Accurate Surrogate Amplitudes with Calibrated Uncertainties

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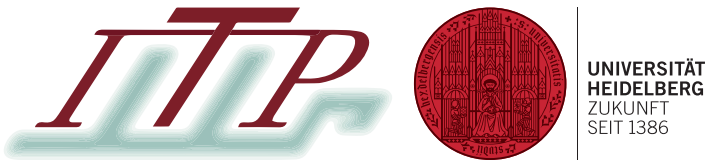
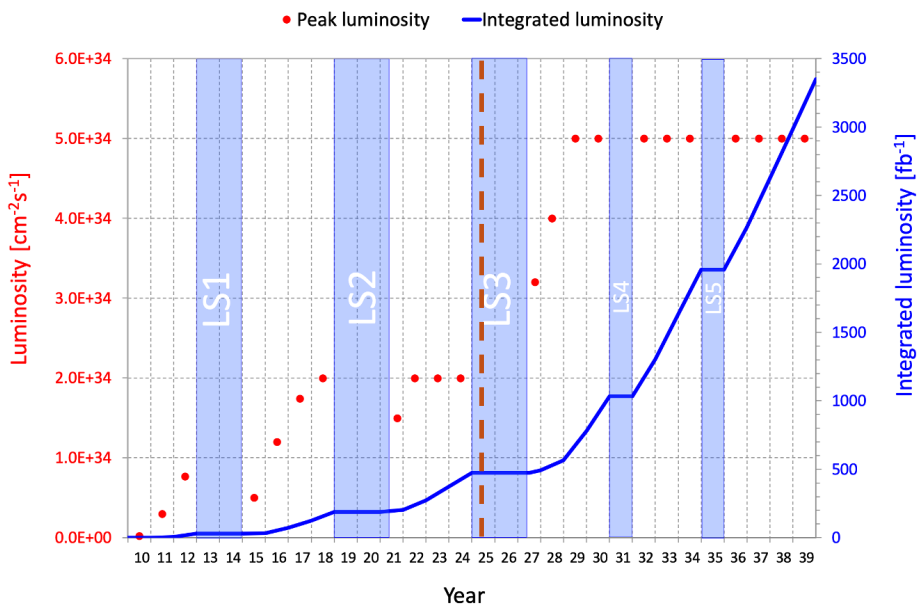
based on
2412.12069 in collaboration with Nina Elmer, Luigi Favaro,
Manuel Haußmann, Tilman Plehn, and Ramon Winterhalder



Particle Theory Seminar, Würzburg, 24.7.2025

The challenge ahead

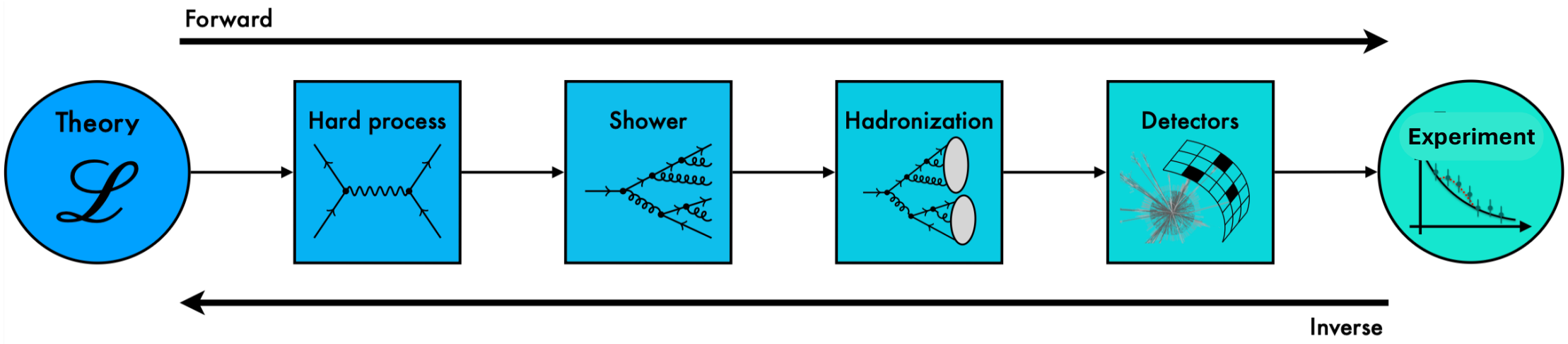
- general trend: larger-and-larger experiments collecting more-and-more data
- e.g. LHC: already enormous dataset will be further enlarged by a factor ~ 10
- costs for future experiments increasing



Fully exploit the available data!

- new analysis methods
- theory precision $\simeq$ experimental precision
- in particular: high-precision MC simulation

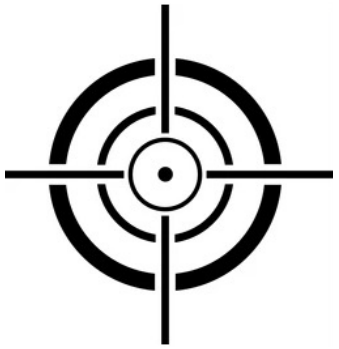
The particle physics workflow



ML can help with each of these steps by increasing

- accuracy/performance and/or
- increase speed

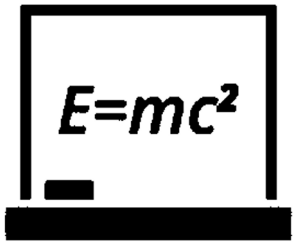
ML for particle physics



precision

speed

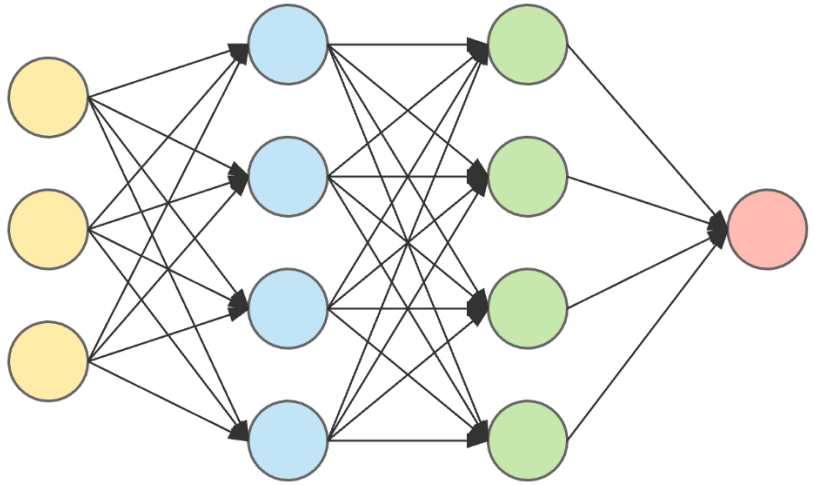
control



physics

Amplitude surrogates

$$|\mathcal{M}|^2 \approx$$



Case study for amplitude surrogates

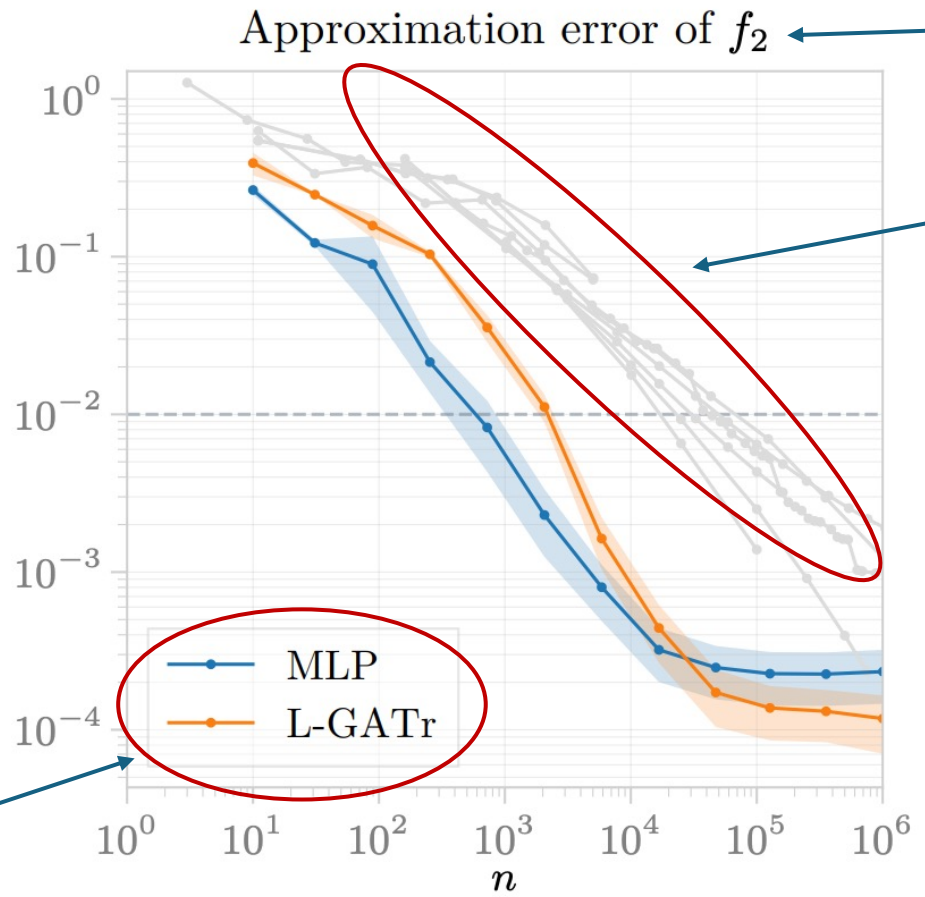
- evaluating analytic expressions for amplitudes $|\mathcal{M}|^2$ can be very expensive due to
  - higher-order corrections
  - large final-state multiplicities

- possible solution:
  - generate small training sample using full analytic expression
  - train a NN to approximate $|\mathcal{M}|^2$
  - generate events using NN surrogate, which is much faster to evaluate

➡ Does this work?

Comparison to classical interpolation

[Bresó et al., 2412.09534]



NLO $q\bar{q} \to t\bar{t}H$ amplitude

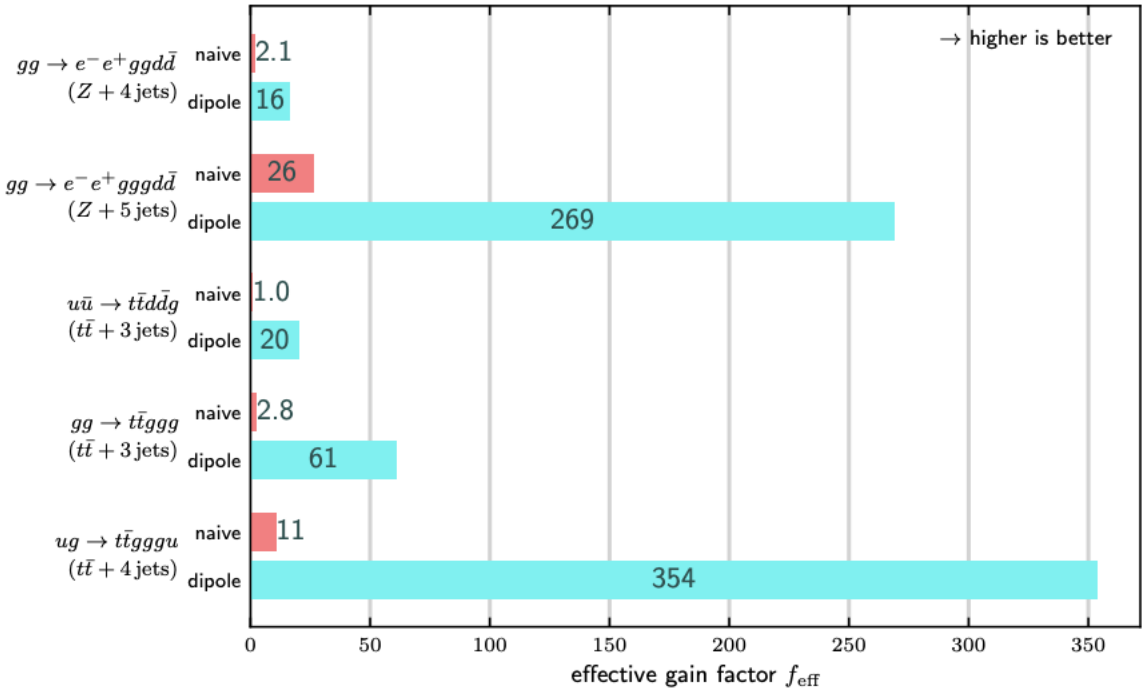
classical interpolation techniques

ML surrogates

ML surrogates outperform classical interpolation techniques

Speed comparison

[Janßen et al.,2301.13562]



	SHERPA default			with dipole-model surrogate				
Process	t_{ME}[ms]	t_{PS}[ms]	ϵ_{full}	t_{surr}[ms]	$x_{\max}$	$\epsilon_{\text{1st,surr}}$	$\epsilon_{\text{2nd,surr}}$	f_{eff}
$gg \to e^- e^+ ggd\bar{d}$	54	0.40	1.411 %	0.14	2.6	1.418 %	39 %	16
$gg \to e^- e^+ gggd\bar{d}$	16 216	5.70	0.076 %	0.20	3.6	0.085 %	29 %	269

$$f_{\text{eff}} = \frac{T_{\text{standard}}}{T_{\text{surrogate}}}$$

dipole vs naïve:
encode singularity structure of amplitudes

→ Large speed-ups possible!

↓

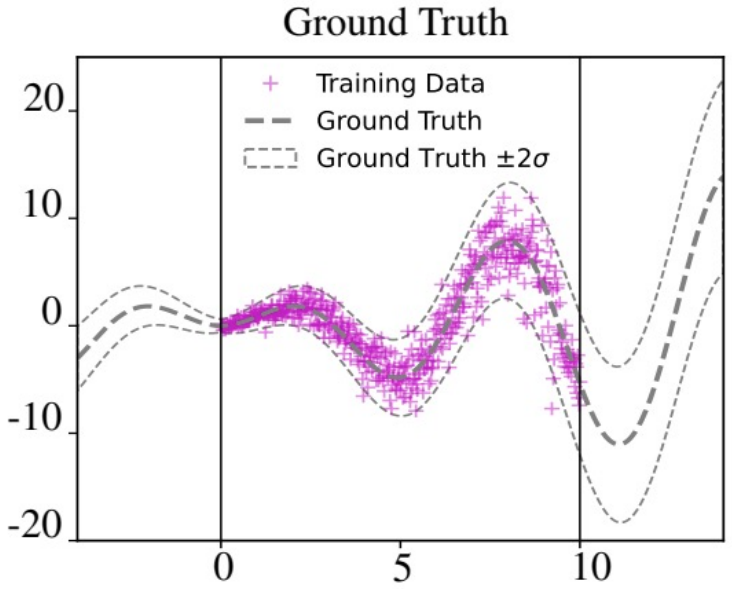
Can we also control the uncertainties?

Learning uncertainties

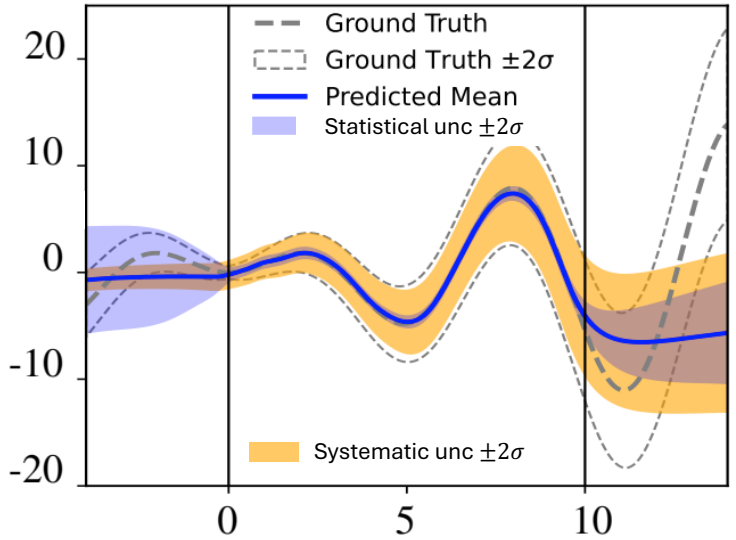
"All models are wrong, but some — those that know when they can be trusted — are useful!"

— George Box (adapted)

Regression with uncertainties



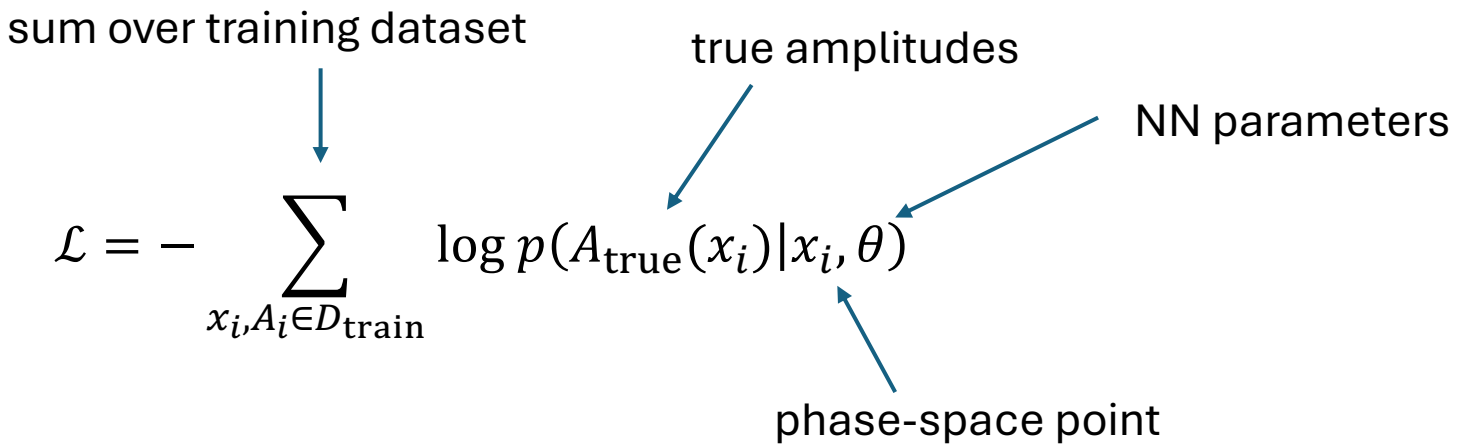
[Yi&Bessa, 2505.02743]



- statistical or epistemic uncertainty ≙ lack of training data
- systematic or aleatoric uncertainty ≙ noise in the data, lack in model expressivity

Systematic uncertainty: heteroskedastic loss

- log-likelihood loss:



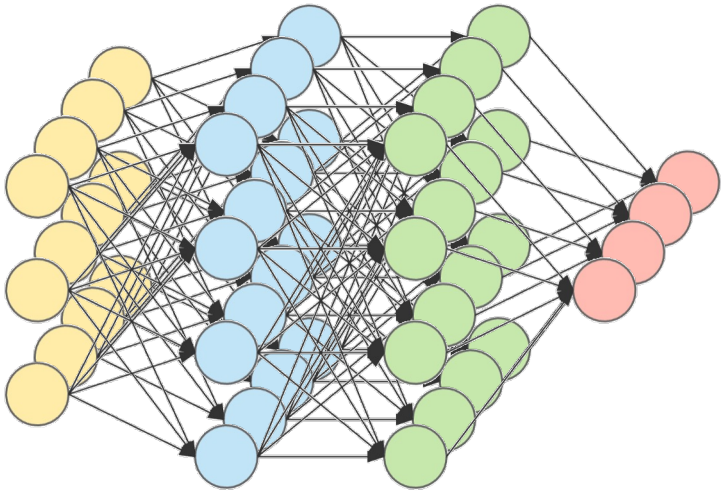
- assume Gaussian likelihood: $p(A|x,\theta) = \mathcal{N}(\overline{A}(x), \sigma^2_{\text{syst}}(x))$
- NN learns both: $\overline{A}(x)$ and $\sigma_{\text{syst}}(x)$

$$\Rightarrow \text{heteroskedastic loss: } \mathcal{L} = \sum_i \left[\frac{\left(\overline{A}(x_i) - A_{\text{true}}(x_i)\right)^2}{2\sigma^2_{\text{syst}}(x_i)} + \log\left(\sigma_{\text{syst}}(x_i)\right) \right]$$

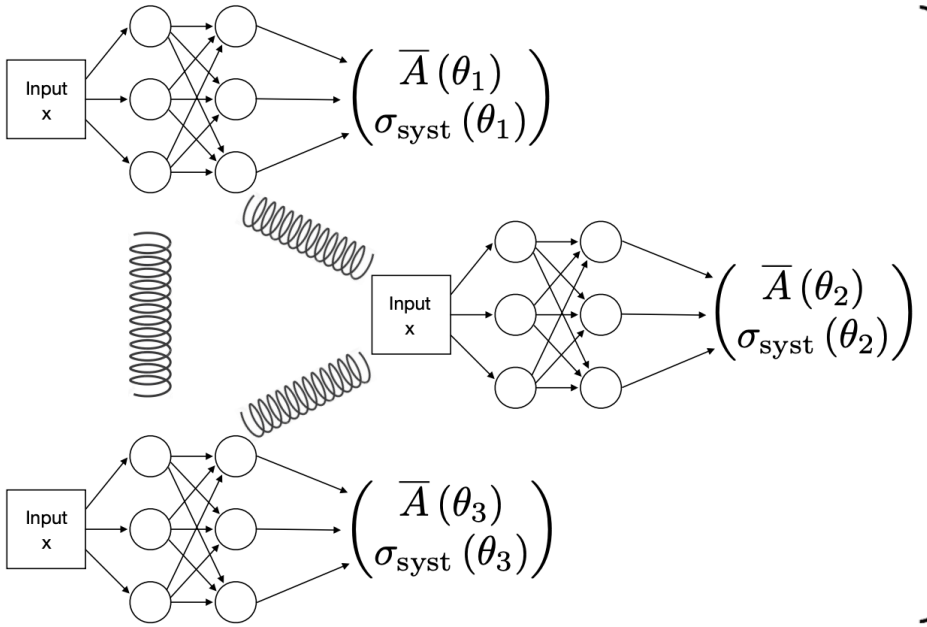
- constant $\sigma_{\text{syst}} \rightarrow$ recovers MSE loss

Statistical uncertainty: repulsive ensemble

- train ensemble of networks
- ensure convergence to correct posterior via repulsive interaction between ensemble members
- each networks leads to slightly different result
- spread of network predictions ~ statistical uncertainty
- less data → higher spread



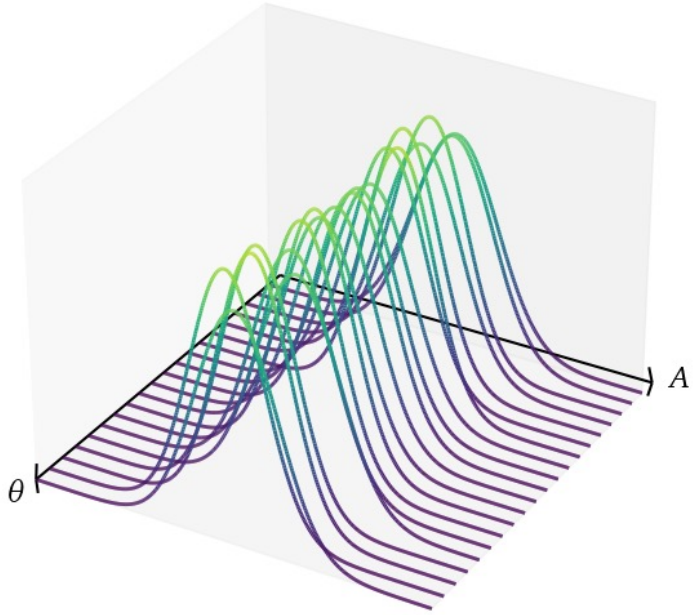
Repulsive ensemble + heteroskedastic loss



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

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

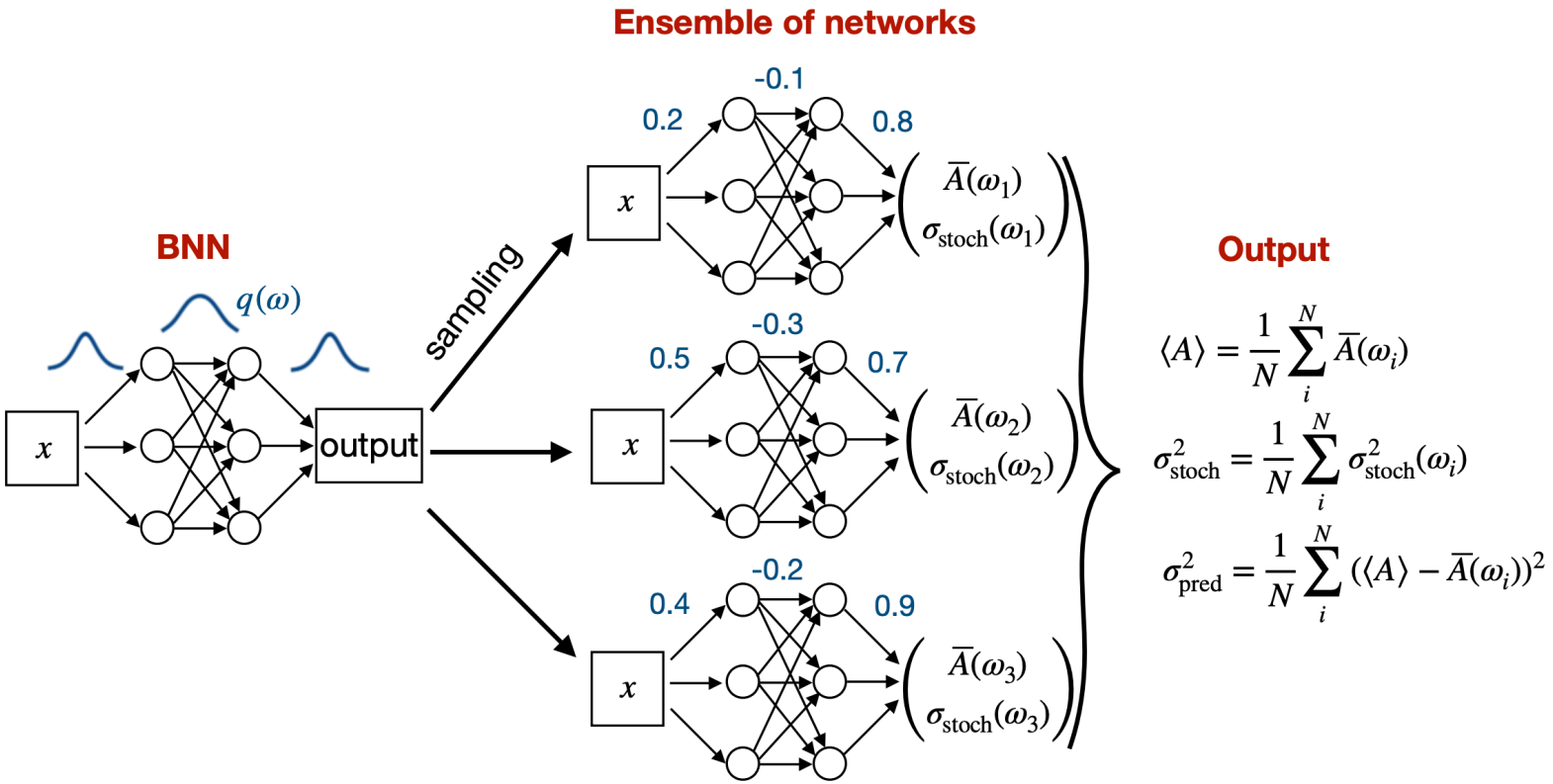
$$\sigma^2_{\text{stat}} = \frac{1}{N} \sum_i^N \left(\langle A \rangle - \overline{A}(\theta_i) \right)^2$$



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

Combined learnable modelling of systematic and statistical uncertainties!

Alternative: Bayesian NNs



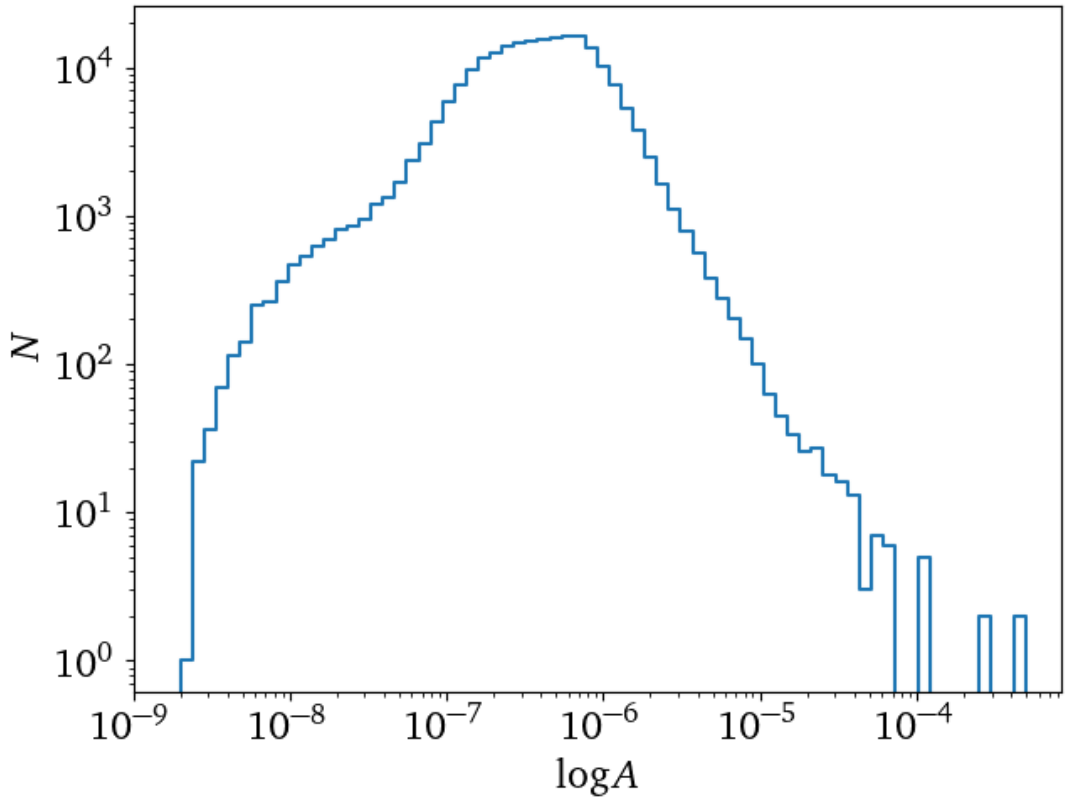
- promote NN parameters to Gaussians $q(\theta)$
- for each evaluation, sample from Gaussians
- learn means and widths

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

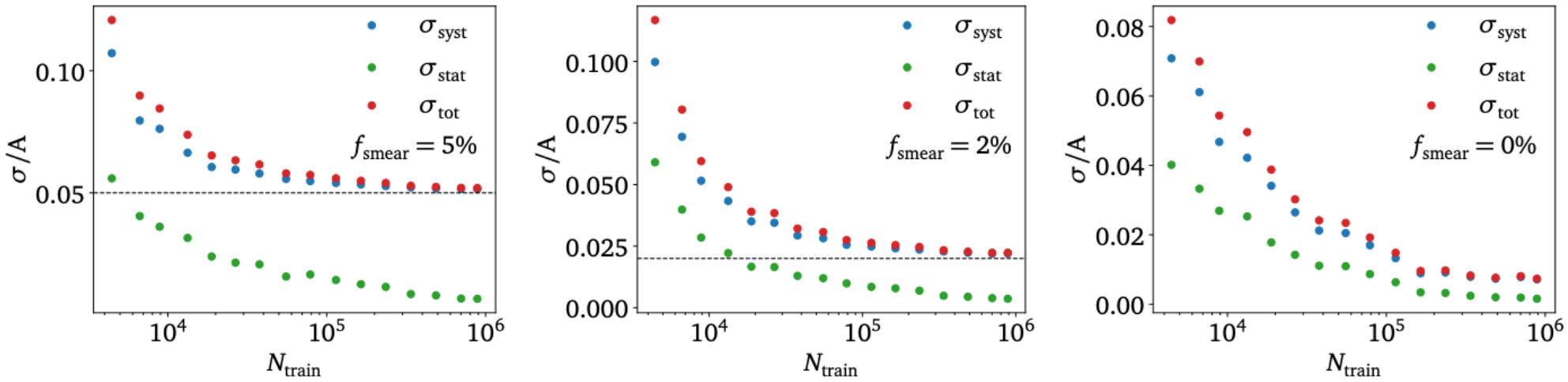
prior

$gg \to \gamma\gamma g$ dataset

- generated using Sherpa+Njet
- 1.1 million events, 70% used for training
- preprocessing:
  - learn logarithm of amplitude
  - rescale inputs and log-amplitudes to have zero mean and unit standard deviation
- amplitude symmetries
  - Lorentz-invariant
  - permutation-invariance w.r.t. identical particles



Behavior of learned uncertainties



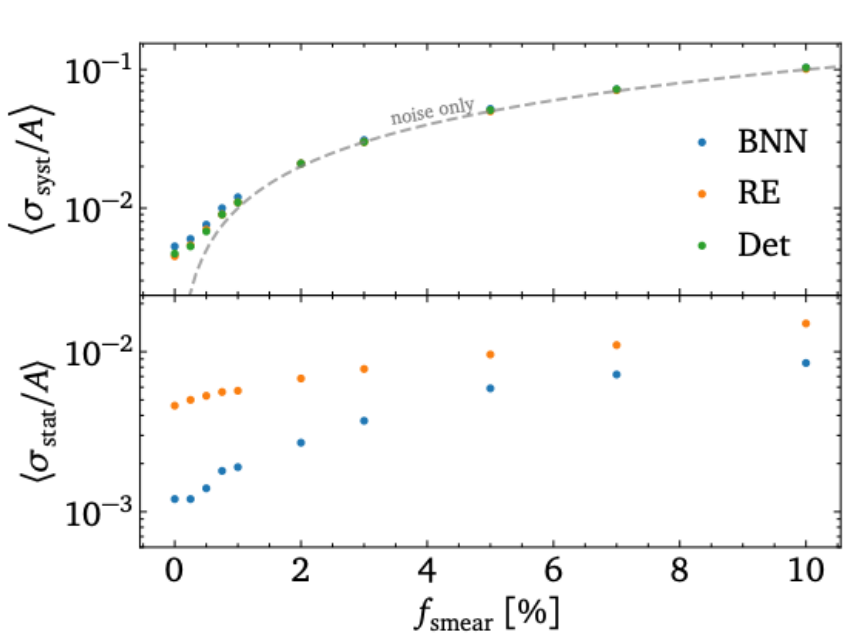
Test: apply different levels of Gaussian noise to amplitudes

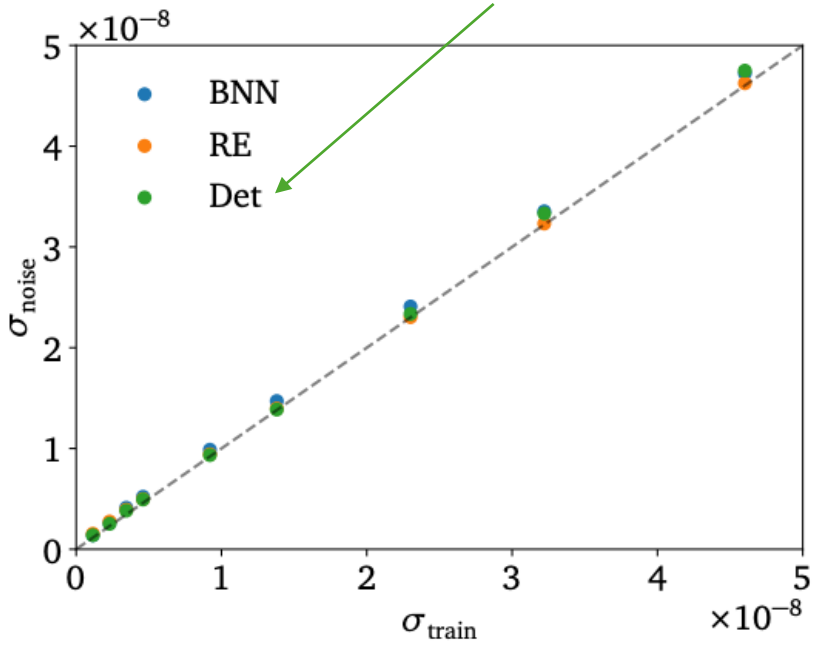
- statistical uncertainty decreases with more training data
- systematic uncertainty converges to level of applied noise

$$A_{\text{train}} \sim \mathcal{N}(A_{\text{true}}, \sigma^2_{\text{train}})$$
$$\sigma_{\text{train}} = f_{\text{smear}} A_{\text{true}}$$

Extracting the noise level

only heteroskedastic loss, no σ_{stat}





with $\sigma^2_{\text{noise}} = \sigma^2_{\text{syst}} - \sigma^2_{\text{syst},0}$ and $\sigma^2_{\text{syst},0}$ being the systematic unc. due to limited NN expressivity.

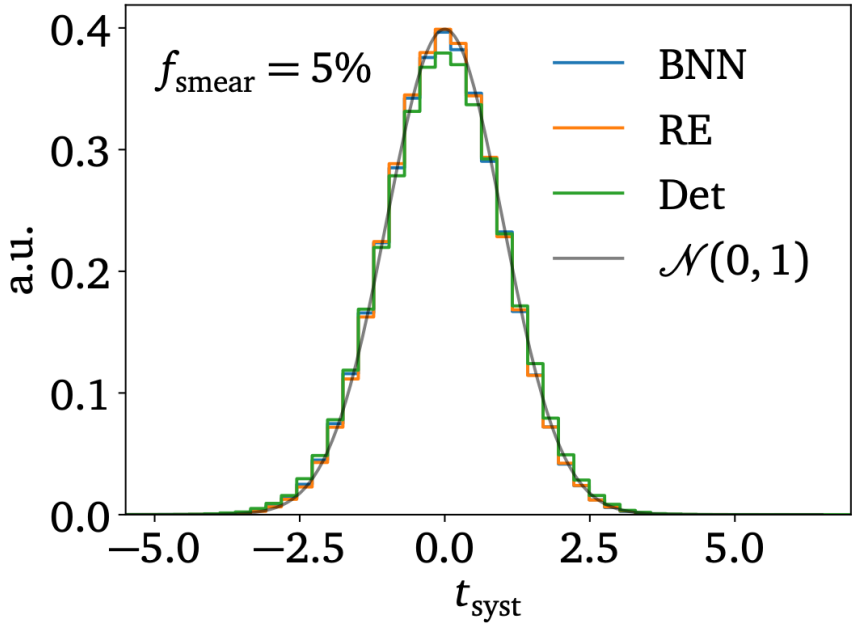
Able to reliably extract noise level!

Are these uncertainties calibrated?

- statistical uncertainties play minor role for amplitude regression
- define systematic pull:

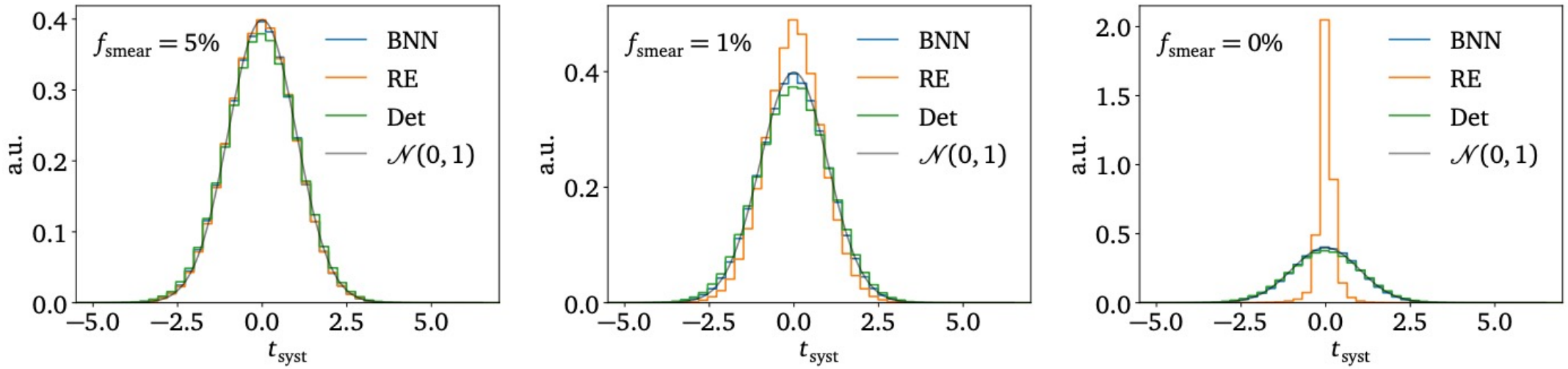
$$t_{\text{syst}} = \frac{\langle A \rangle(x) - A_{\text{train}}(x)}{\sigma_{\text{syst}}(x)}$$

- if calibrated, t_{syst} distribution should follow $\mathcal{N}(0, 1)$



Almost perfectly calibration → reliable uncertainty estimate

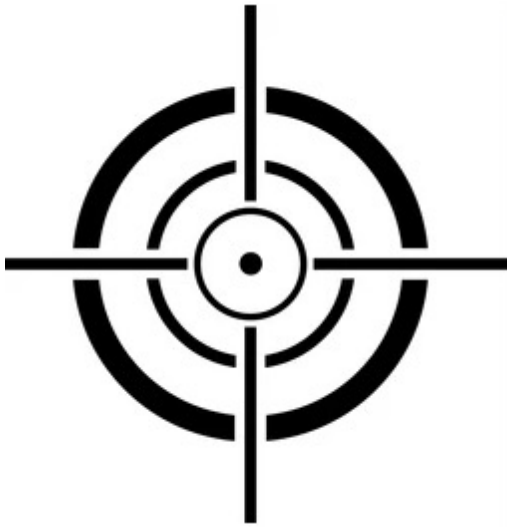
Dependence on smearing



- BNN and deterministic models
  → well calibrated for different smearing levels

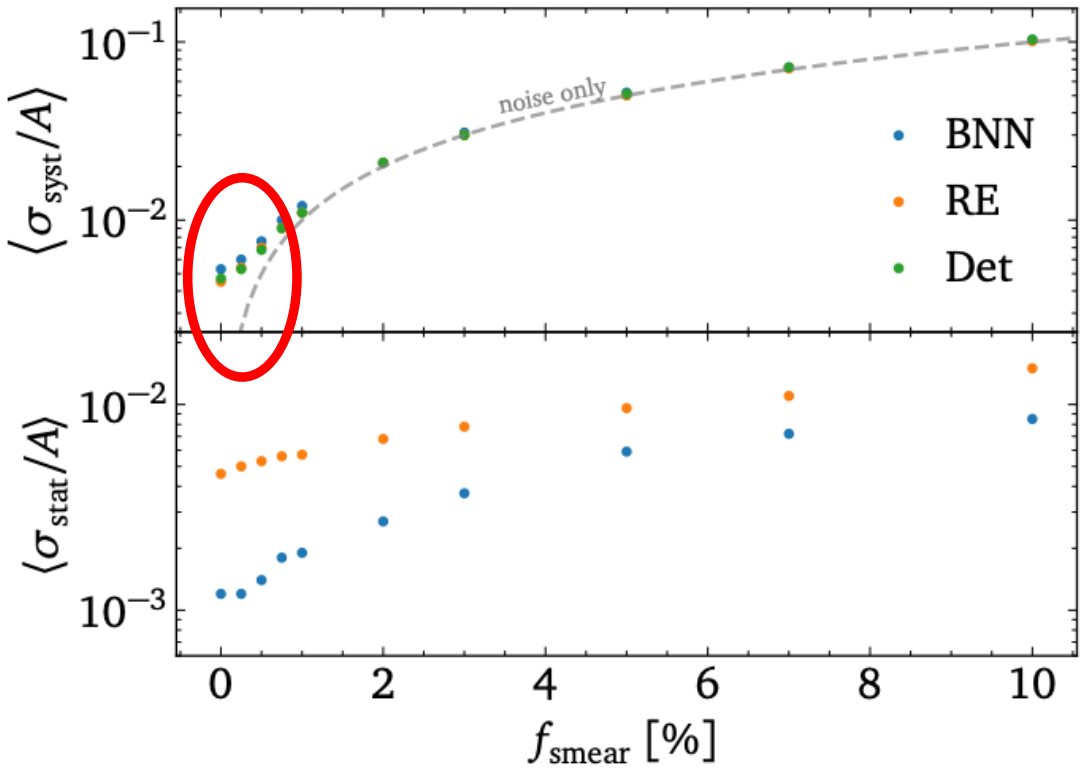
- repulsive ensemble overestimates uncertainty for low smearing
  → see below

Pushing for precision



activations, layers, and domain knowledge

Enhancing NN expressivity

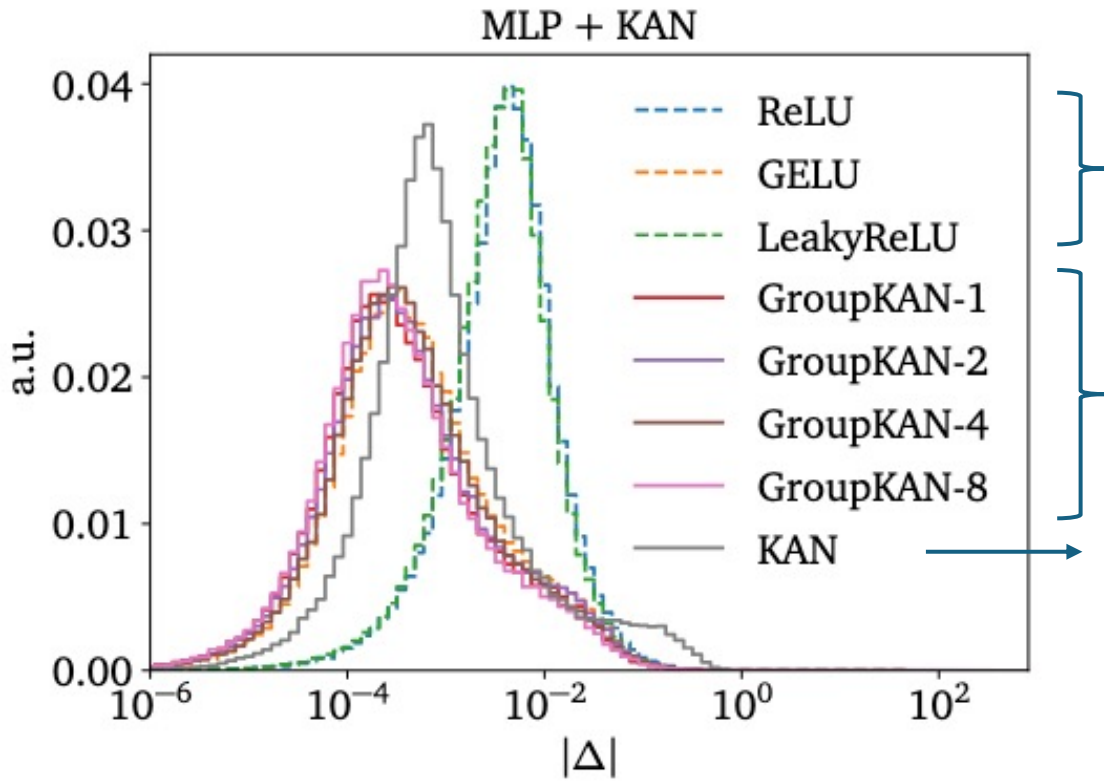


Can we improve accuracy for low smearing?

Improve NN expressivity:

- different activations, NN structures
- more layers,
- exploit symmetries

Activation functions and NN structure



static activation functions

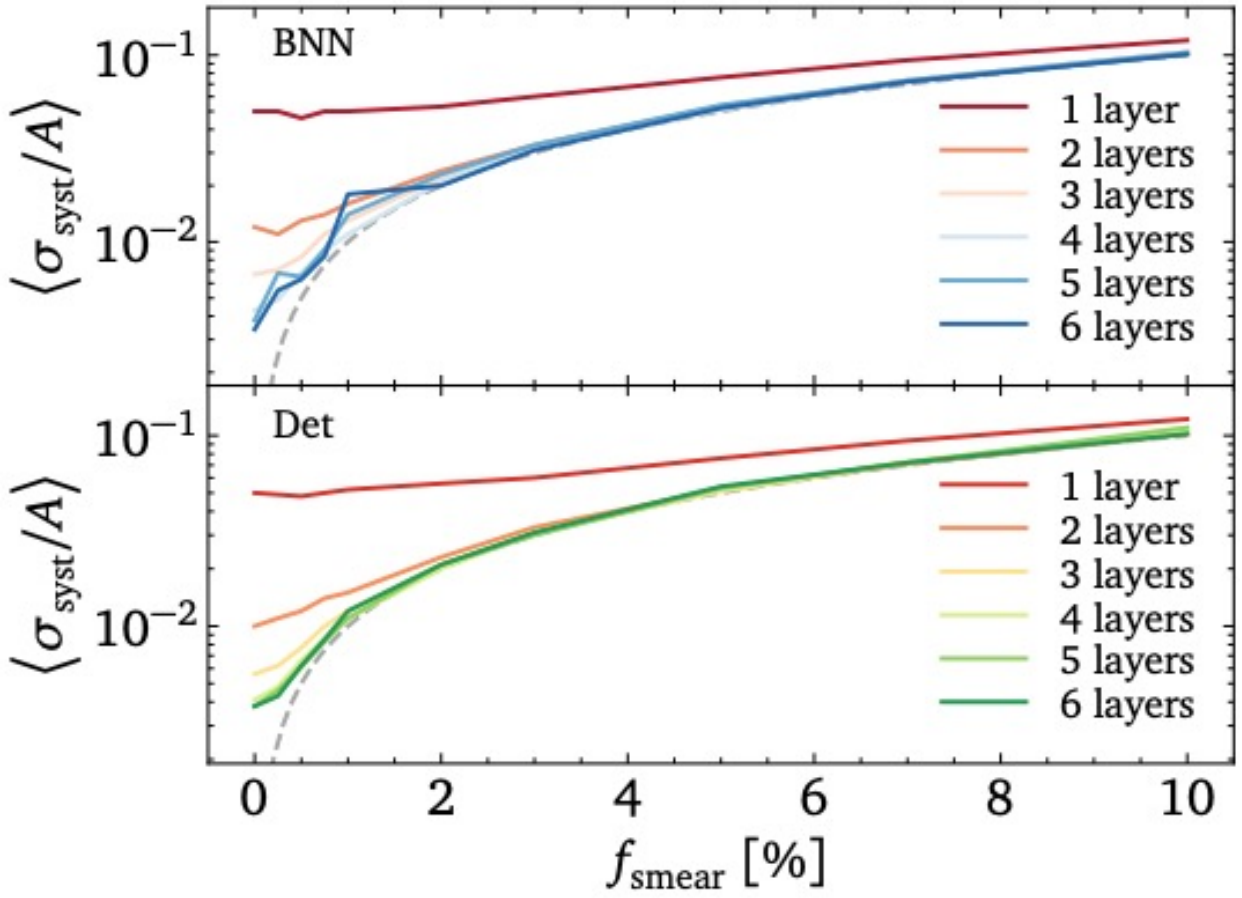
learned activation functions

Kolmogorov-Arnold Network

relative deviation: $\Delta = \frac{A_{\mathrm{NN}} - A_{\mathrm{true}}}{A_{\mathrm{true}}}$

well-chosen activation function can significantly improve performance

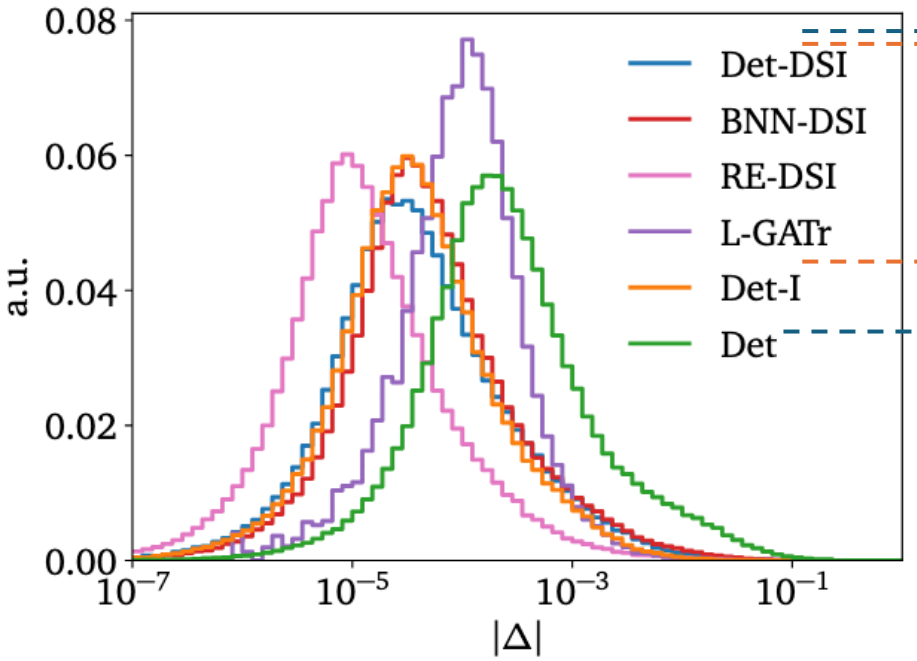
Adding more layers



adding more layers

convergence towards noise level

Encoding our physics knowledge

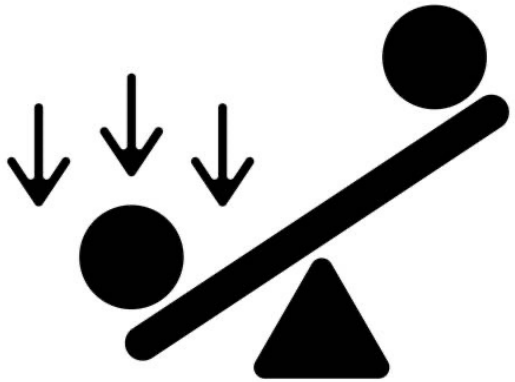


permutation invariance

Lorentz invariance

relative deviation: $\Delta = \frac{A_{\mathrm{NN}} - A_{\mathrm{true}}}{A_{\mathrm{true}}}$

Large gain in NN accuracy! Also found uncertainties still to be well calibrated.



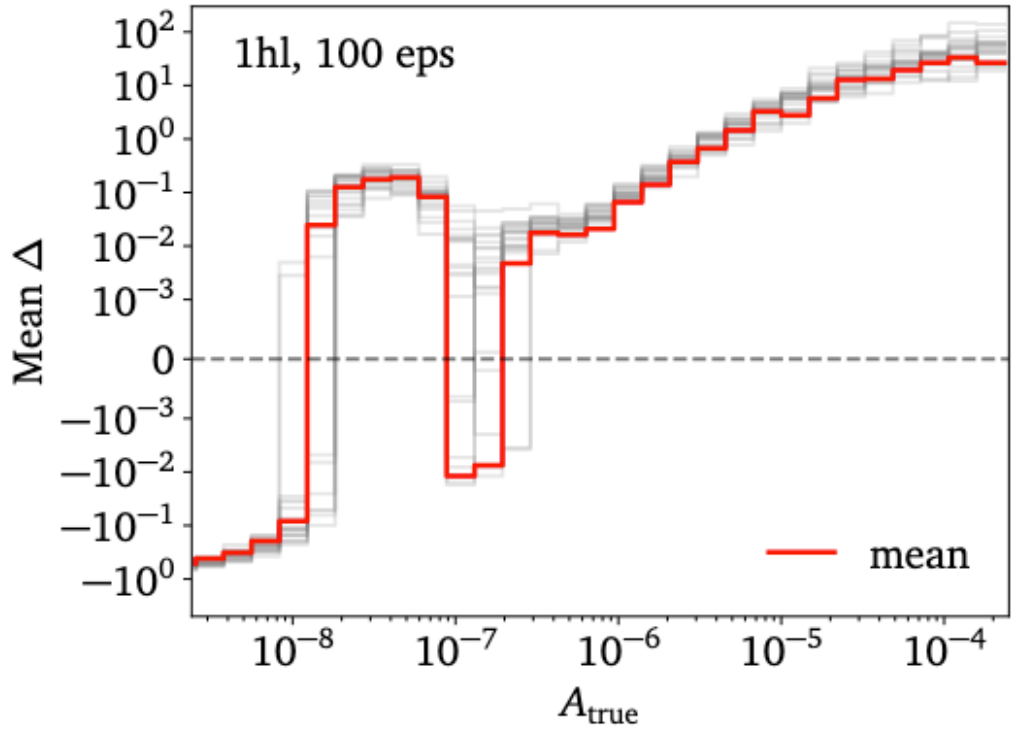
Ensembling and biases

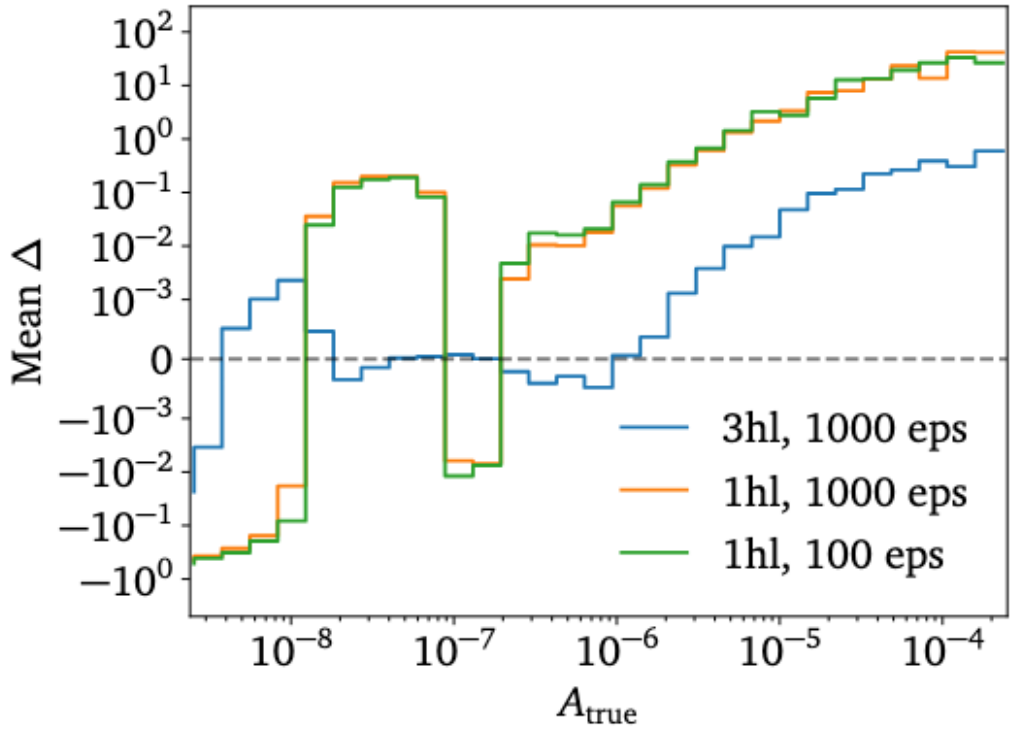
The wisdom (and biases) of the crowd.

[HB, Elmer, Plehn, Winterhalder, to appear]

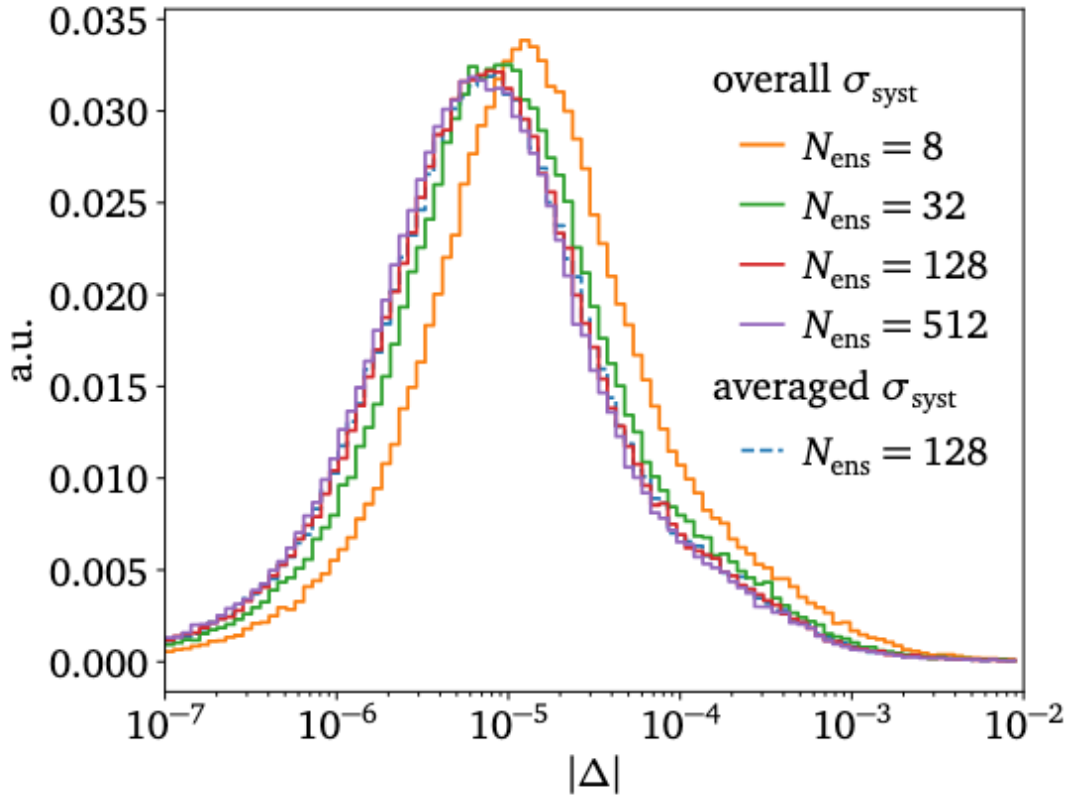
Ensembling and biases

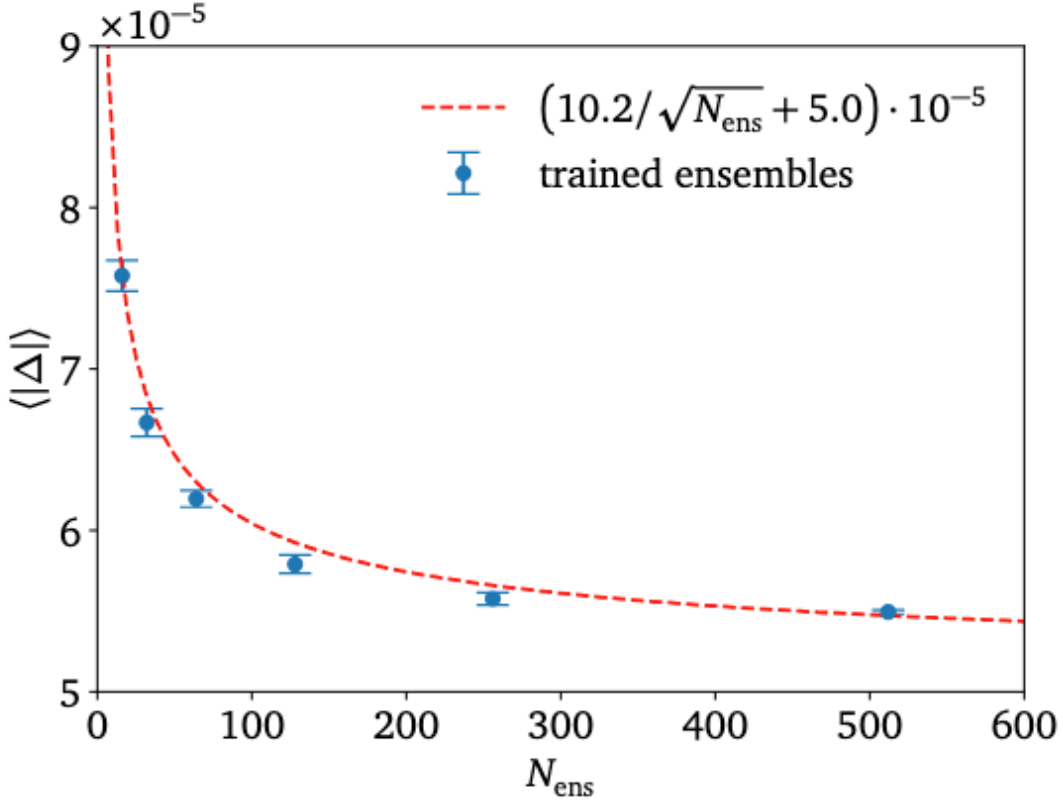
- ensembling averages out noise → widely used
- but, their can be systematic biases





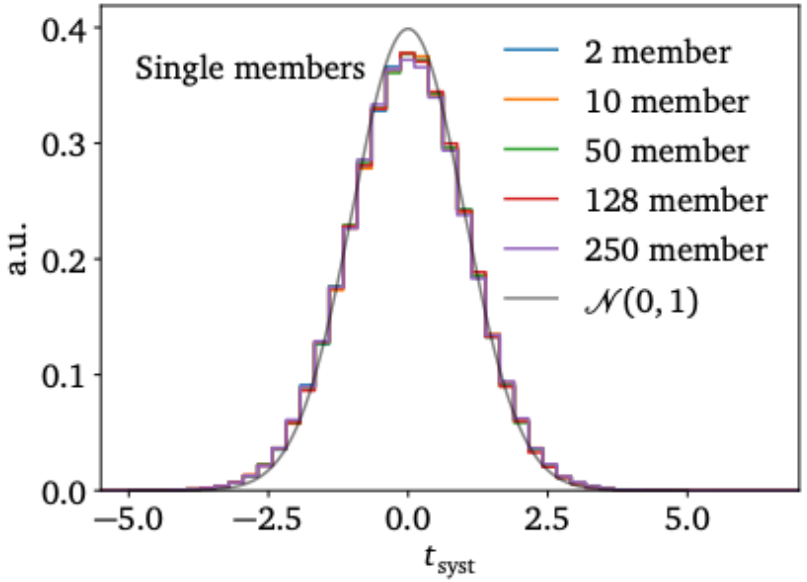
Extracting the biases

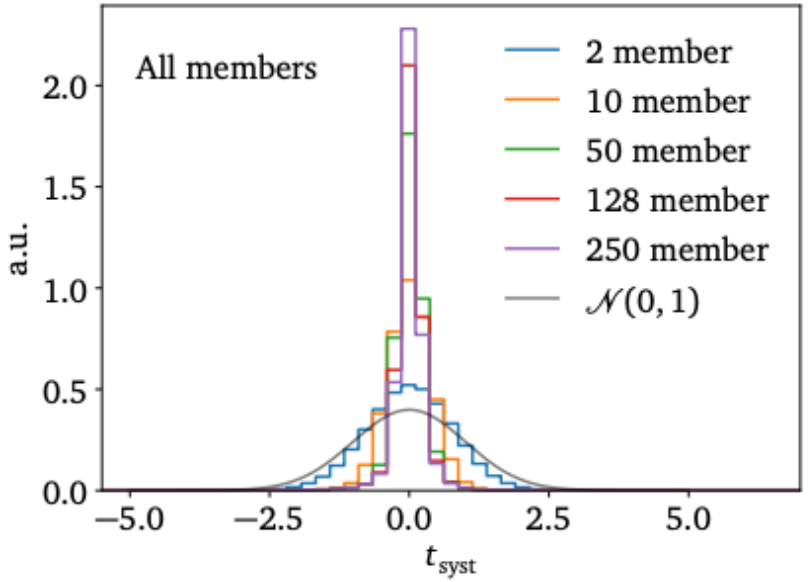




ensembling increases precision, but gains level off for $N_{\text{ens}} \gtrsim 100$

Miscalibration of ensemble systematic





$$A_{\text{NN}}(x) = \frac{1}{N_{\text{ens}}} \sum_{i=1}^{N_{\text{ens}}} A_{\text{NN},i}(x)$$

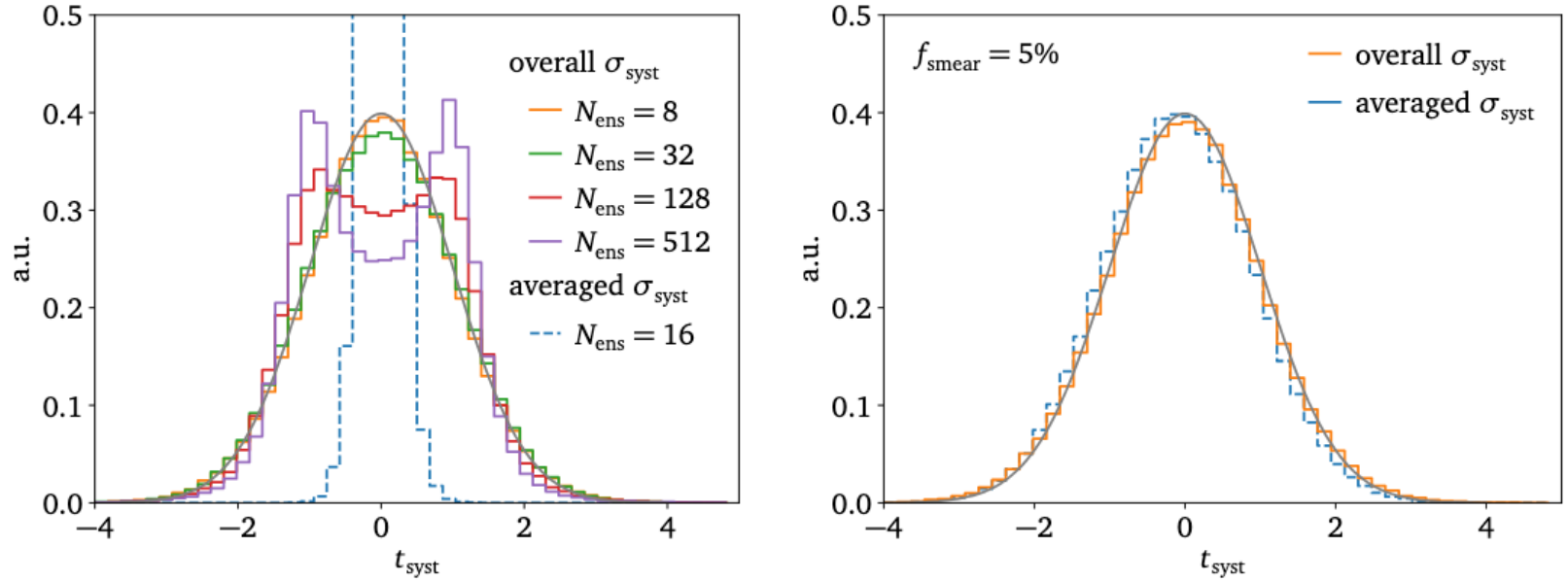
$$\sigma^2(x) = \frac{1}{N_{\text{ens}}} \sum_{i=1}^{N_{\text{ens}}} \sigma_i^2(x)\,.$$

- averaging systematic unc. of ensemble members ~ average uncertainty of each member
- but ensemble more precise

Fixing ensemble systematic unc.

$$A_{\mathrm{NN}}(x) = \frac{1}{N_{\mathrm{ens}}} \sum_{i=1}^{N_{\mathrm{ens}}} A_{\mathrm{NN},i}(x) \qquad \mathcal{L}_\sigma = \frac{1}{B} \sum_{b=1}^{B} \left[\frac{|A_{\mathrm{train}}(x_b) - A_{\mathrm{NN}}(x_b)|^2}{2\sigma^2(x_b)} + \log \sigma(x_b) \right]$$

solution: train separate network with loss $\mathcal{L}_\sigma$ to predict systematic uncertainty of ensemble



lower noise levels → non-Gaussian biases become visible

Localized smearing

Is the systematic uncertainty able to pick-up local noise?

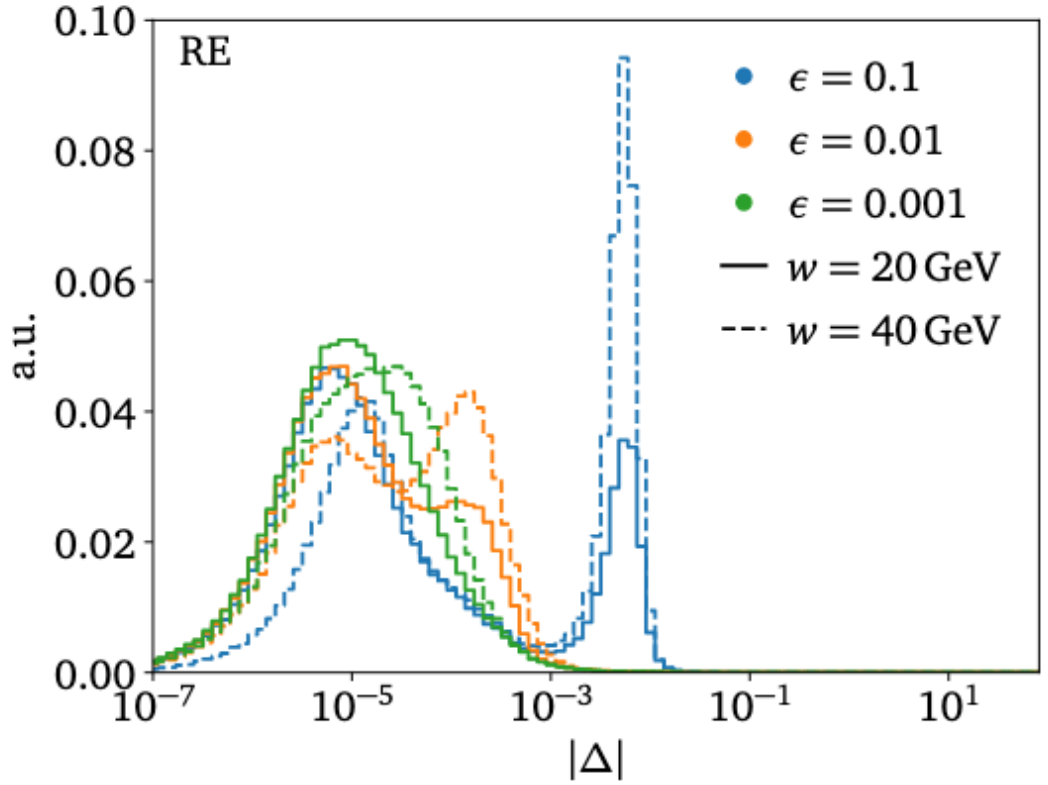
[HB et al., to appear]

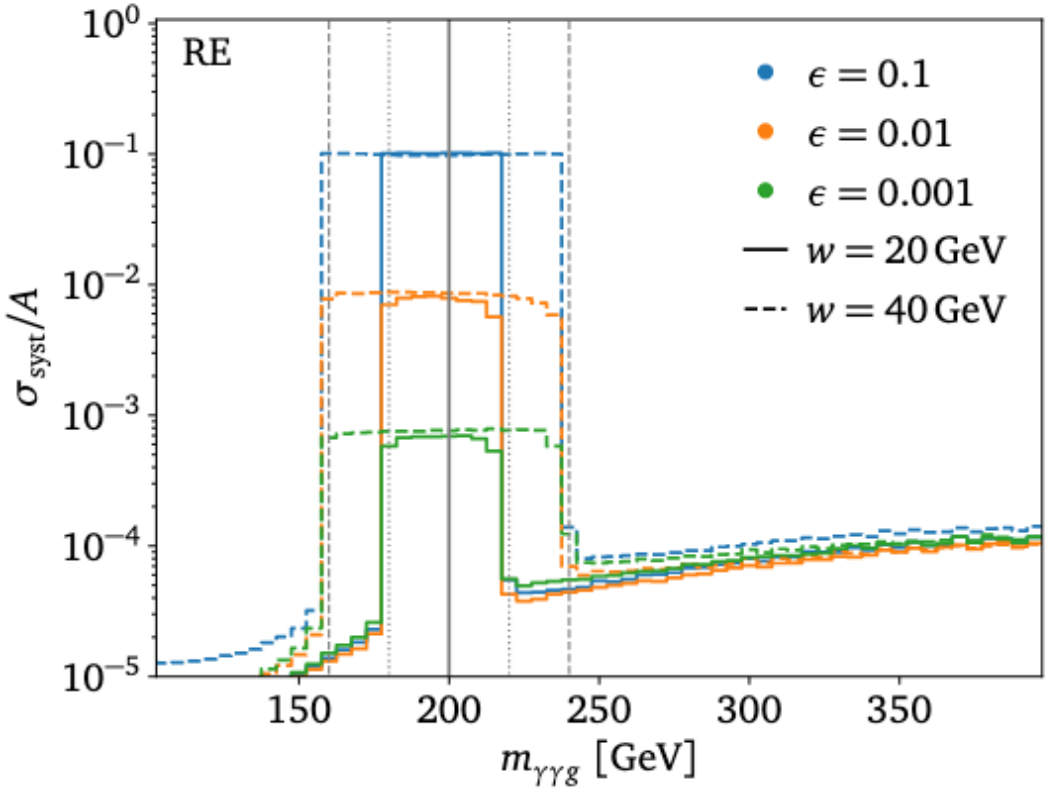
Box smearing

- analytic amplitude evaluation might loss precision close to thresholds, kinematic edges, …
- can the learned systematic uncertainties pick this up?
- test this by inducing local noise to our amplitudes
- simple start: box smearing with $m_{\text{thresh}} = 200\ \text{GeV}$

$$A_{\text{train}}(x) = \begin{cases} \mathcal{N}\left(A_{\text{true}}(x), \epsilon A_{\text{true}}(x)\right) & \text{if } |m_{\gamma\gamma g}(x) - m_{\text{thresh}}| < w \\ A_{\text{true}} & \text{if } |m_{\gamma\gamma g}(x) - m_{\text{thresh}}| \geq w \end{cases}$$

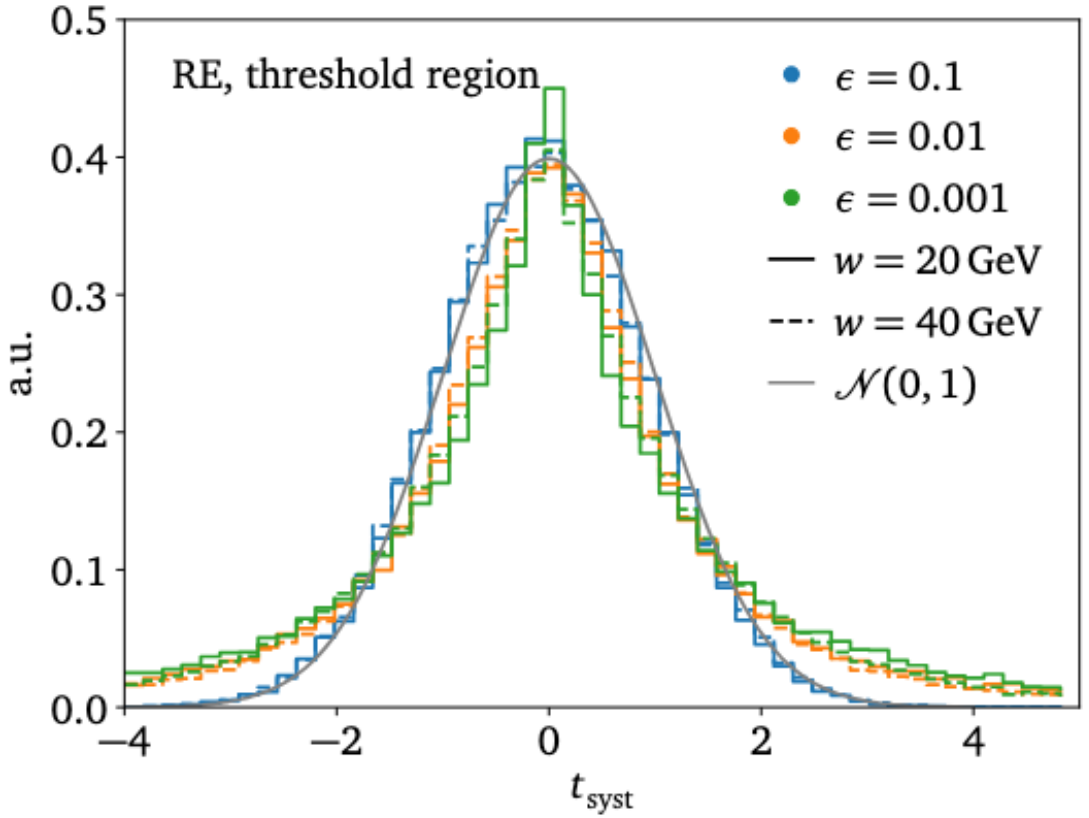
Box smearing — results

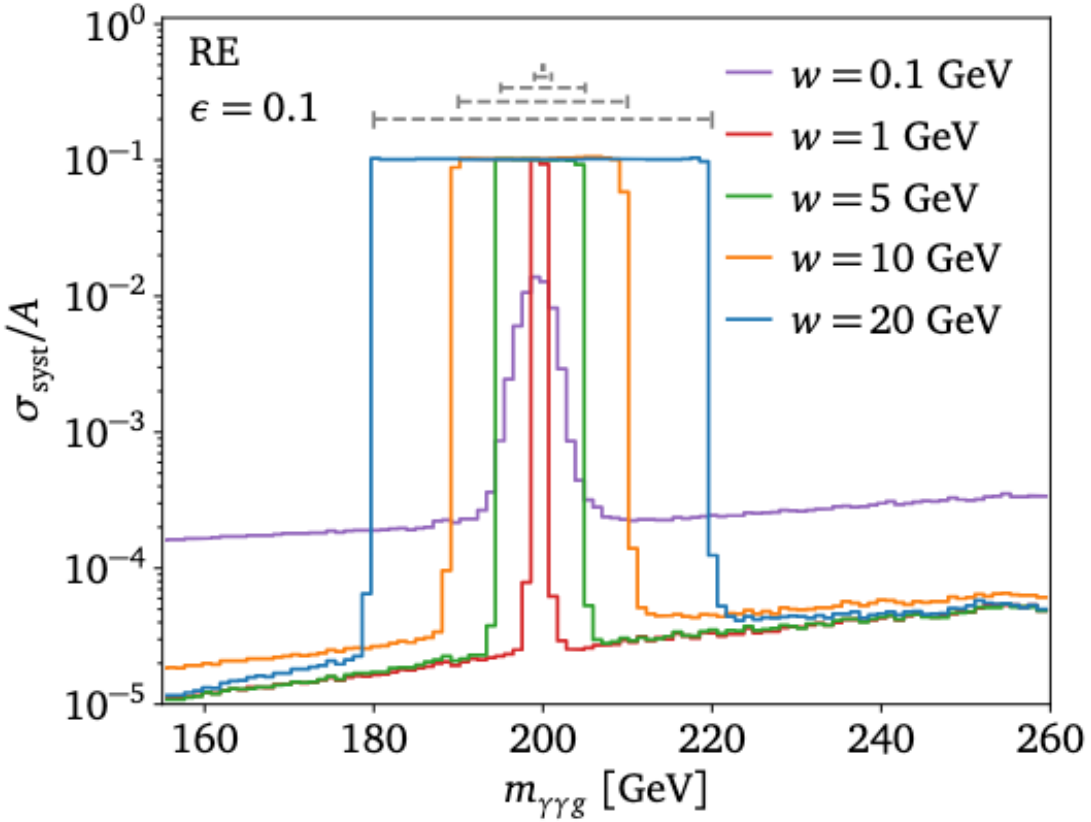




σ_{syst} closely follows expected behavior

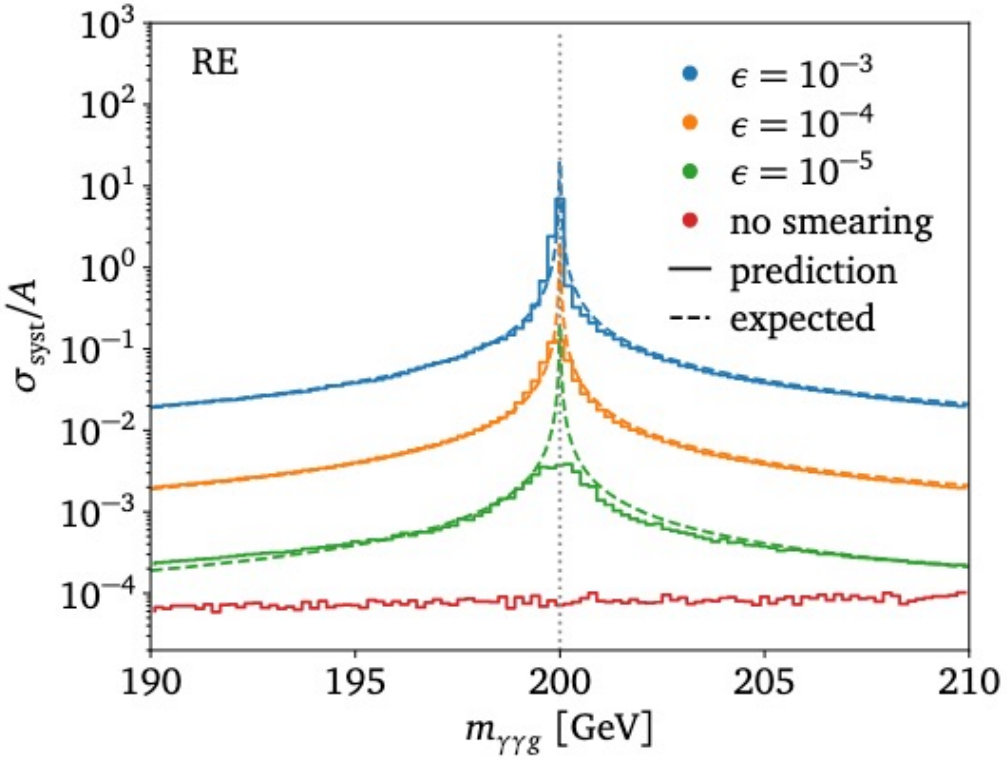
Box smearing — calibration

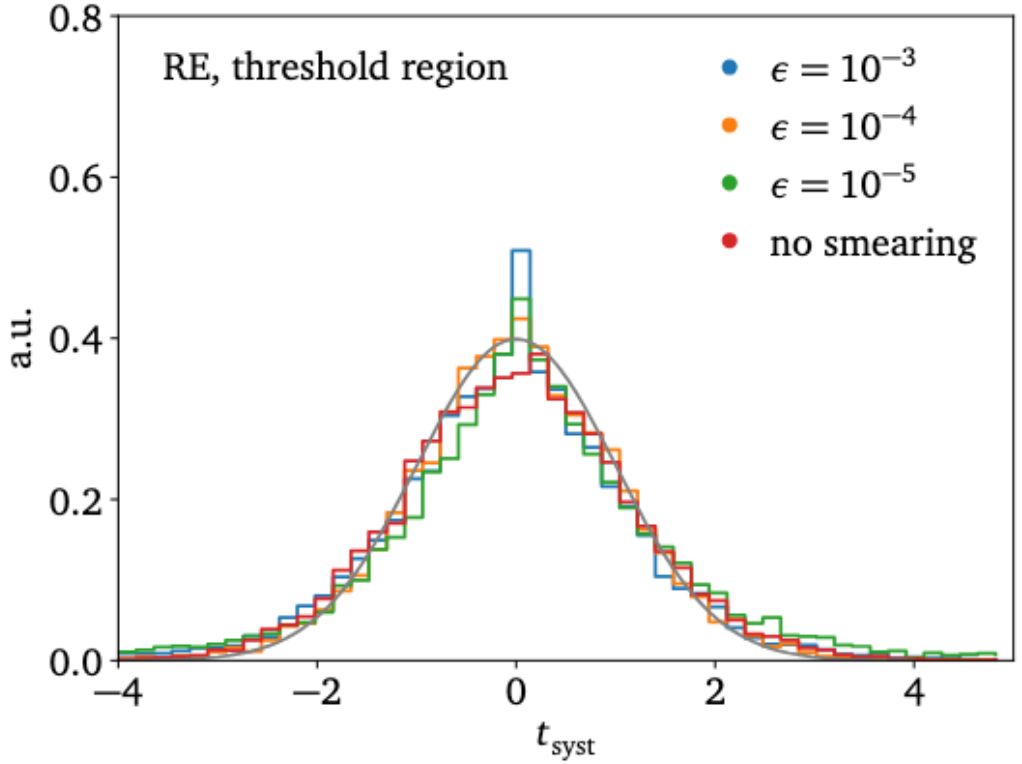




also good calibration

Peaked smearing





$$A_{\text{train}}(x) = \mathcal{N}\left(A_{\text{true}}(x), \frac{\epsilon\, m_{\text{thresh}}}{|m_{\gamma\gamma g}(x) - m_{\text{thresh}}|} A_{\text{true}}(x)\right)$$

well captured by systematic uncertainties

Conclusions

Conclusions

- amplitude surrogates → speed up MC generation
- uncertainty-aware NNs allow for controlled modelling of
  - systematic uncertainties: data-inherent noise + model expressivity
  - statistical uncertainties: lack of data
- methods: heteroskedastic loss, repulsive ensemble, Bayesian NNs
- learned uncertainties reflect actual deviations from truth well
- encoding physics knowledge increase accuracy with still well-calibrated unc.

same techniques also applicable to all kind of other problems

Appendix

Kolmogorov-Arnold theorem

Any $f: [0,1]^n \to \mathbb{R}$ can be written as a finite decomposition of univariate functions and addition.

$$f(x) = f(x_1, \ldots, x_n) = \sum_{q=1}^{2n+1} \Phi_q \left(\sum_{p=1}^{n} \phi_{q,p}(x_p) \right)$$

where $\phi_{q,p} : [0,1] \to \mathbb{R}$ and $\Phi_q : \mathbb{R} \to \mathbb{R}$.

Kolmogorov-Arnold Networks (KANs)

- KAN layer: $$x_{l+1} = \underbrace{\begin{pmatrix} \phi_{l,1,1}(\cdot) & \phi_{l,1,2}(\cdot) & \cdots & \phi_{l,1,n_l}(\cdot) \\ \phi_{l,2,1}(\cdot) & \phi_{l,2,2}(\cdot) & \cdots & \phi_{l,2,n_l}(\cdot) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_{l,n_{l+1},1}(\cdot) & \phi_{l,n_{l+1},2}(\cdot) & \cdots & \phi_{l,n_{l+1},n_l}(\cdot) \end{pmatrix}}_{\equiv \Phi_l} x_l \,,$$

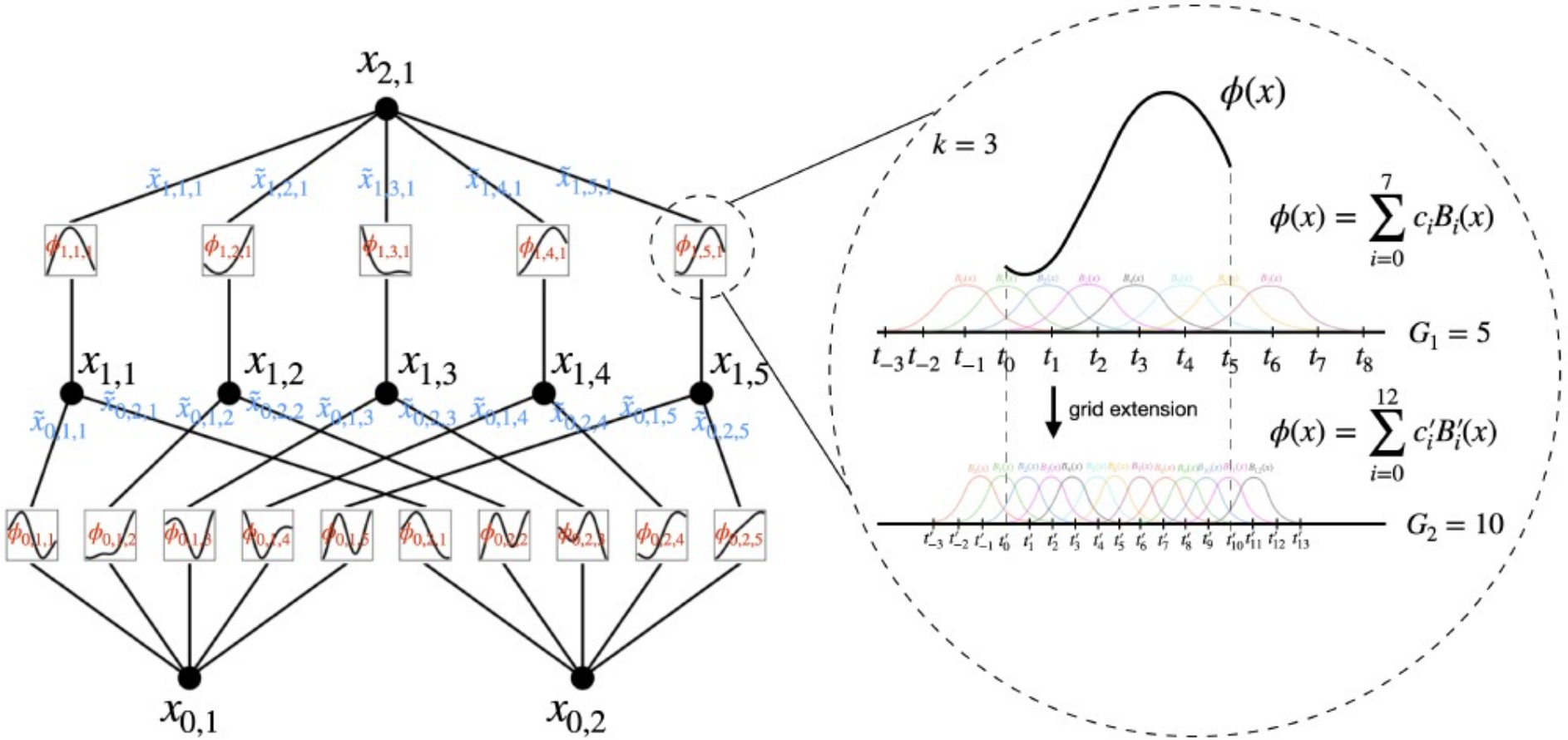
- KAN network: $$\mathrm{KAN}(x) = (\Phi_{L-1} \circ \Phi_{L-2} \circ \ldots \circ \Phi_1 \circ \Phi_0)x$$

- GroupKAN layer: $$\mathrm{activation}(x) \to \mathrm{GroupKANlayer}_l(x) = \begin{pmatrix} \phi_{l,g_l(1)}(x_1) \\ \phi_{l,g_l(2)}(x_2) \\ \vdots \\ \phi_{l,g_l(n_l)}(x_{n_l}) \end{pmatrix}$$

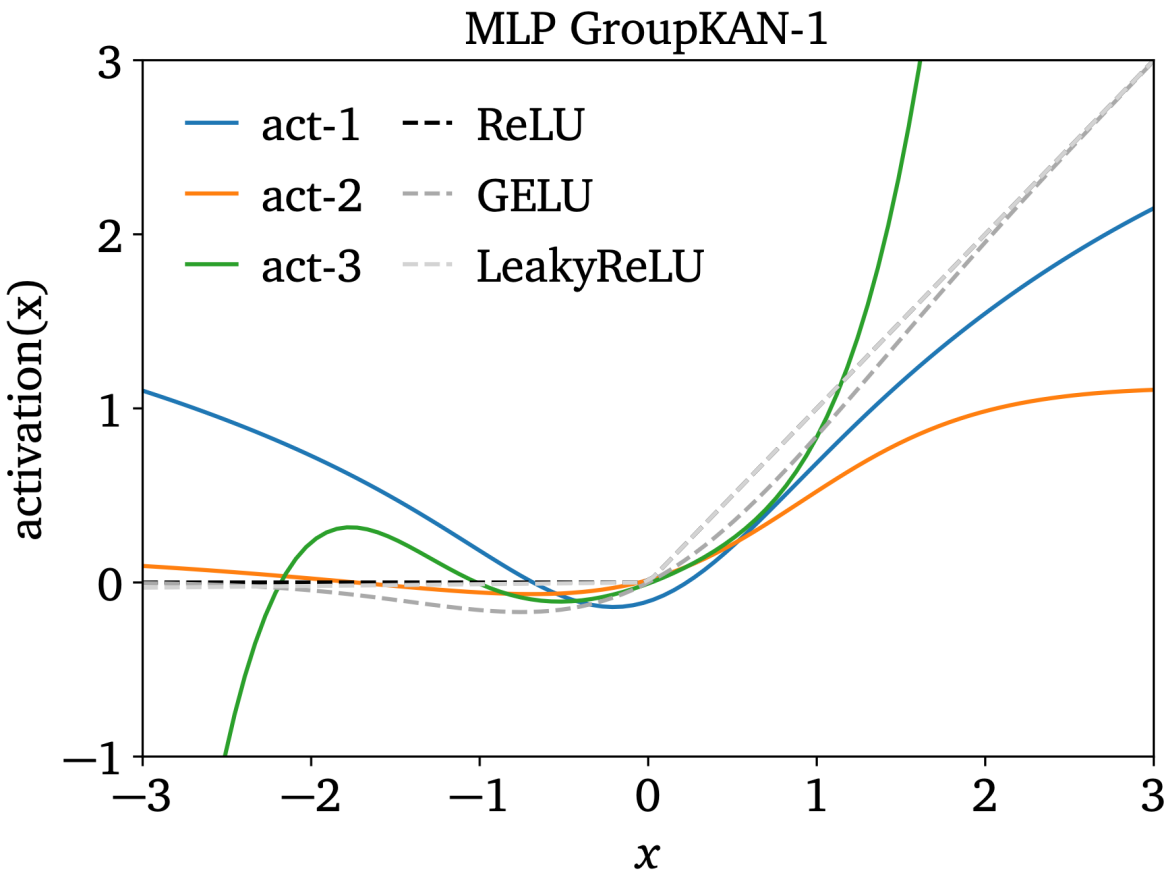
- GroupKAN network: $$\mathrm{GroupKAN}(x) = (W_{L-1} \circ \mathrm{GroupKANlayer}_{L-2} \circ W_{L-2} \circ \ldots \circ \mathrm{GroupKANlayer}_0 \circ W_0)x$$

- Normal MLP network $$\mathrm{MLP}(x) = (W_{L-1} \circ \mathrm{activation} \circ W_{L-2} \circ \ldots \circ \mathrm{activation} \circ W_0)x$$

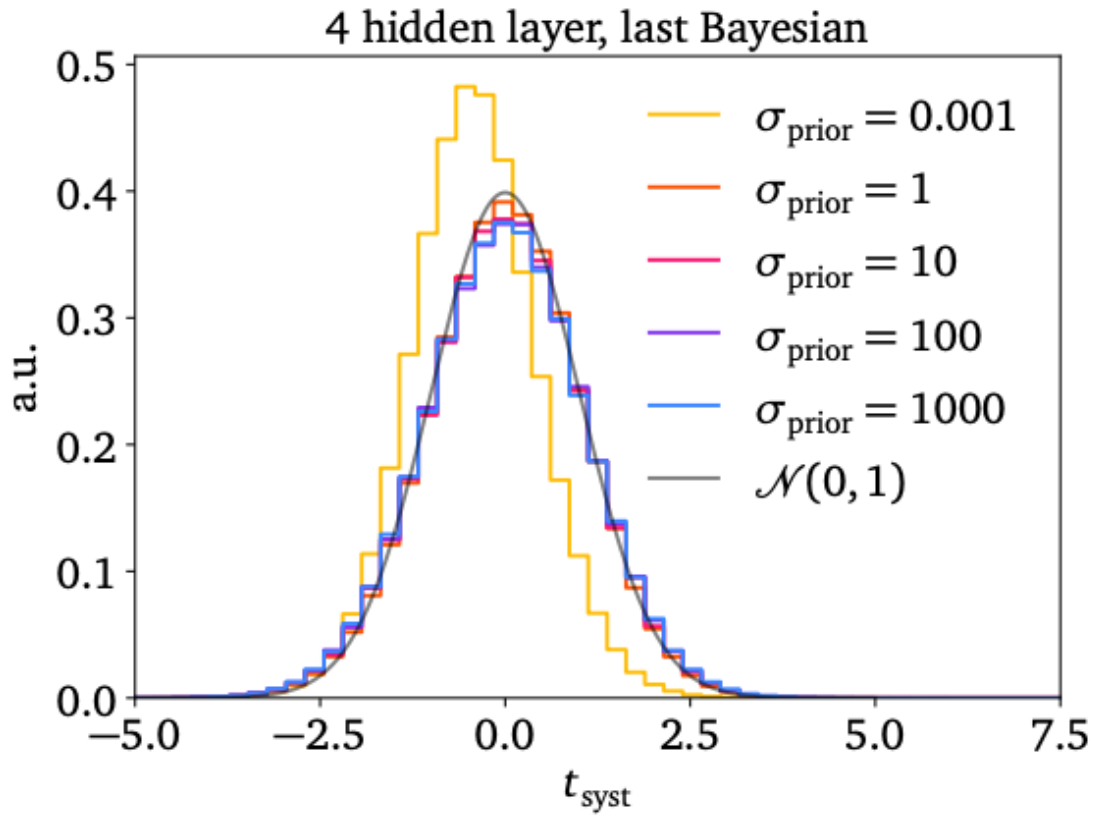
Kolmogorov-Arnold Networks (KANs)

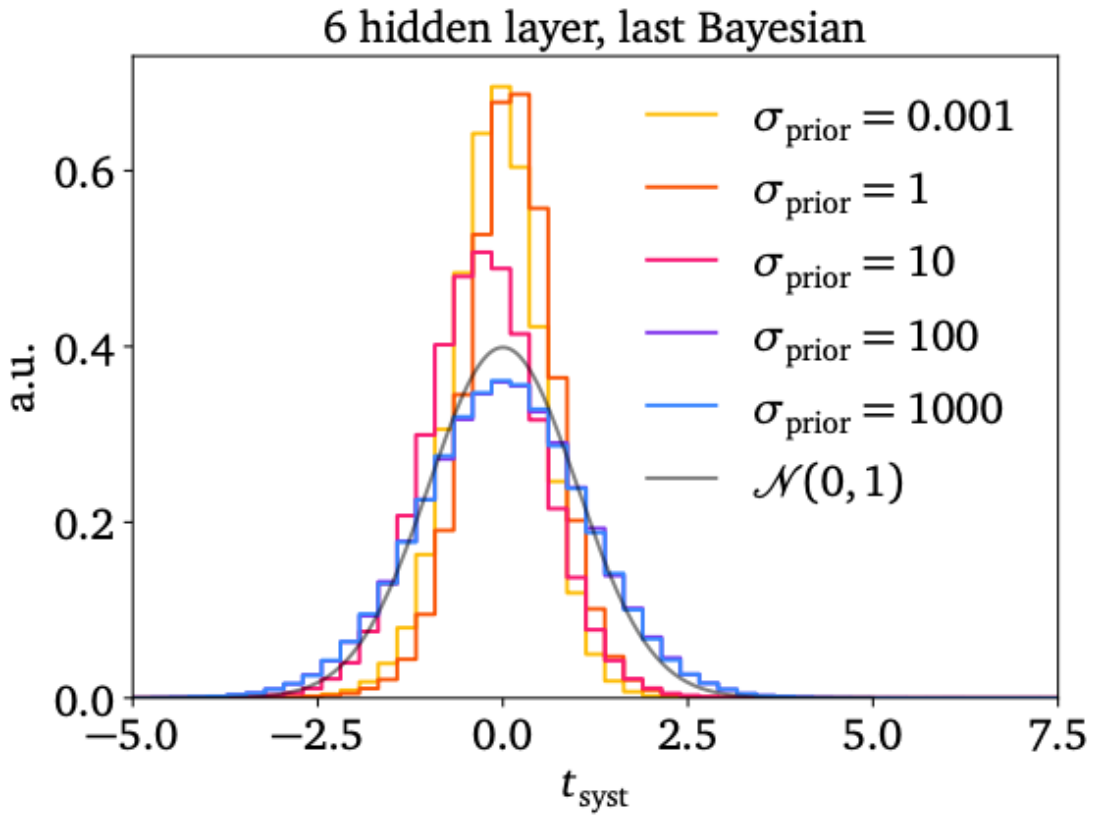


Learned activation functions



BNN prior dependence





Uncertainty overview