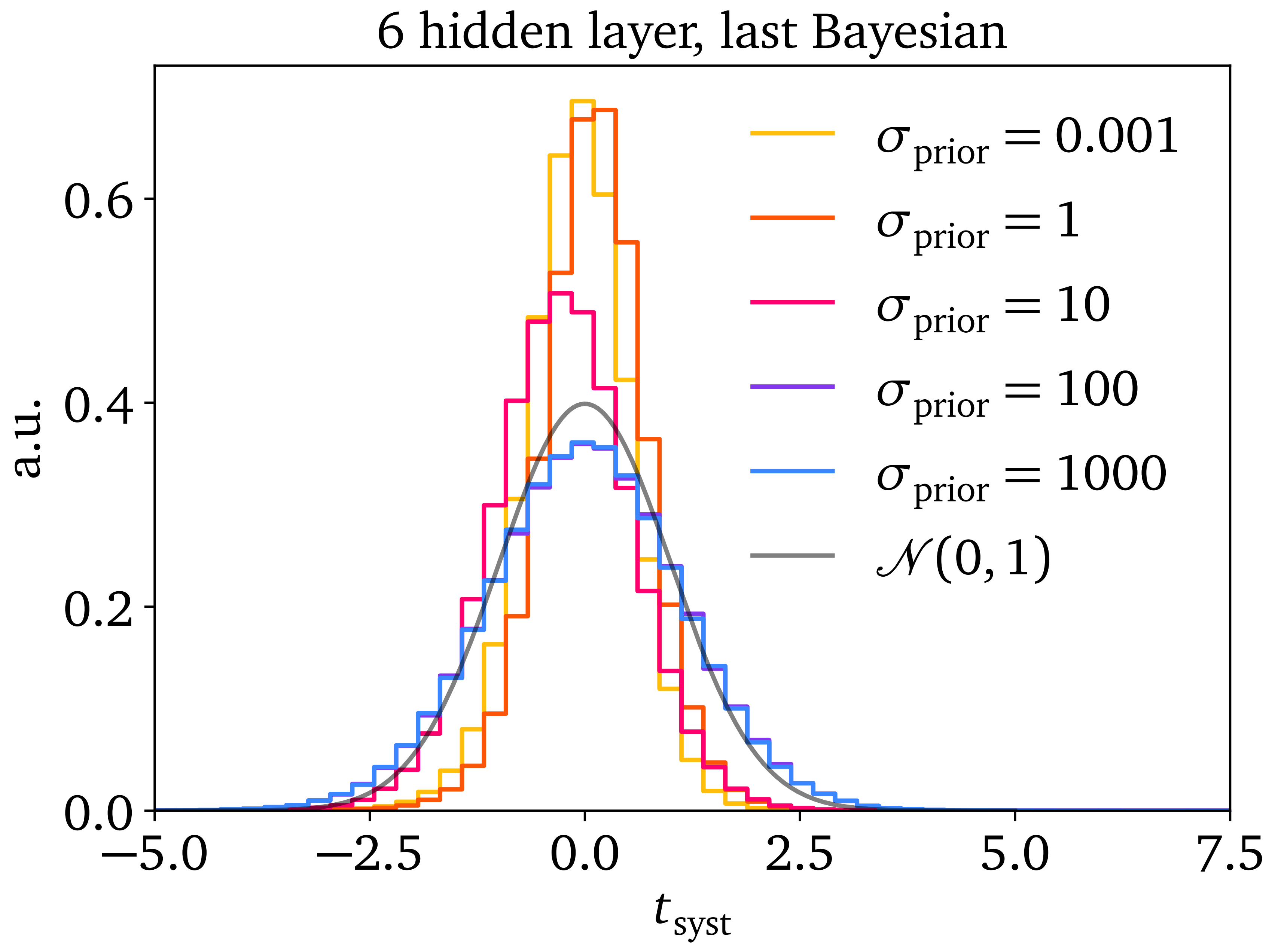
➡ **More expressivity** and better **sensitivity** for small noise with more layers

➡ Improvement of intrinsic uncertainty to 0.3%

Prior influence in the BNN





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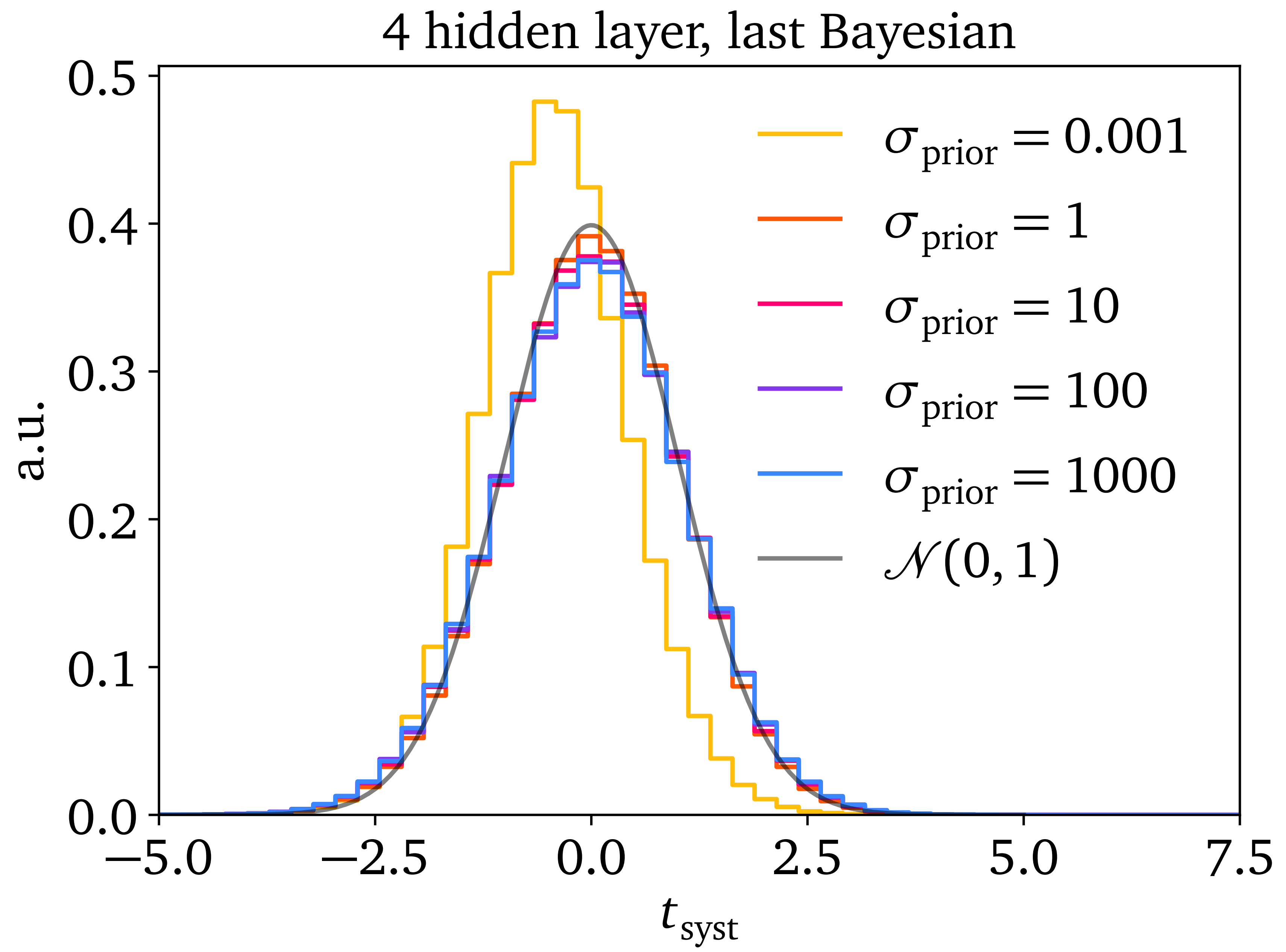
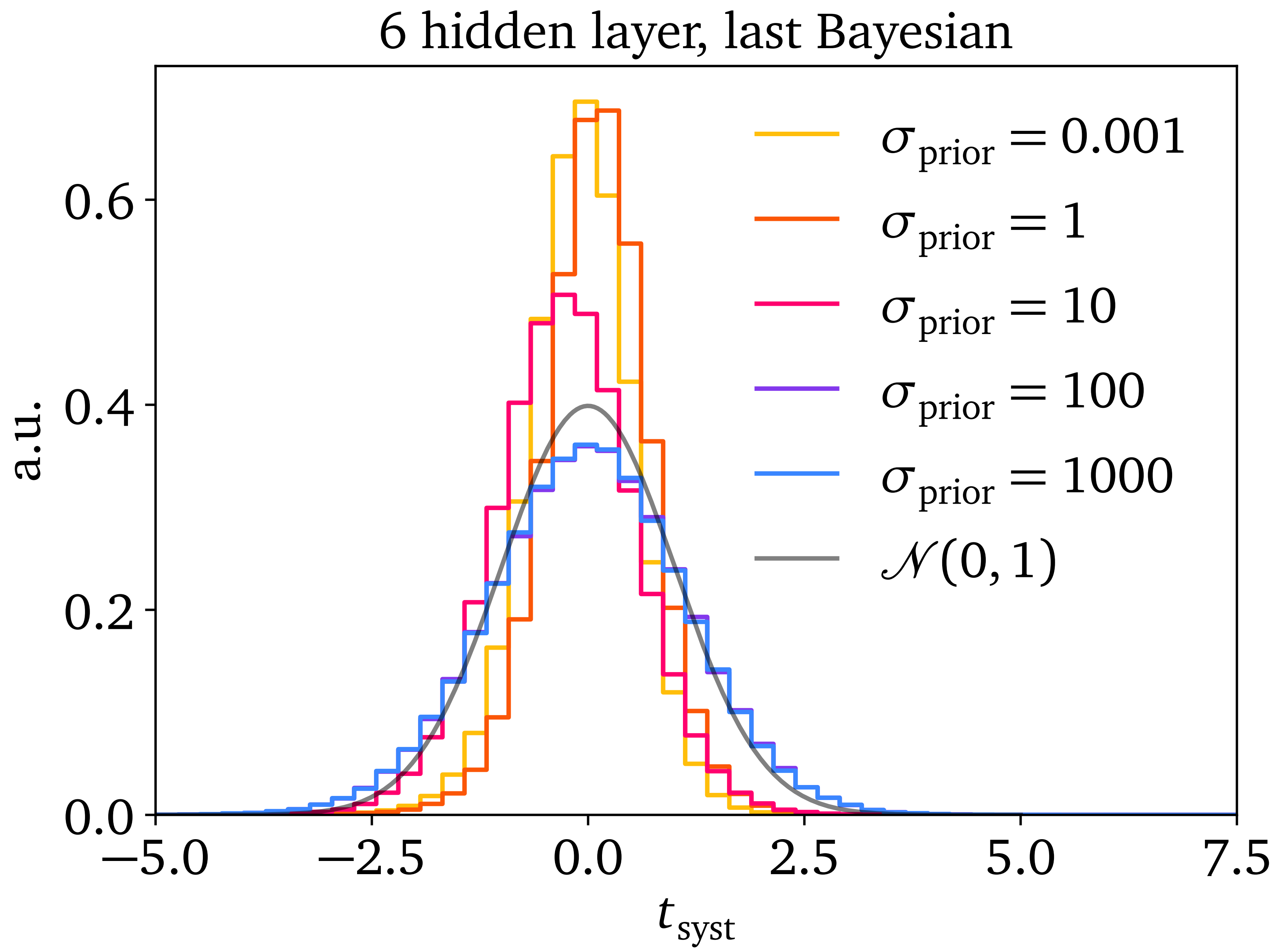




➡ Results don't depend on prior

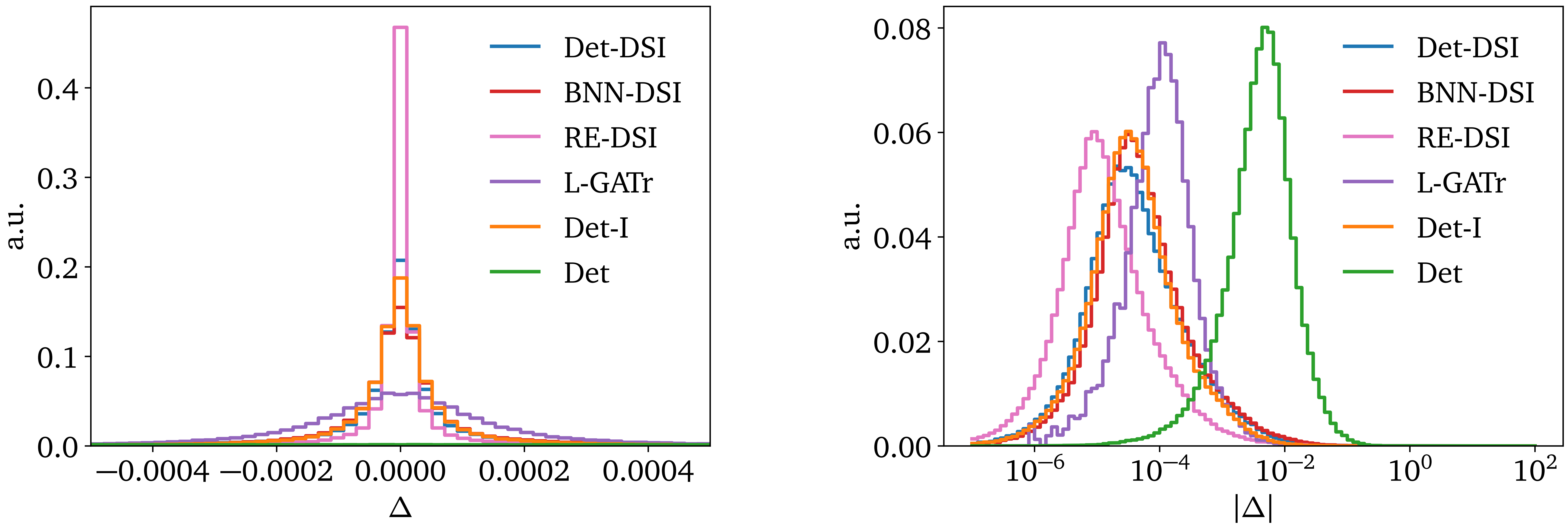
➡ For more layers a larger prior is needed

Testing 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]

Advanced architectures - Accuracy



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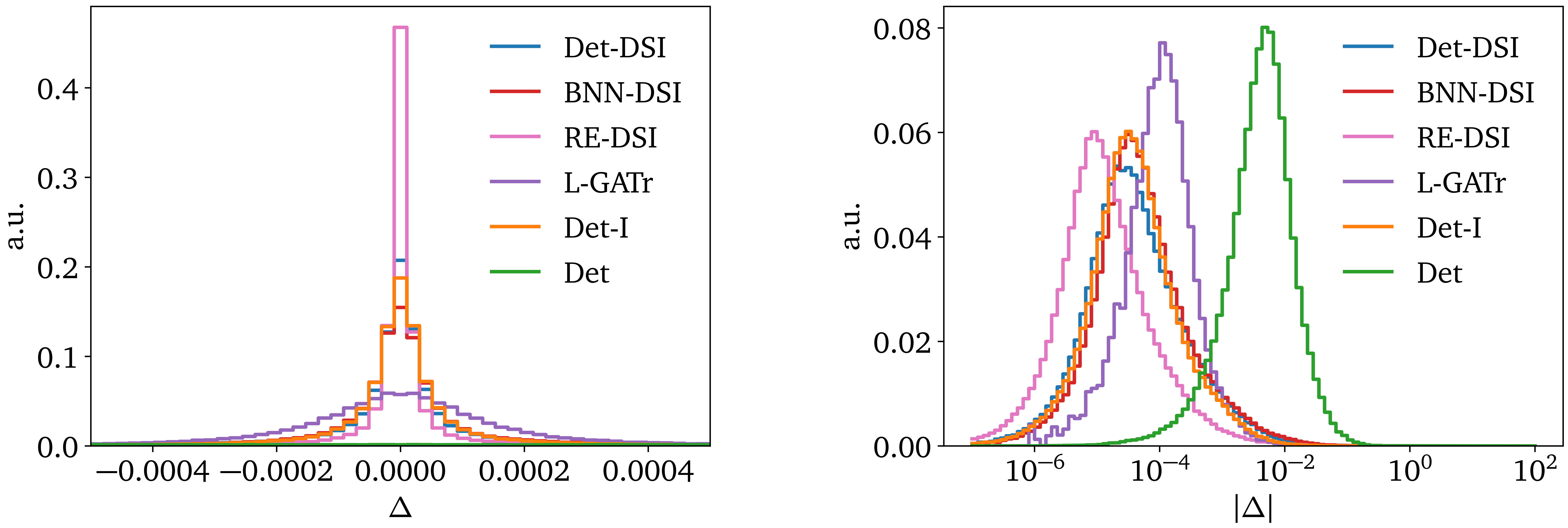
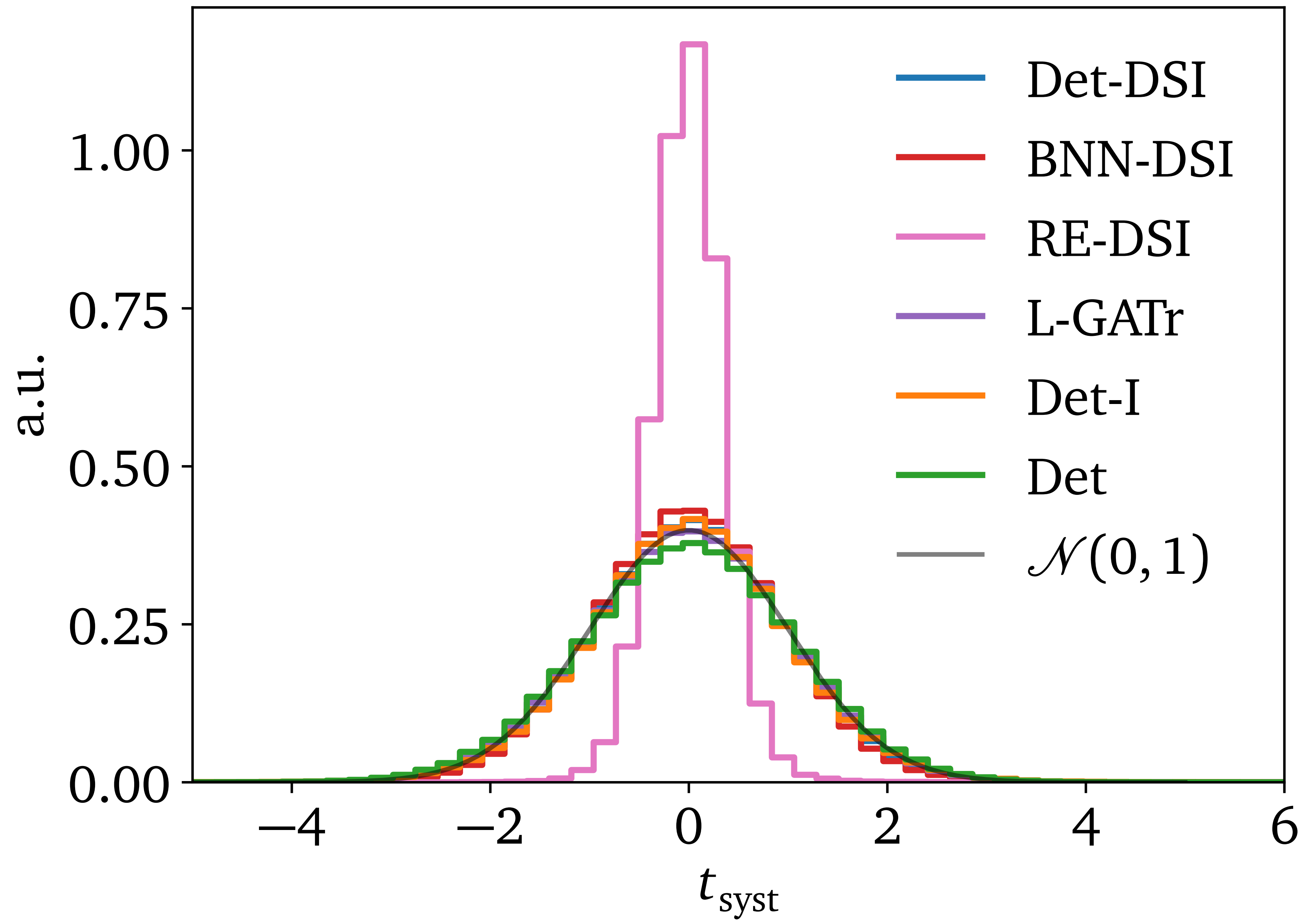
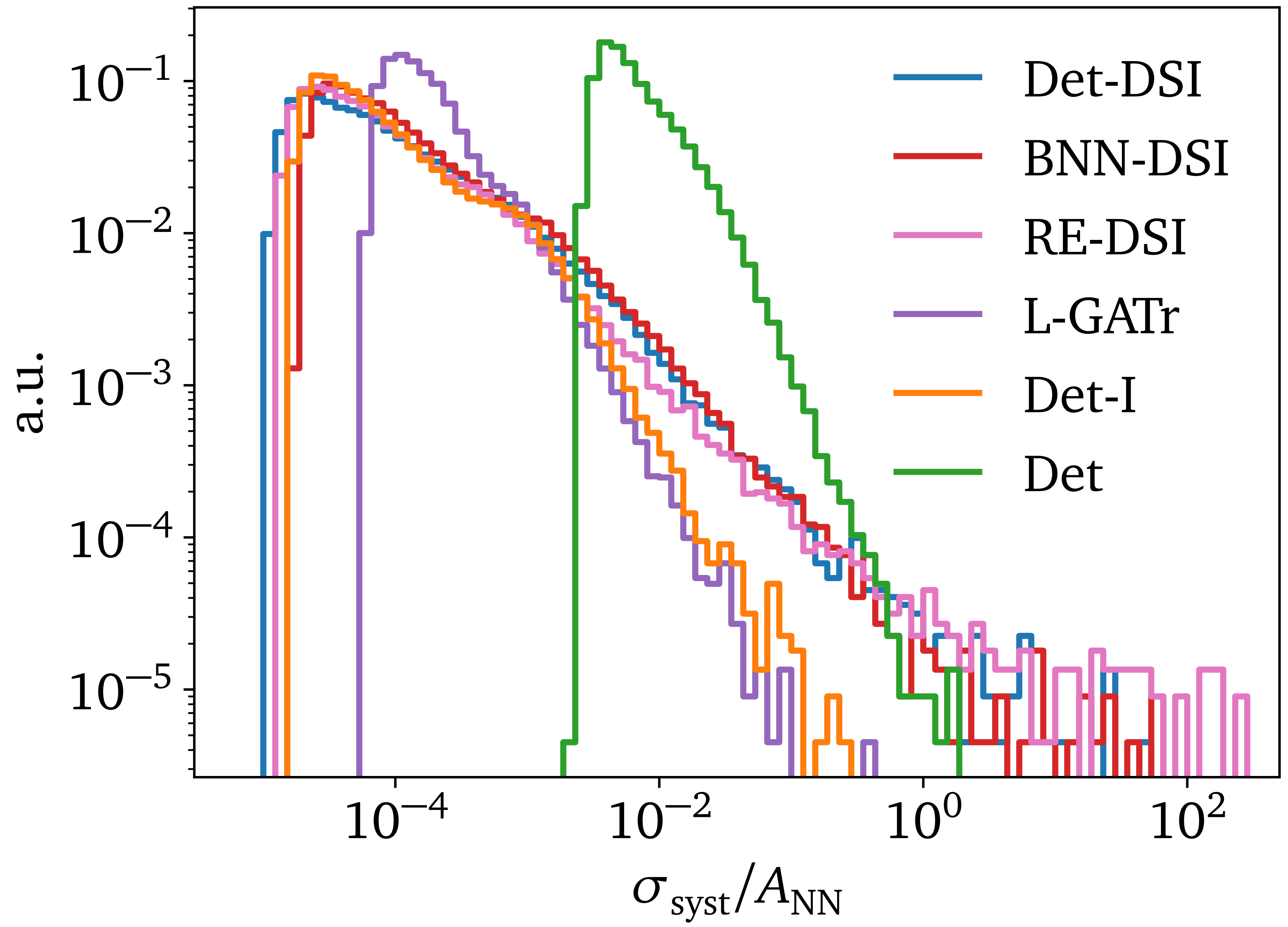


➡**Controlled accuracy** to 10^{-5} level

Advanced architectures - Uncertainties





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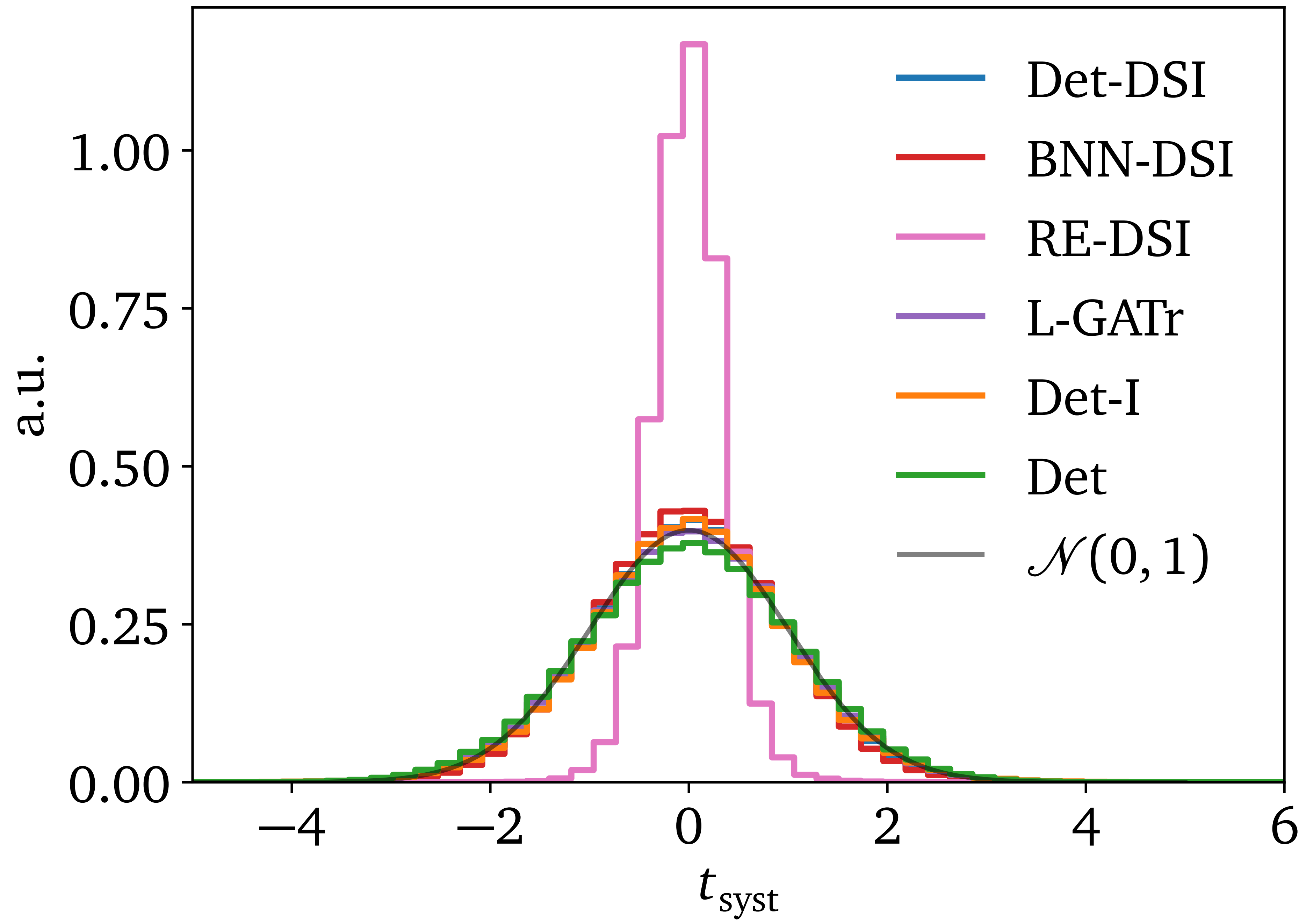
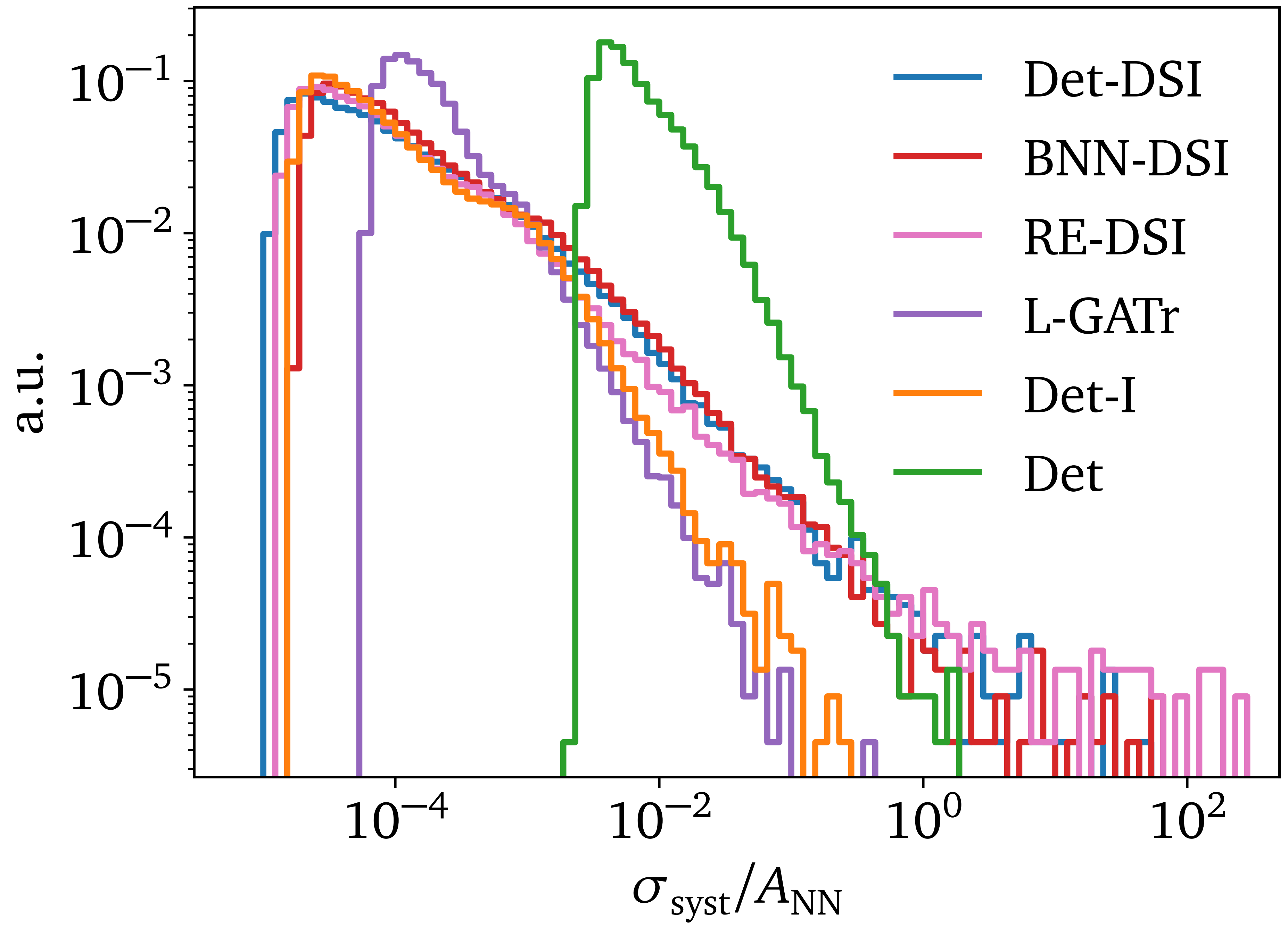




➡ **Calibrated uncertainty** with **precision** on 10^{-5} level

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

Conclusion

1. Able to track systematic and statistical uncertainties
2. Networks are calibrated (if not: calibration possible)
3. RE benefits from ensemble nature in precision
4. Networks are able to give controlled accuracy on 10^{-5} level

Conclusion

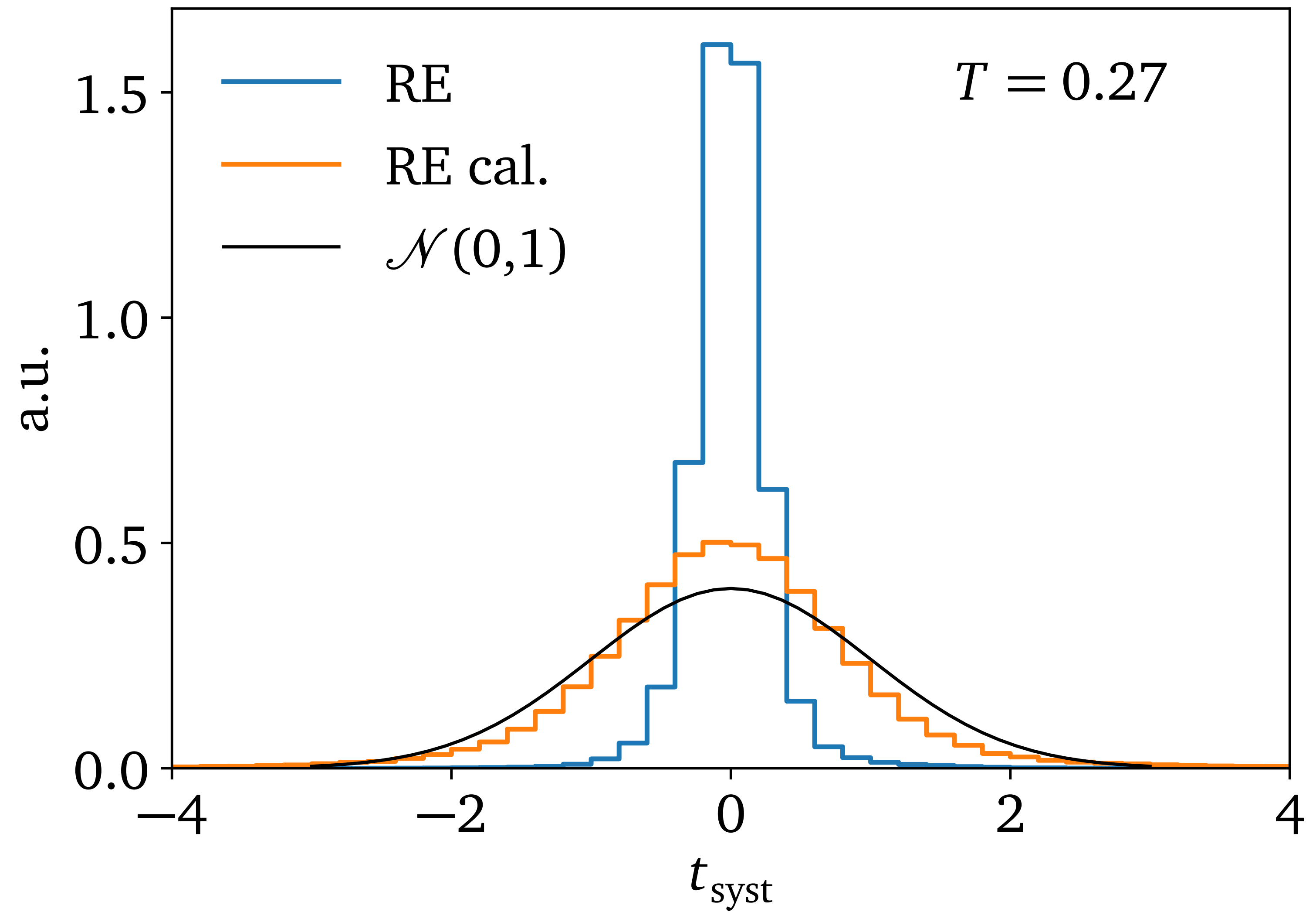
1. Able to track systematic and statistical uncertainties
2. Networks are calibrated (if not: calibration possible)
3. RE benefits from ensemble nature in precision
4. Networks are able to give controlled accuracy on 10^{-5} level

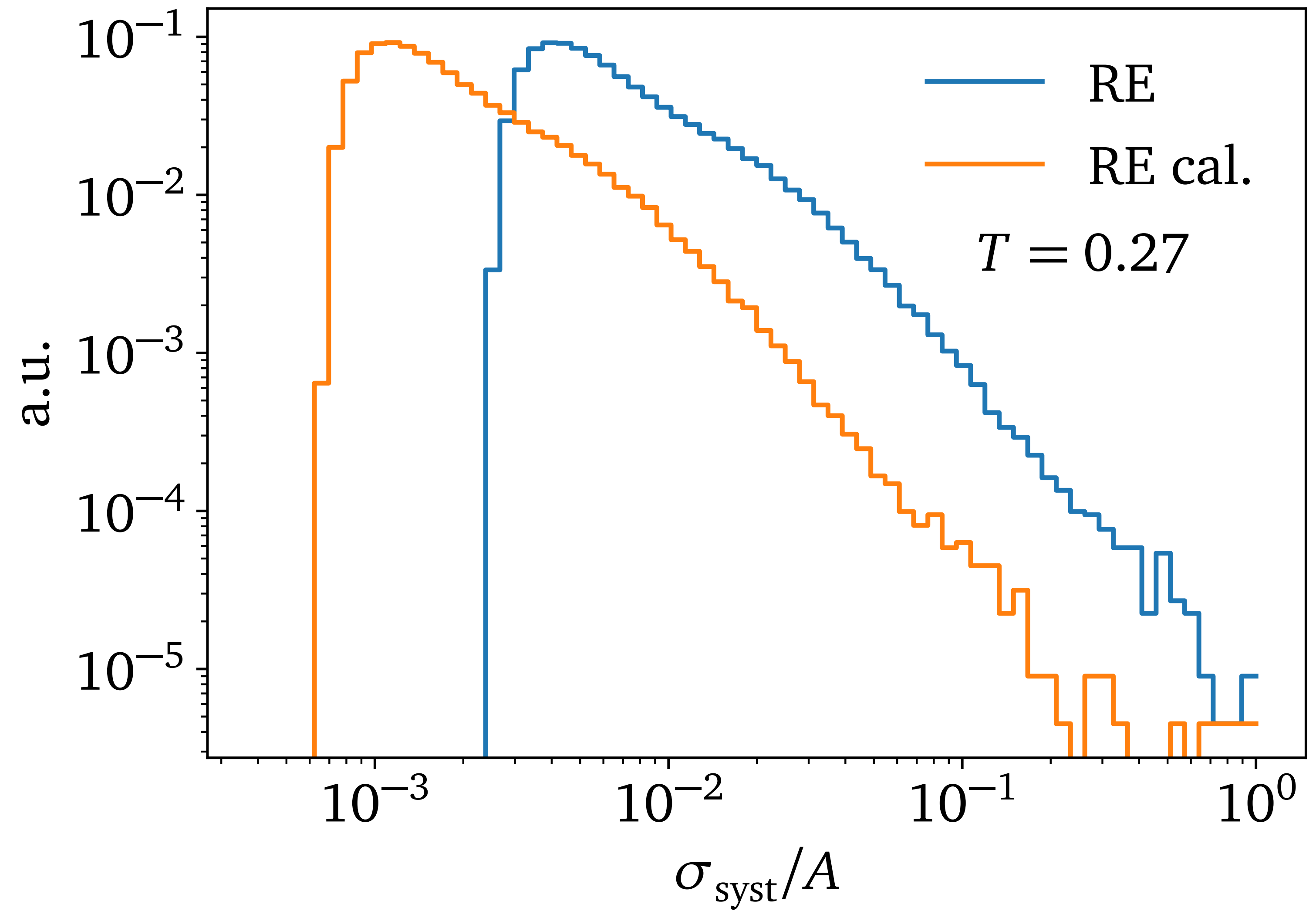
Thank you for your attention!

Back up / Additional material

Calibration of networks

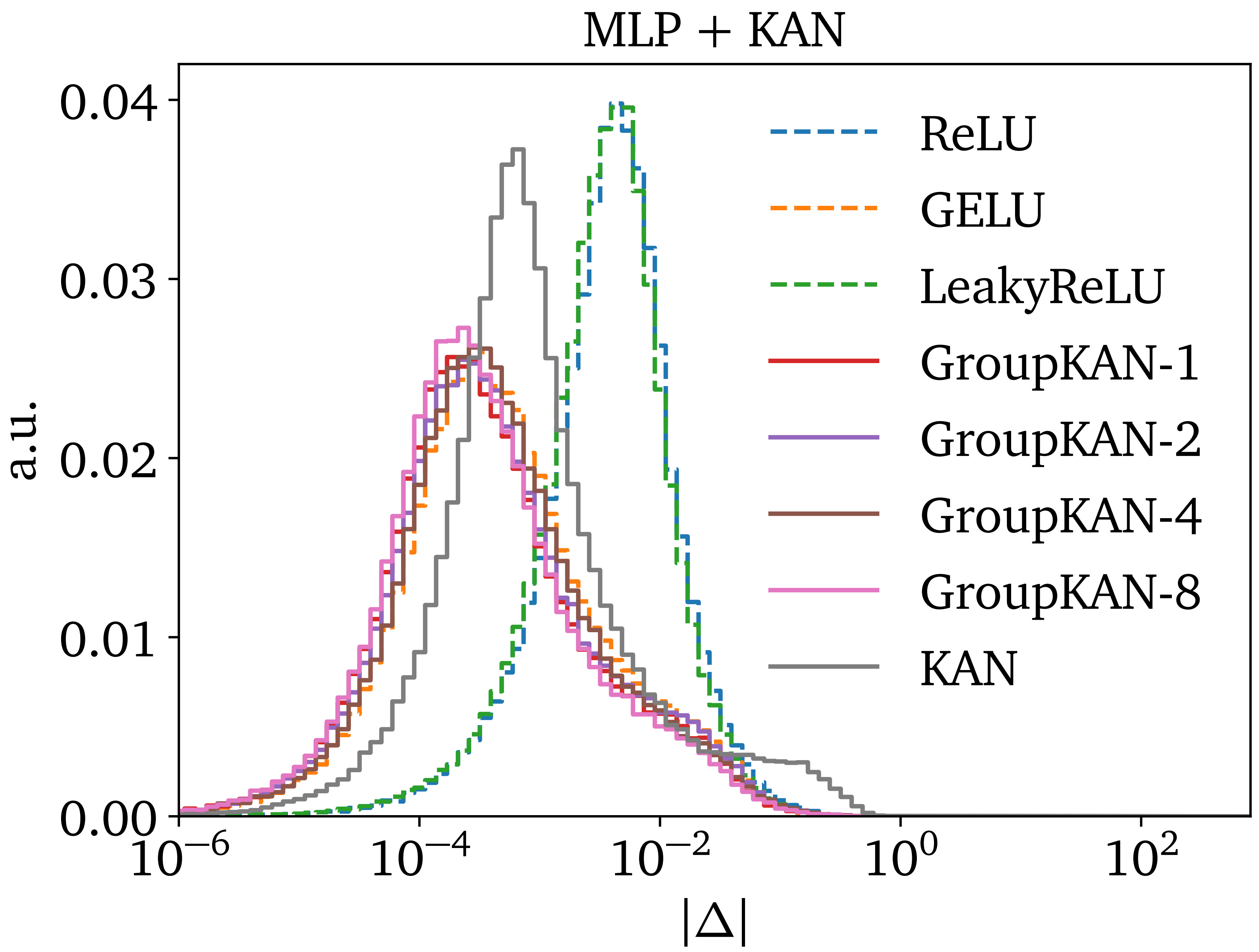
- Calibrate RE by introducing scaling parameter T: $\sigma_{\text{syst}} \to \sigma_{\text{syst}} \times T$
- T estimated by using stochastic gradient descent $\mathcal{L}_T(x) = \left\langle \frac{|A_{\text{true}}(x) - \bar{A}(x)|^2}{2\sigma^2(x)T^2} + \log \sigma(x) T \right\rangle_{x \sim D_{\text{train}}}$

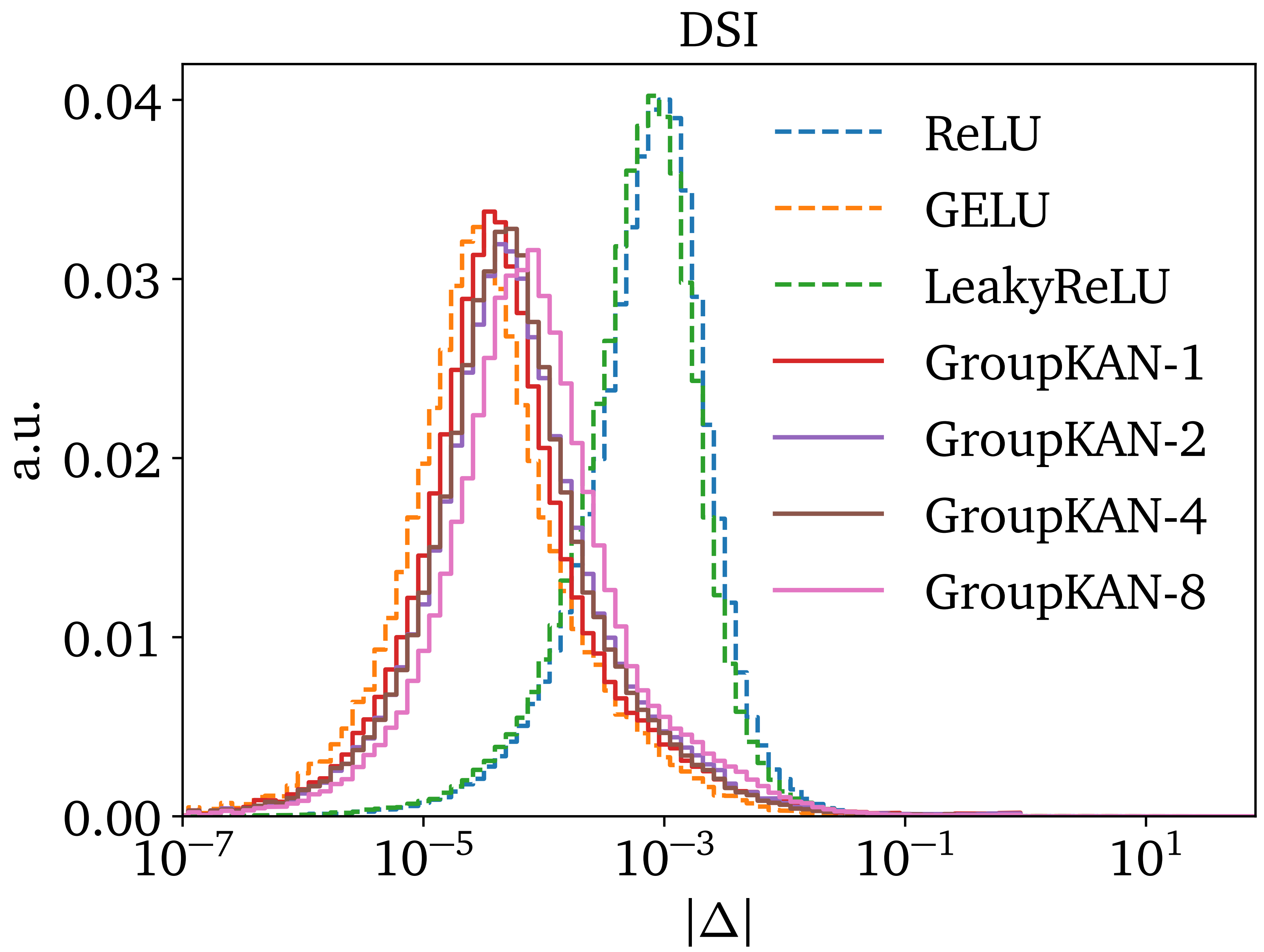




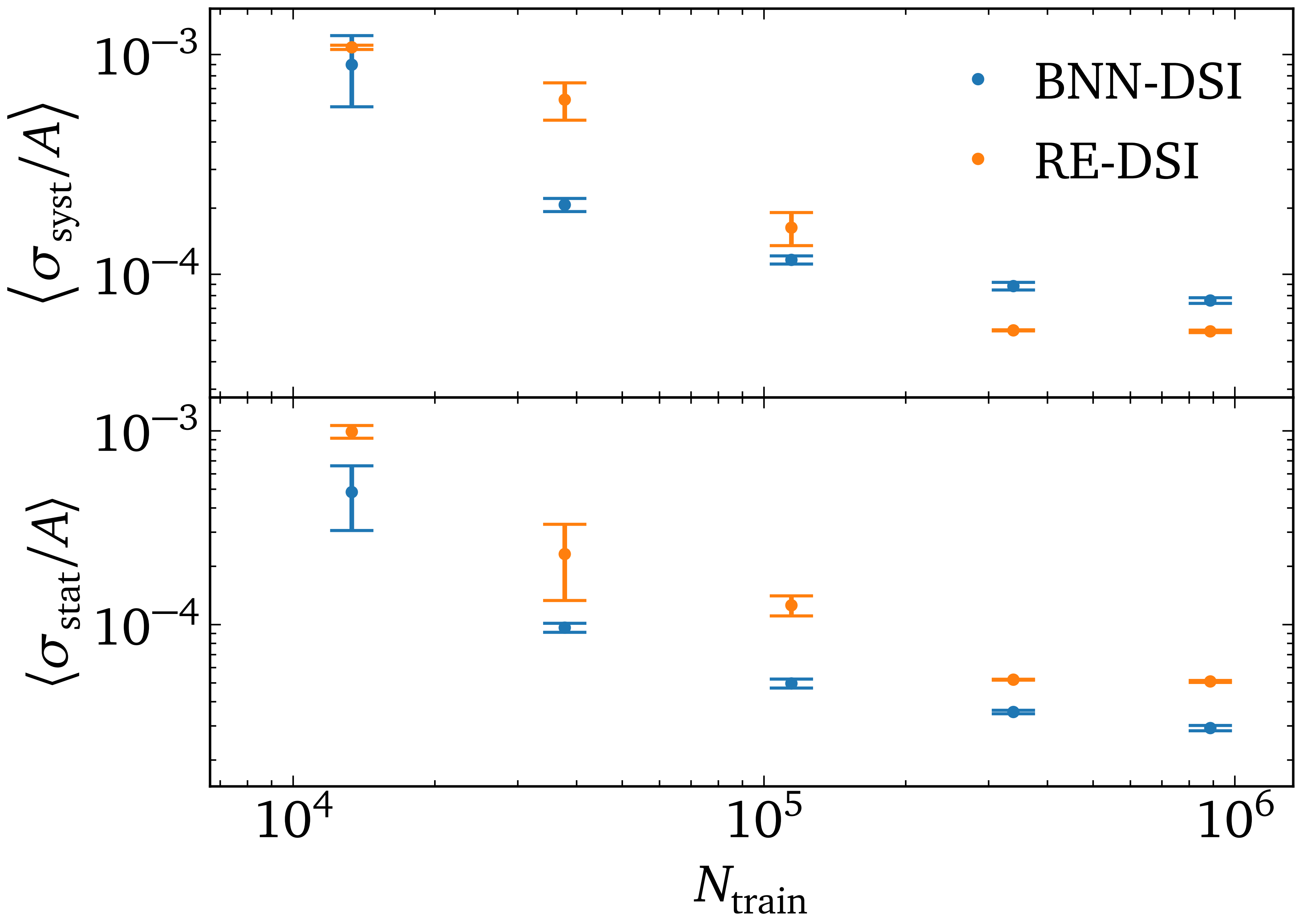
Kolmogorov-Arnold networks (KANs)

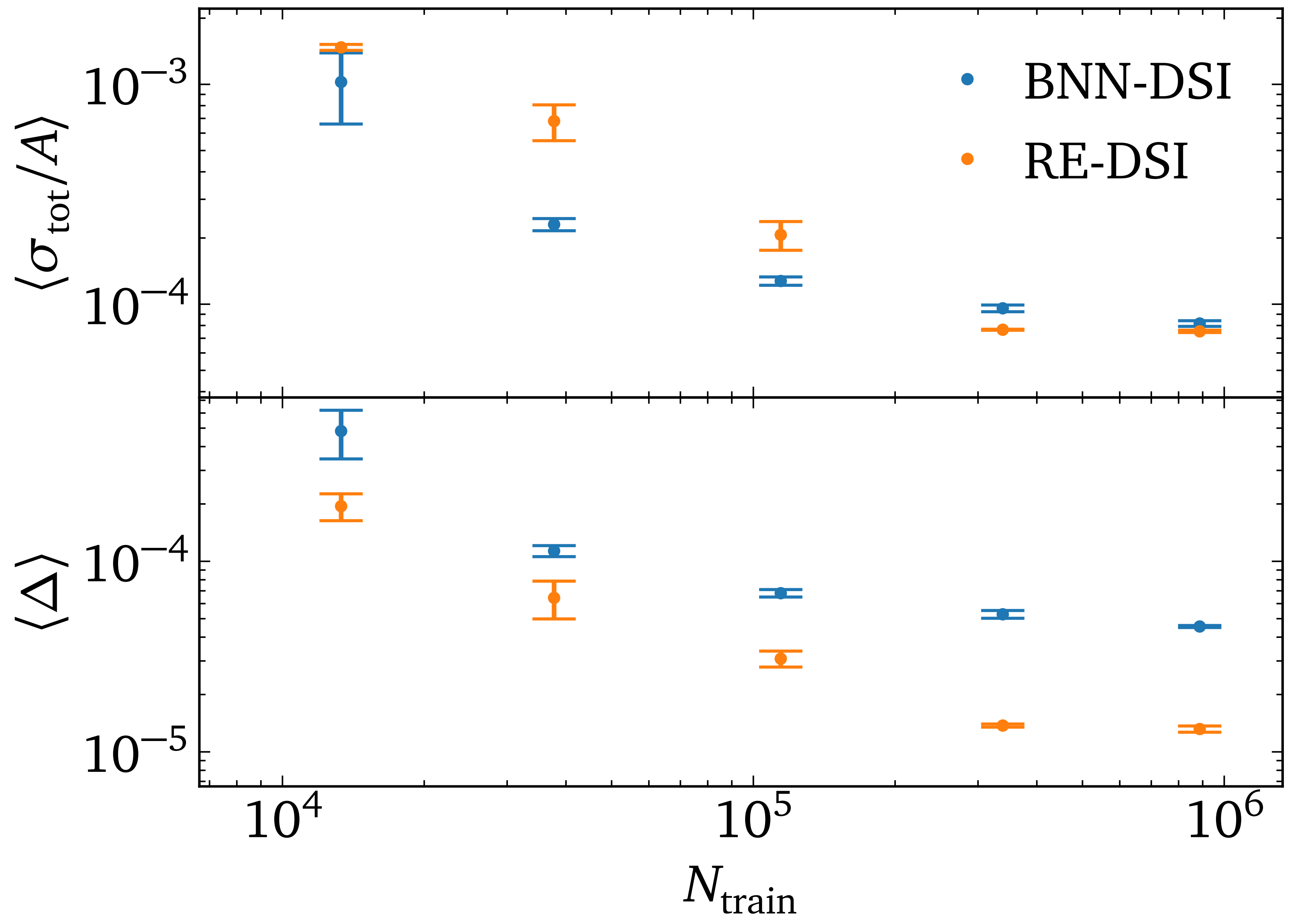
- Use KANs for calibration
- GroupKANs allow for learnable activation functions





Relative uncertainty vs training size





➡ σ_{syst} always larger

➡ Difference in σ_{tot} for small data

➡ σ larger for RE-DSI than BNN-DSI

➡ RE-DSI more accurate in prediction