The Good, the Bad, and the Bayesian

How networks learn uncertainties

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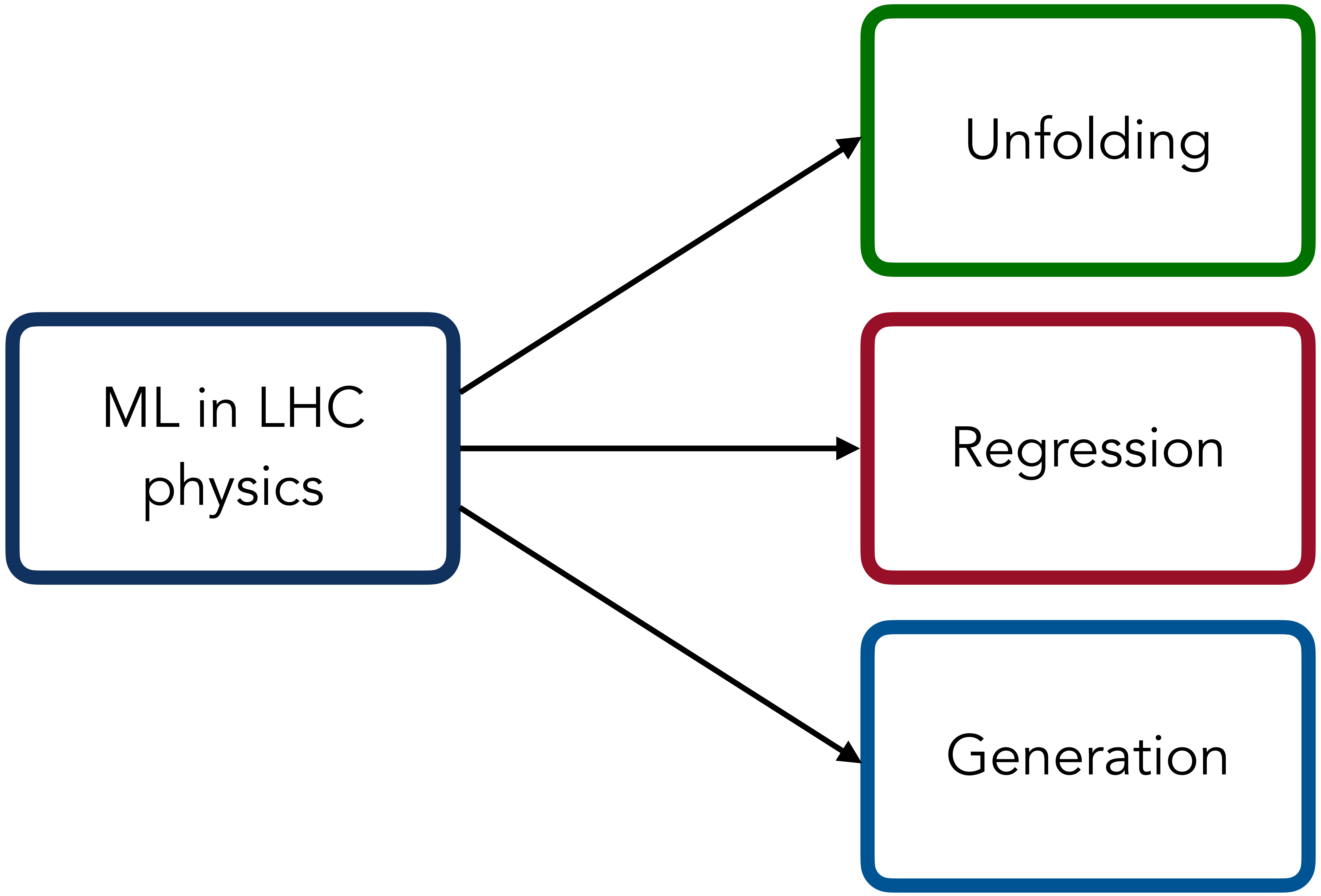
IMPRS
for Precision Tests of Fundamental Symmetries
INTERNATIONAL MAX PLANCK RESEARCH SCHOOL

Motivation



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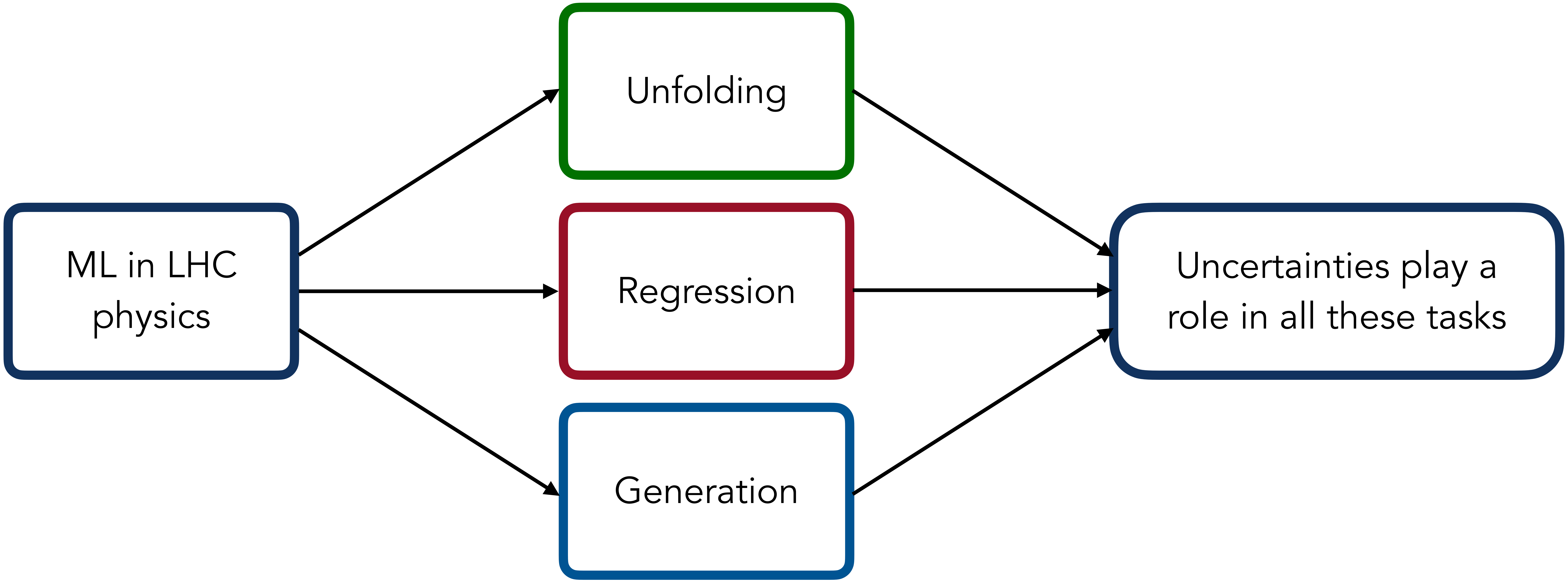
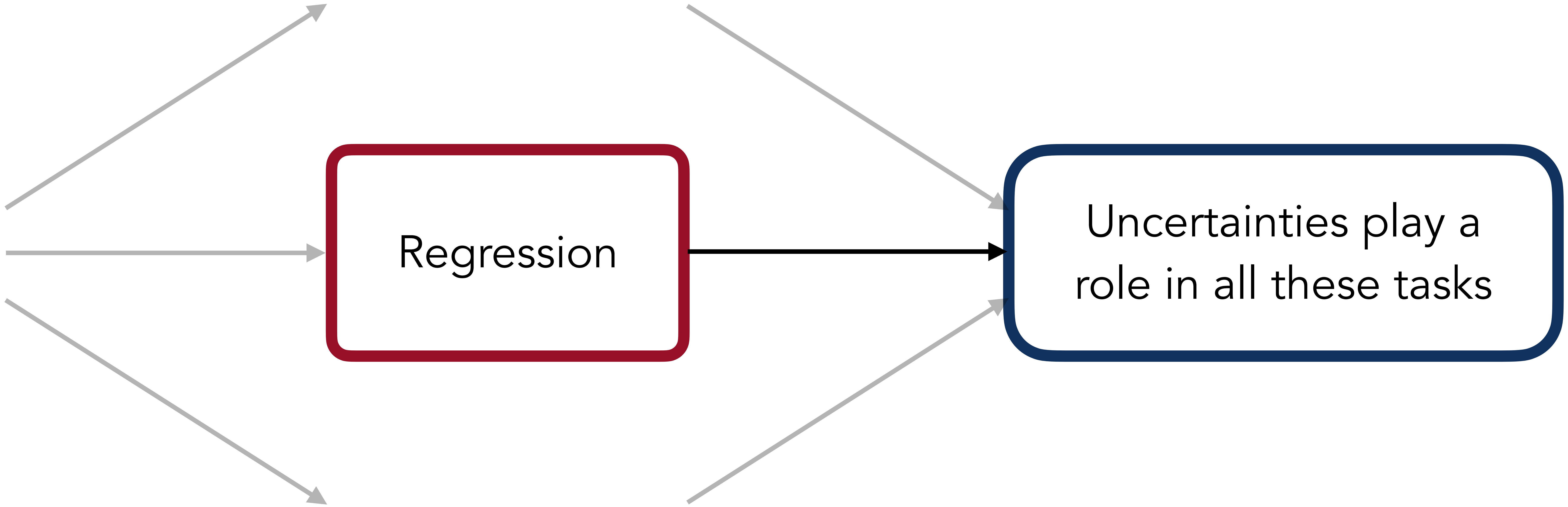

ML in LHC physics
Unfolding
Regression
Generation
Uncertainties play a role in all these tasks

Motivation



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network output

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

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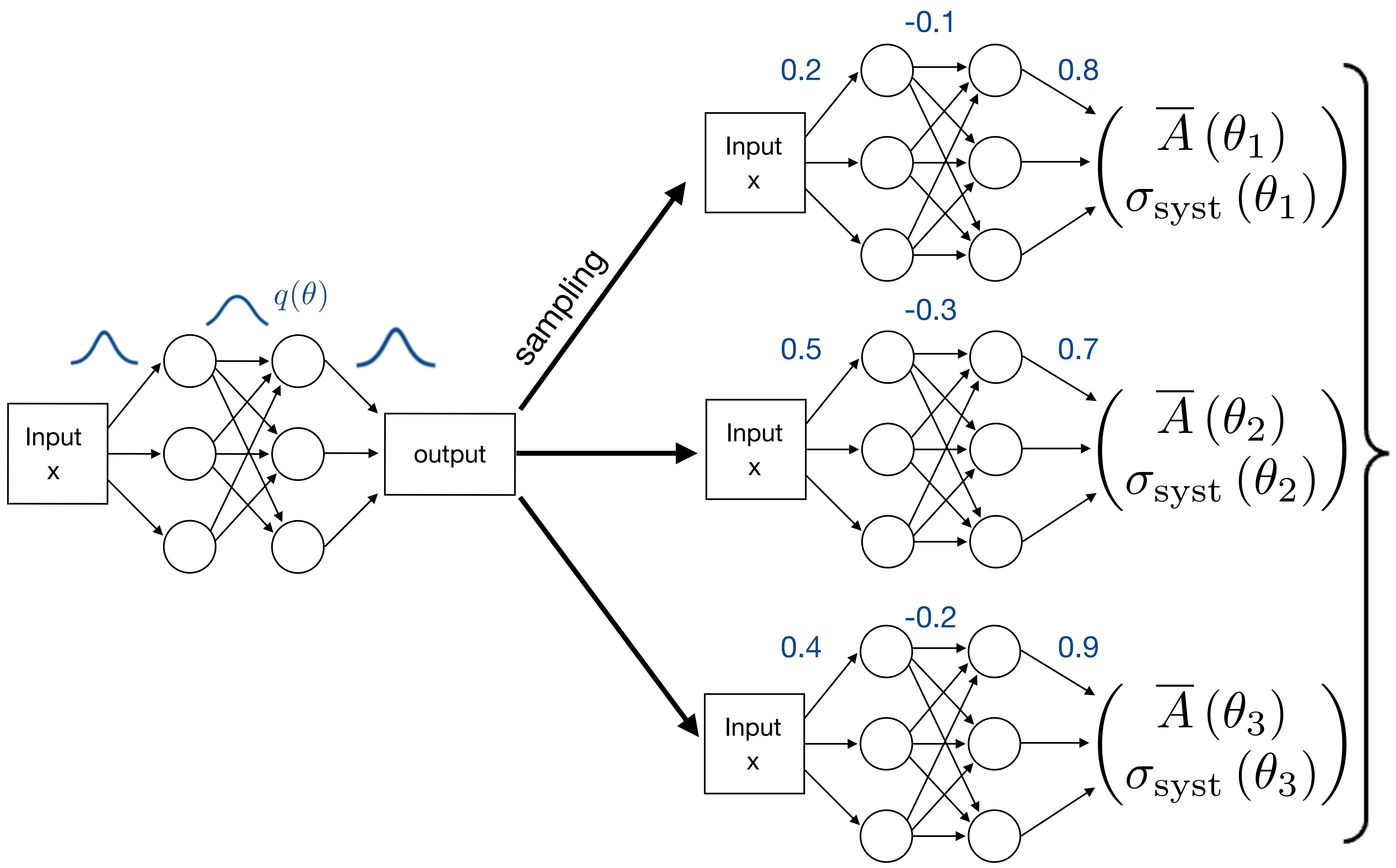
Gaussian uncertainty in heteroscedastic loss: $\mathscr{L}_{\text{heteroscedastic}} = \sum_i \frac{|f(x_i) - f_\theta(x_i)|^2}{2\sigma(x_i)^2} + \log \sigma(x_i) + \ldots$

Bayesian neural network (BNN)

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



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

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

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

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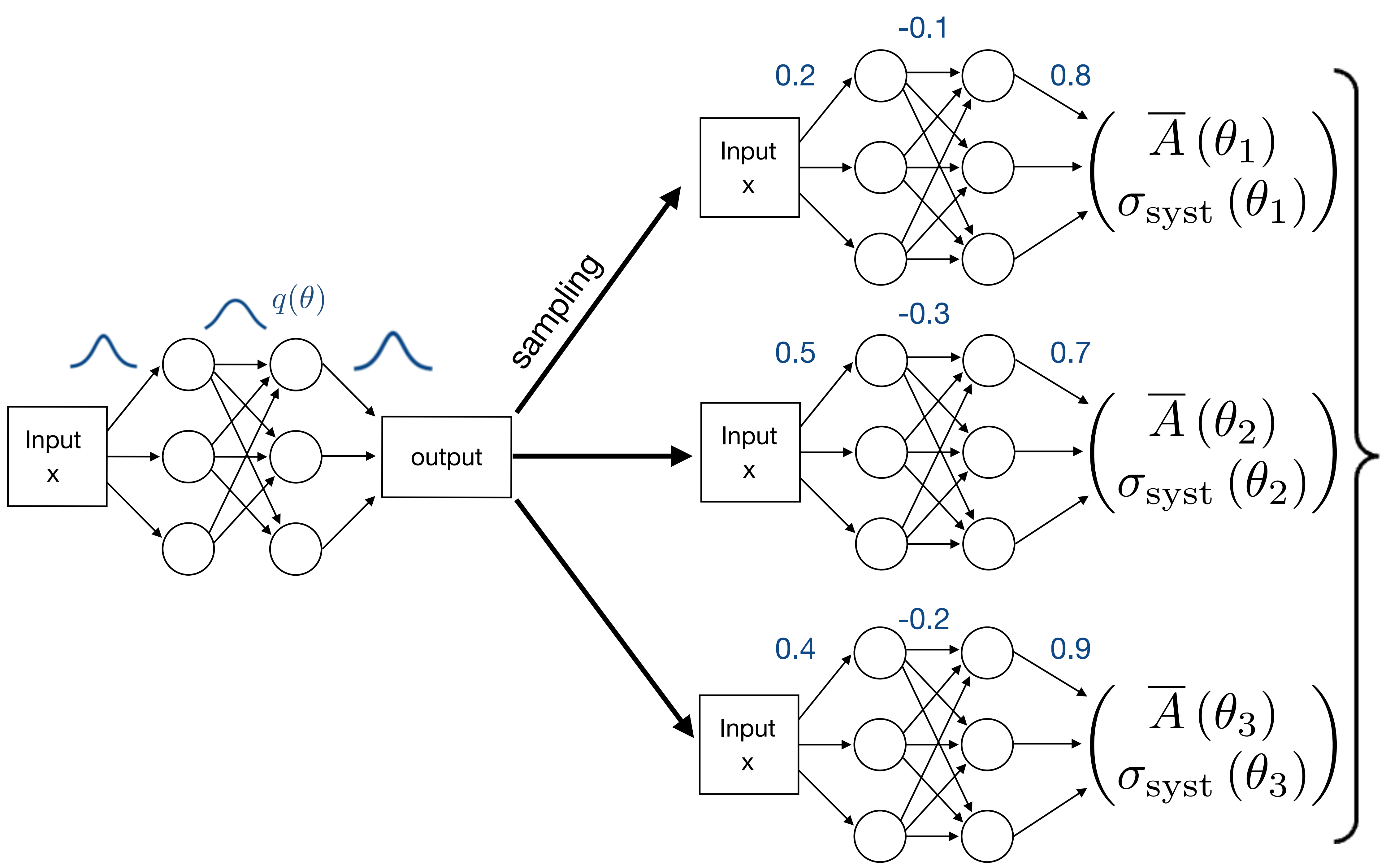

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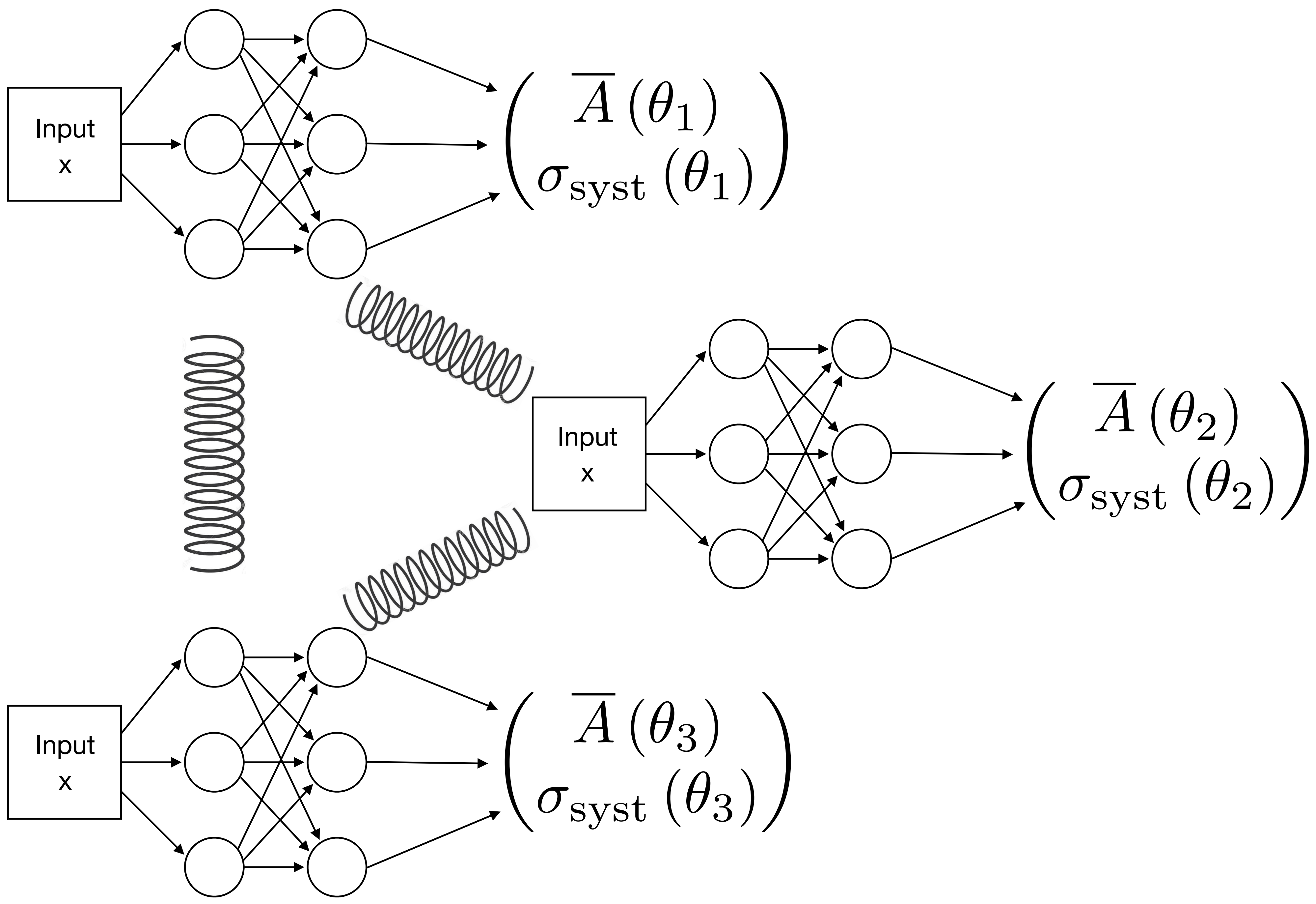
- Parameters: **Network weights $q(\theta)$**
- $q(\theta)$ params of a Gaussian distribution
- Ensemble: Sample from weight distribution

Repulsive ensemble (RE)

Ensemble of networks **Output**



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

Repulsive ensemble (RE)

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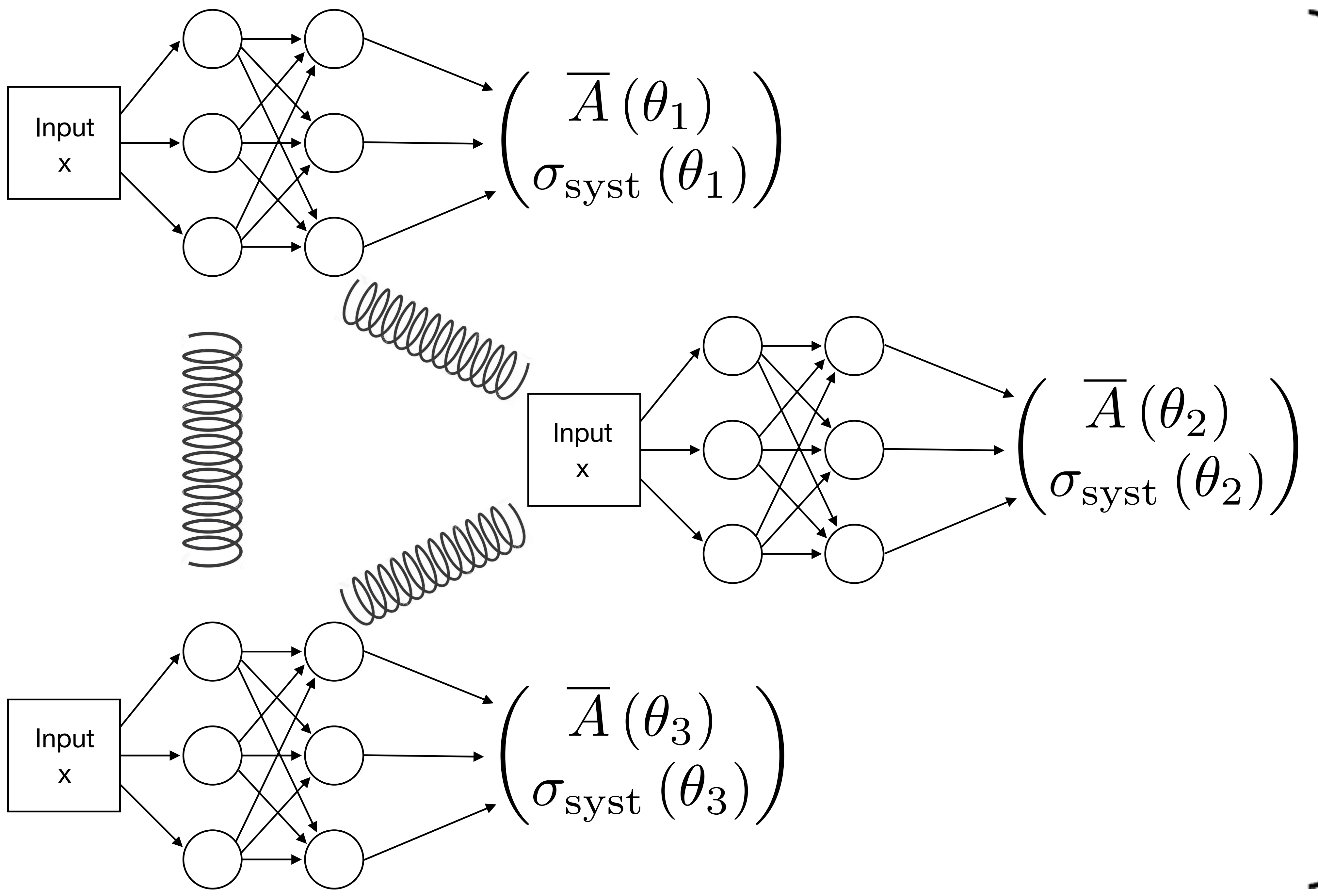

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- Repulsive term: Cover full posterior distribution
- Ensemble members **trained simultaneously**

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Learning amplitudes

- Learning only Amplitudes for different training sizes
- Compare full data to all but 10% largest

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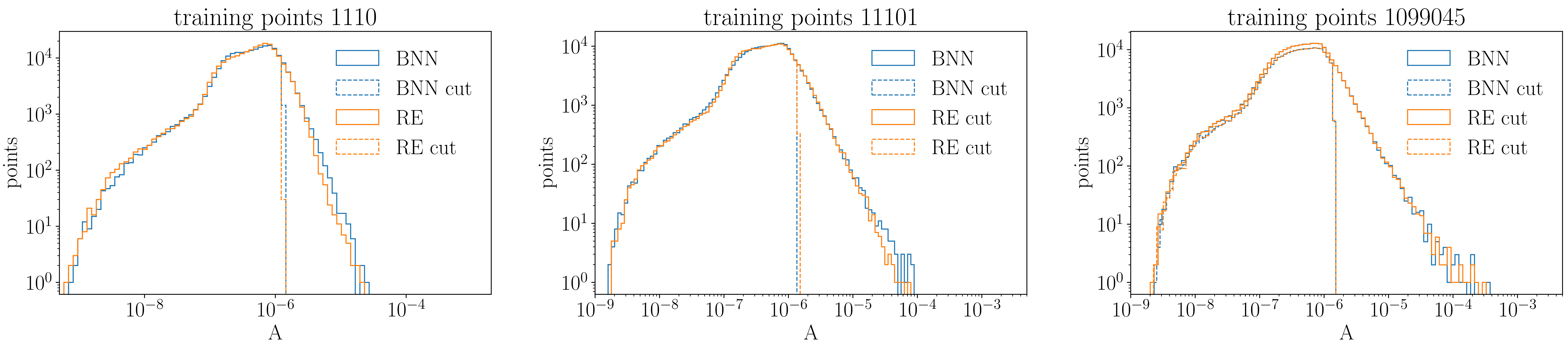

Uncertainties

Two uncertainty types:

Systematic and **statistical**

Plateaus for perfect training

Vanishes with perfect training

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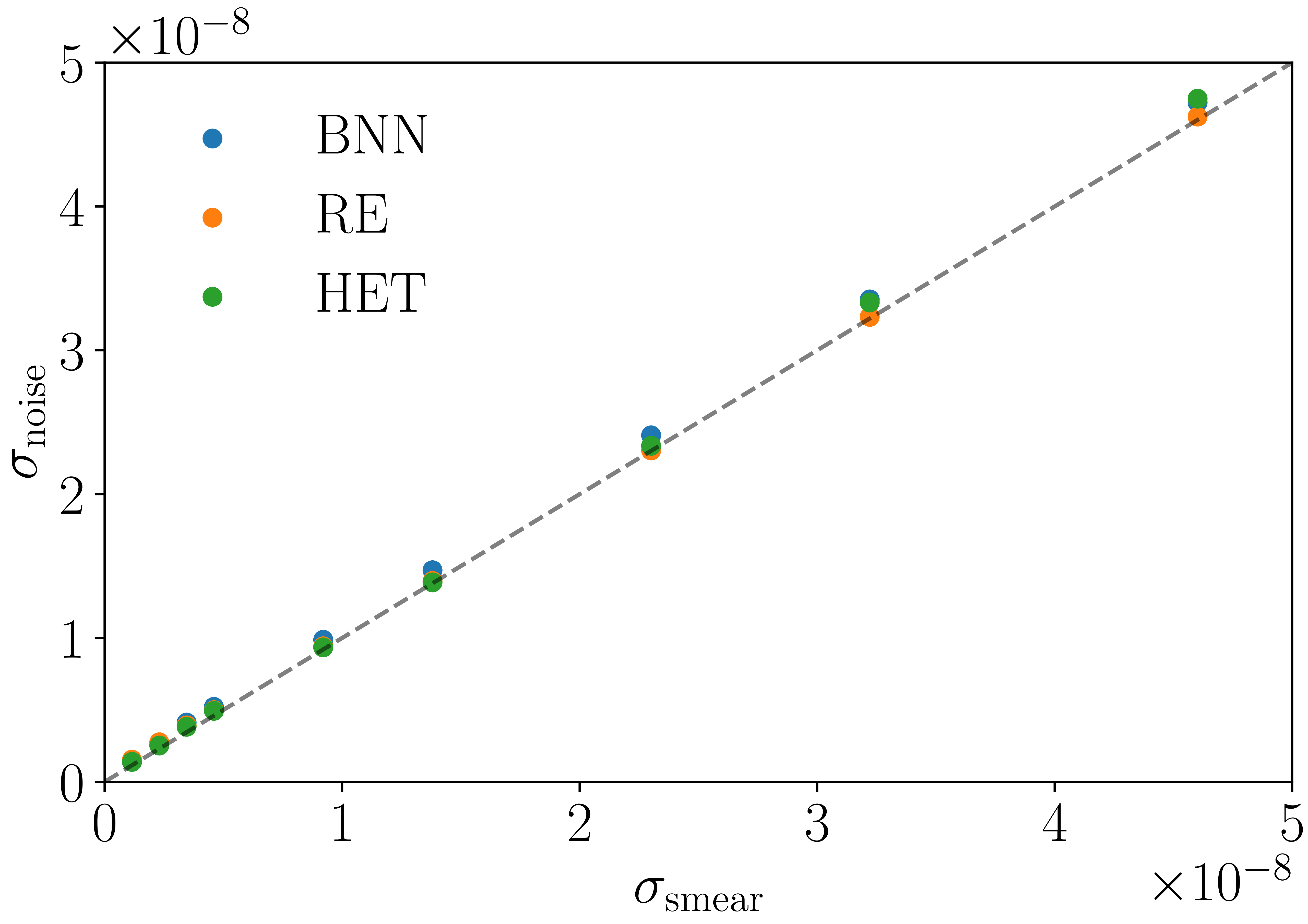
$$\sigma^2_{\text{tot}} \equiv \sigma^2_{\text{syst}} + \sigma^2_{\text{stat}}$$

Adding Gaussian noise

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

$$\sigma_{\text{smear}} = \{0.25, ..., 10\}\% \times A_{\text{truth}}$$



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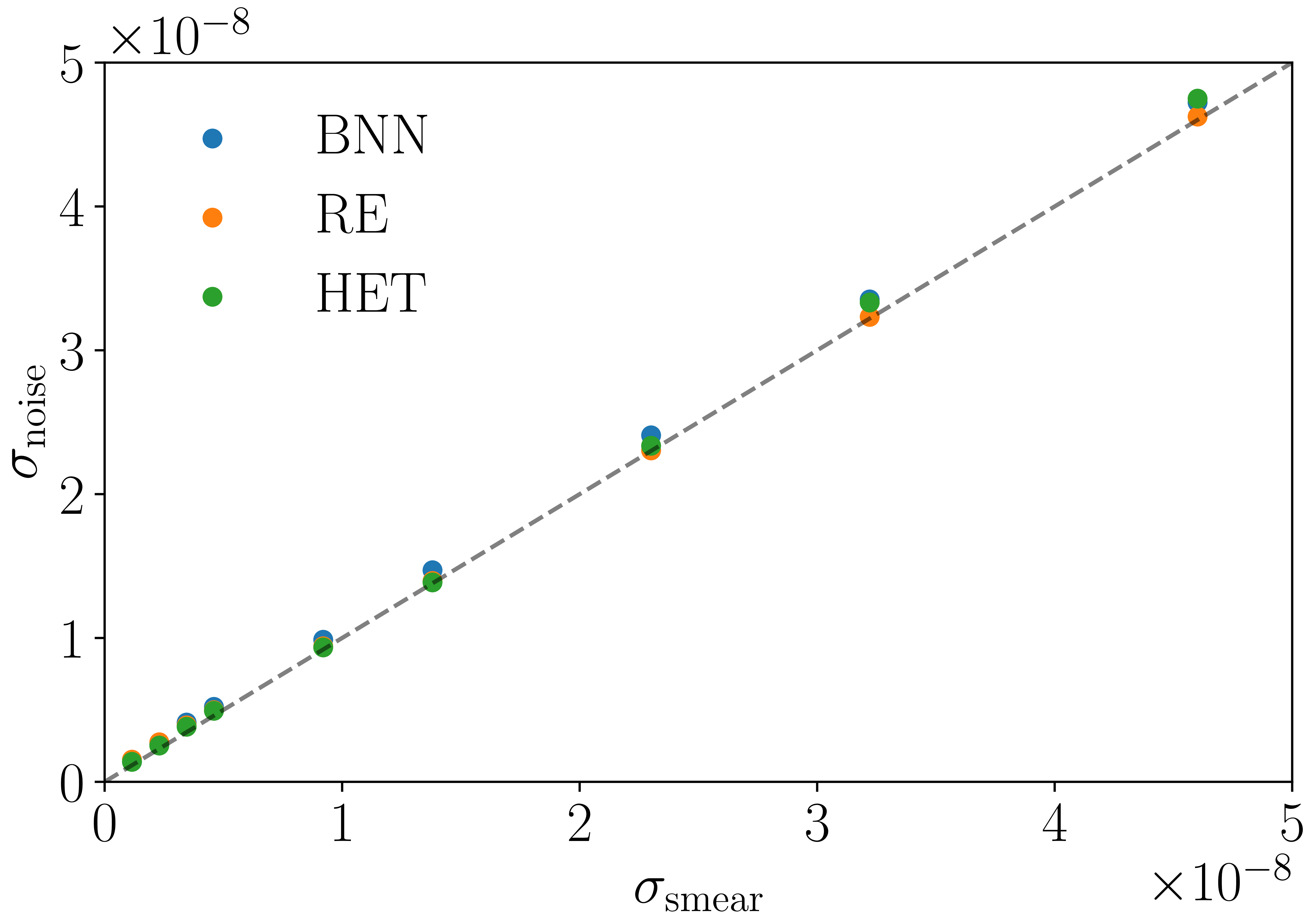
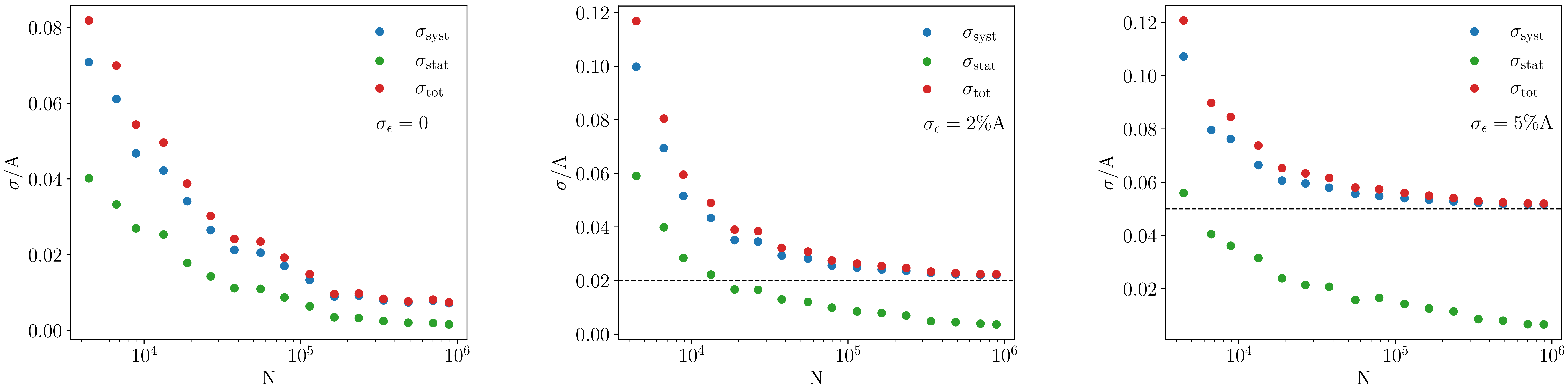
➡Get additional systematic uncertainty

➡Networks learn noise



Adding noise to the data



BNN only

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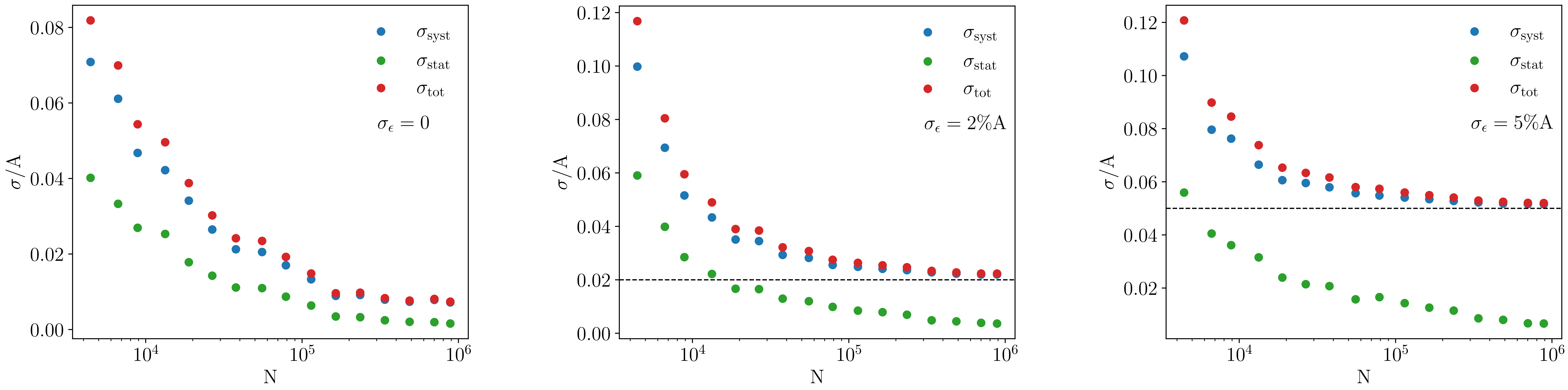

BNN only

1. Statistical uncertainty **independent** of noise
2. Systematic uncertainty **plateaus** on noise level

Pull distribution

Problem:

Uncertainties not comparable for different networks

Are uncertainties correctly learned?

Pull distribution

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Pull distribution

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Correctly learned uncertainty should follow a Gaussian shape

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Pull distribution

Pull distribution

noise	0%	1%	5%	10%
$\langle \sigma_{\text{het}}/A \rangle$	0.005	0.011	0.051	0.104
$\langle \sigma_{\text{syst, BNN}}/A \rangle$	0.006	0.012	0.052	0.103
$\langle \sigma_{\text{syst, RE}}/A \rangle$	0.005	0.011	0.050	0.101

Pull distribution

➡Same relative uncertainty but different pull distribution

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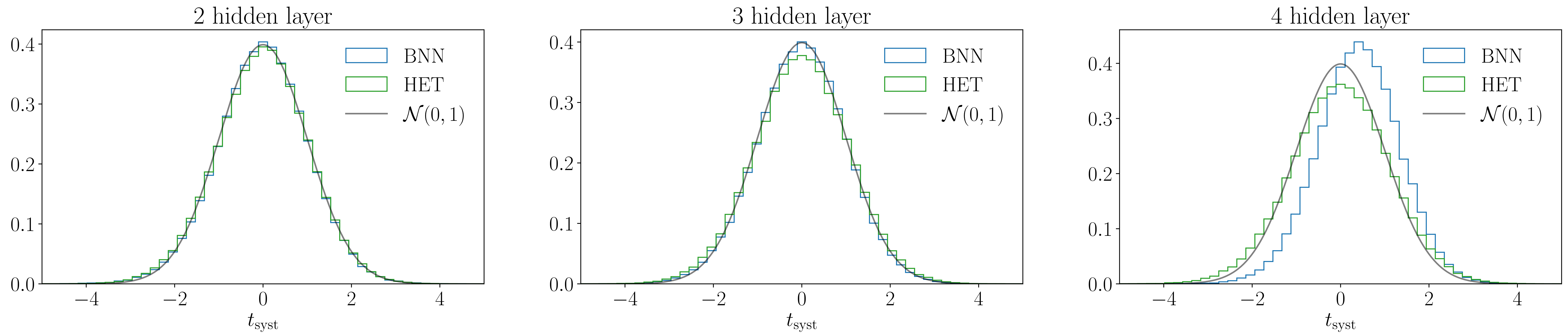

# hl	1	2	3	4	5	6
$\langle \sigma_{\text{het}}/A \rangle$	0.050	0.010	0.0056	0.0041	0.0038	0.0038
$\langle \sigma_{\text{syst, BNN}}/A \rangle$	0.050	0.012	0.0067	0.0076	0.016	0.017

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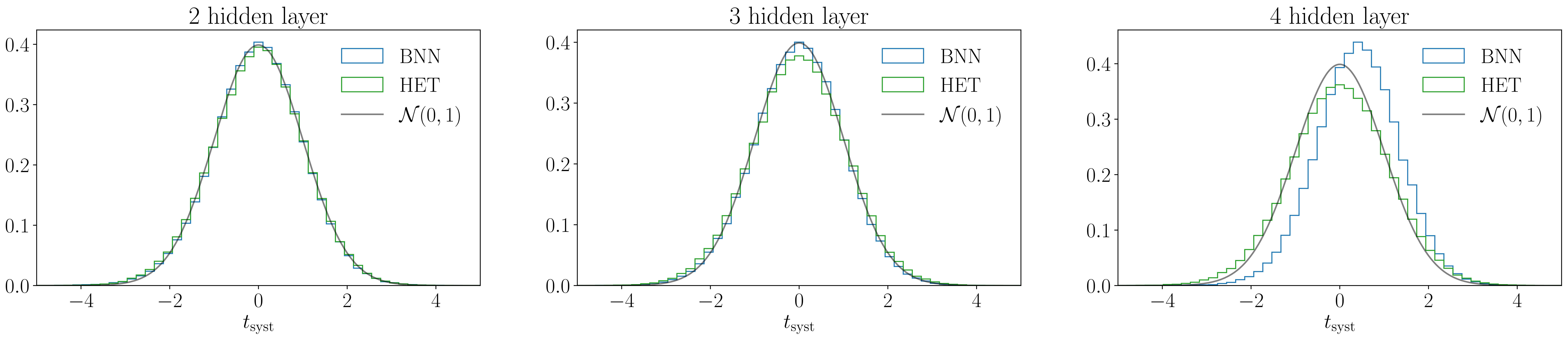

➡ Plateau for systematics from network size for het

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Reduce systematics

- Gain from different architectures
- Use Deep Set Invariants (DSI)
- Compare to heteroscedastic network with **invariant preprocessing**

network	$\langle \sigma / A \rangle$
HET	0.0056
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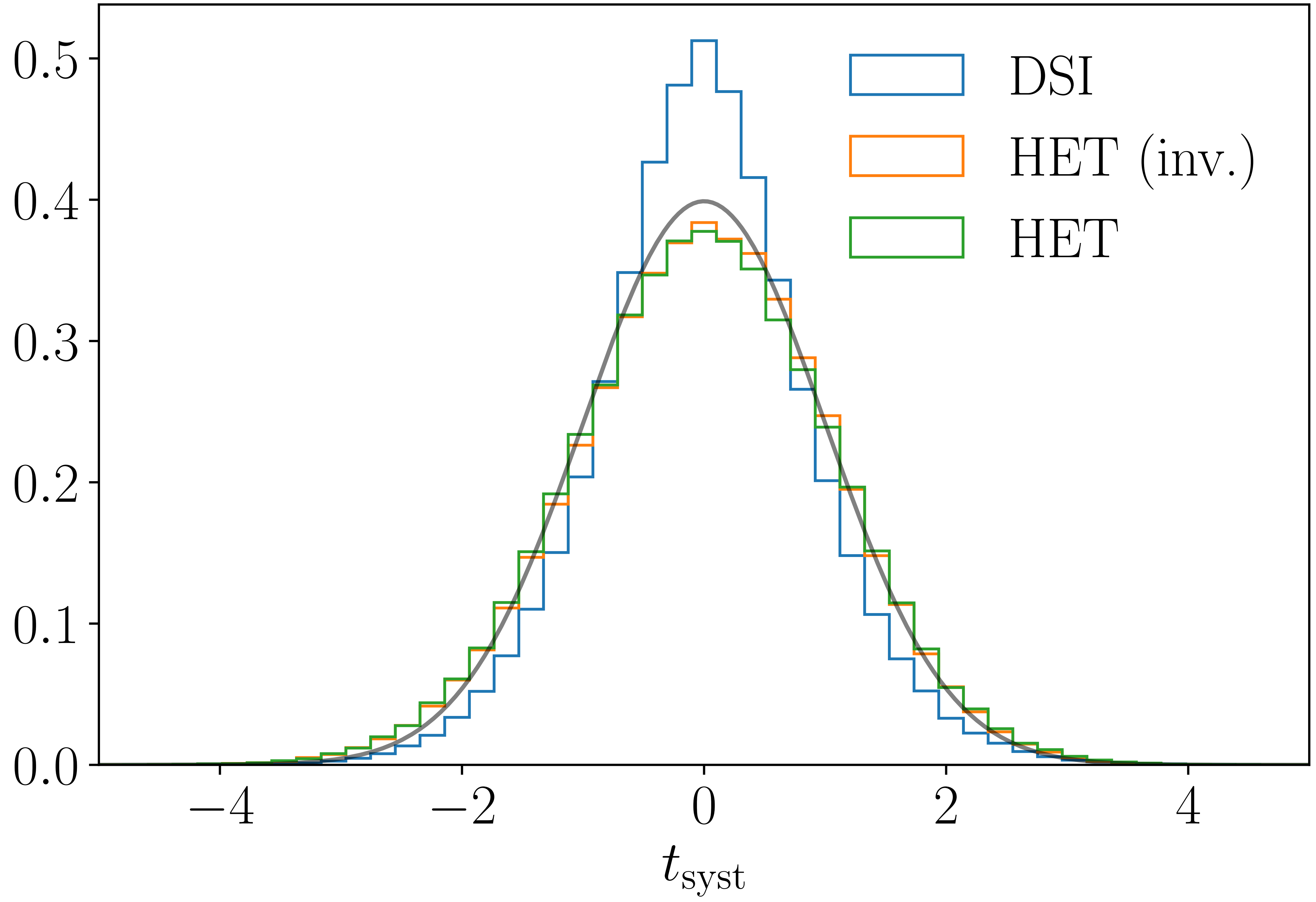

Conclusion and Outlook

1. Networks are able to learn Gaussian noise

2. Relative systematic uncertainties are similar but the pull distribution might look different

3. Reduce systematics by either changing the network size or include symmetries

Next: Look at statistical pull distribution, deeper look into the DSI

Thank you for your attention!