Uncertainty-aware discrimination of BSM signatures in embedding spaces

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Lepton-Photon 2025

Parton Distribution Functions

PDFs describe how the hadron's momentum is carried by the constituents (quarks and gluons), and are defined through factorization theorems.

PLB 139814 2025 for QIS prescription.

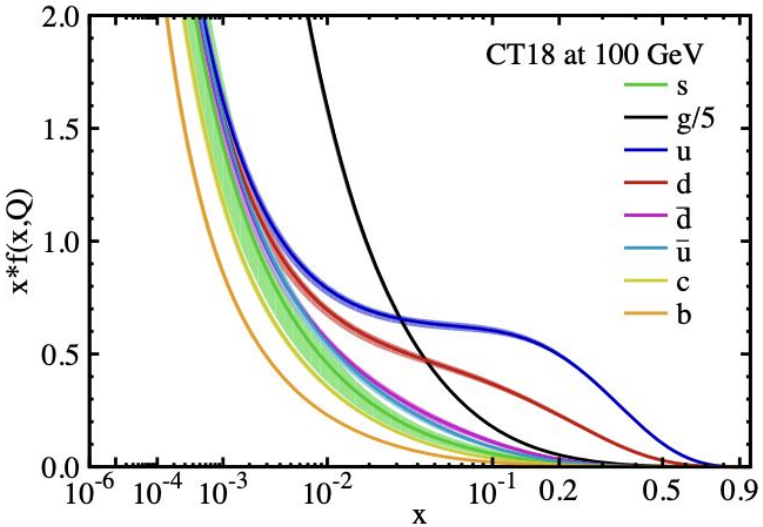
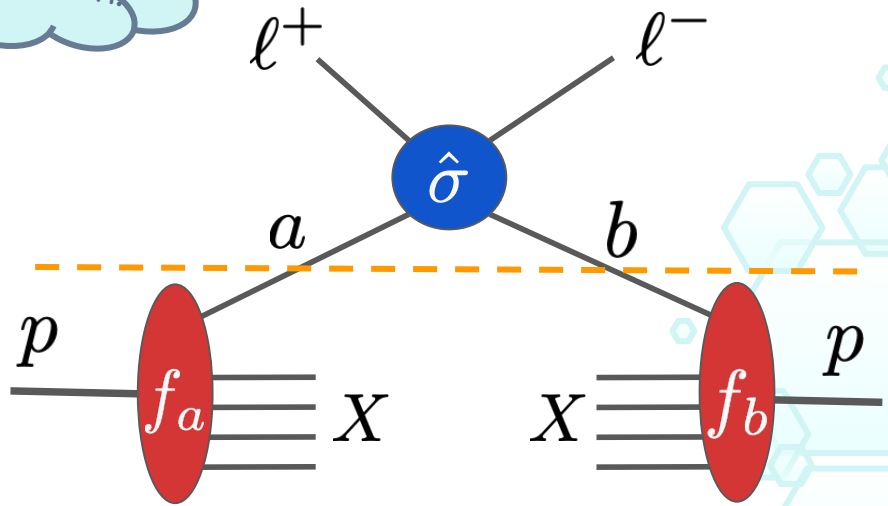


Image credit: PhysRevD.103.014013

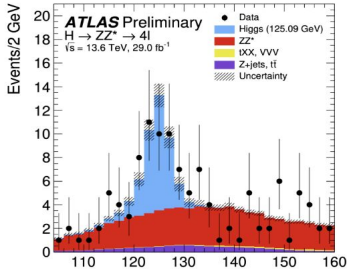
Neutral Current Drell-Yan



$$\sigma = \sum_{a,b} \int dx_a dx_b f_a(x_a) \hat{\sigma}_{ab \to \ell^+ \ell^- + X} f_b(x_b)$$

PDFs are ubiquitous in collider pheno

$gg \to H$



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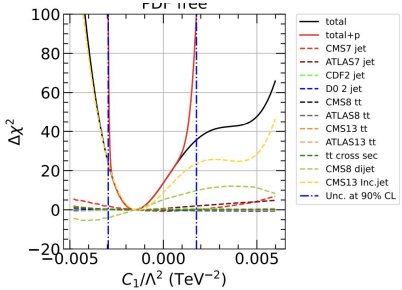
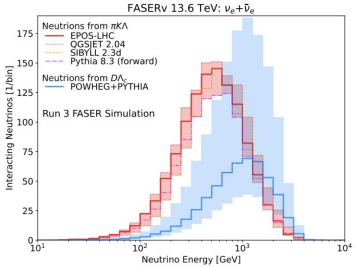
Motivating studies relevant for current and future collider programs like the LHC and EIC.

$gg \to t\bar{t}$



JHEP 05 (2023) 003

$\nu N \to \ell X$



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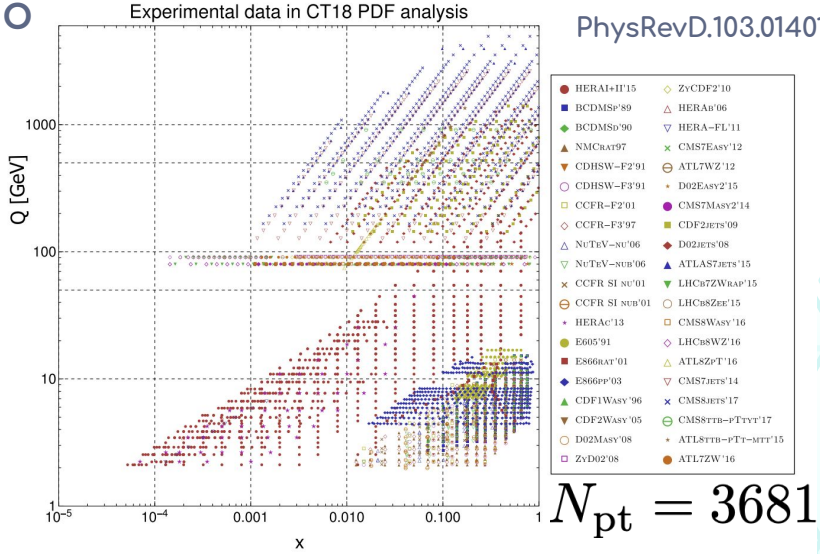


PhysRevD.103.014013

$N_{\rm pt} = 3681$

Global PDF fits unify data across all sectors of the SM, building a robust picture of hadron structure and effectively mediating our knowledge / or lack thereof of fundamental interactions.

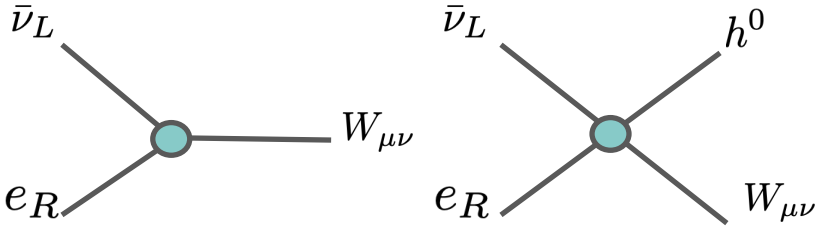
PDFs (Hadronic QCFs) + SMEFT / BSM (fit contaminations)

We know that the SM is incomplete! What is the particle nature of the new physics (NP)?

$$\mathcal{L}_{\text{SMEFT}} = \mathcal{L}_{\text{SM}} + \sum_{d>4} \sum_{i} \frac{C_i^{(d)}}{\Lambda^{d-4}} \mathcal{Q}_i^{(d)}$$

SM Effective Field Theory (SMEFT) provides a model agnostic framework to insert signatures of heavy new physics. For example:

$$\mathcal{Q}_{eW} = (\bar{\ell}_L \sigma^{\mu\nu} e_R) \sigma^a \varphi W^a_{\mu\nu}$$

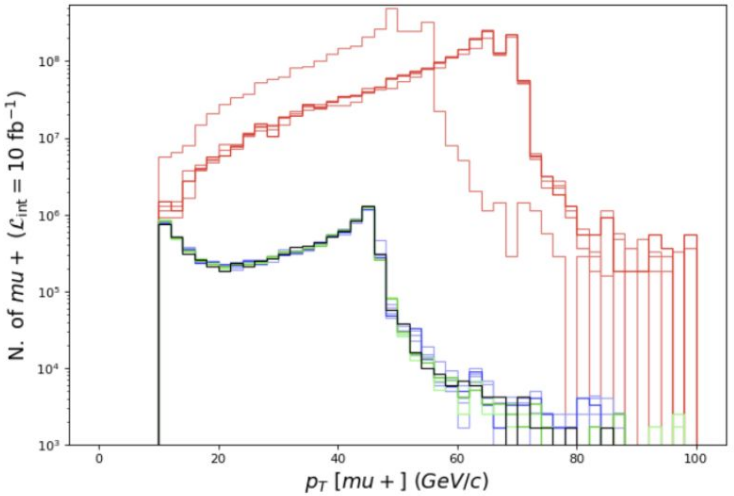


Hammou, et al JEHP 11 (2023) 090

Can PDFs absorb signatures of NP?

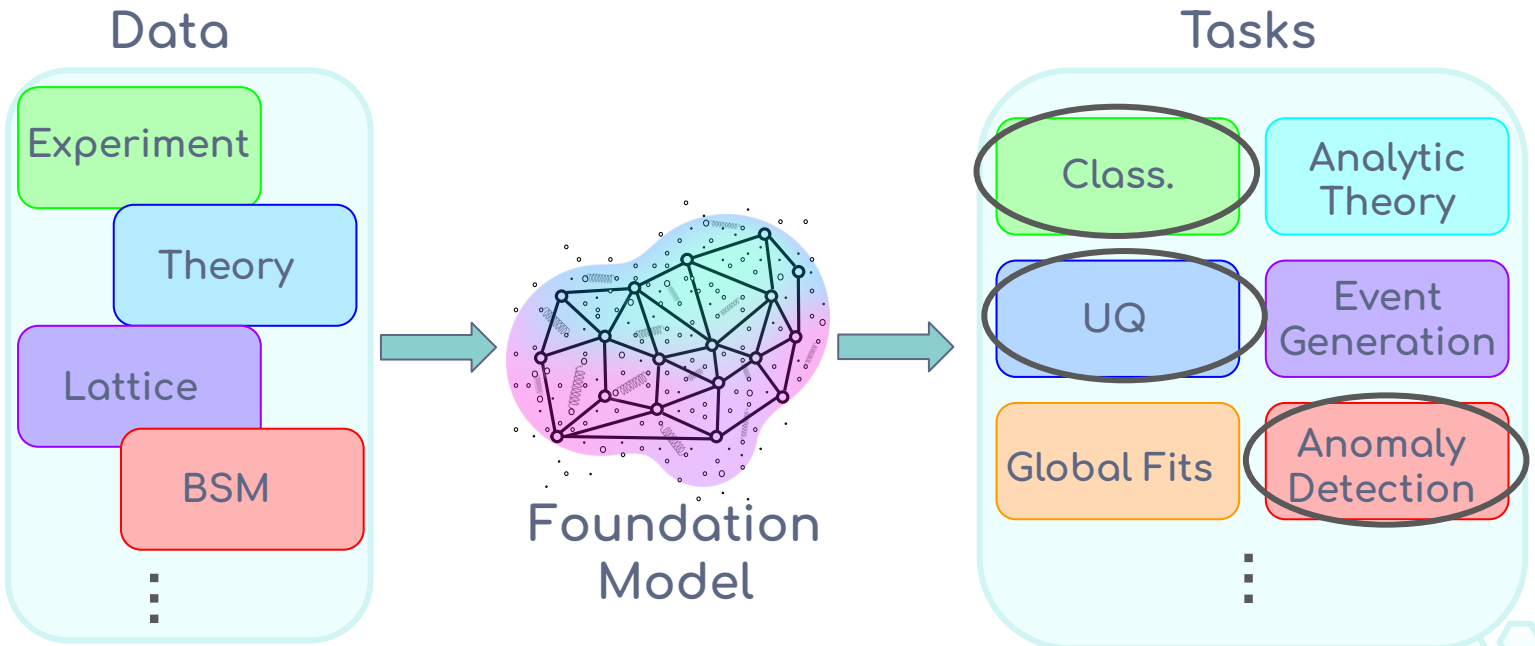
There are a lot of SMEFT parameters to try 30+. Can we compare many scenarios?

A Baniecki, TJ Hobbs, BK arXiv:25XX.XXXXX



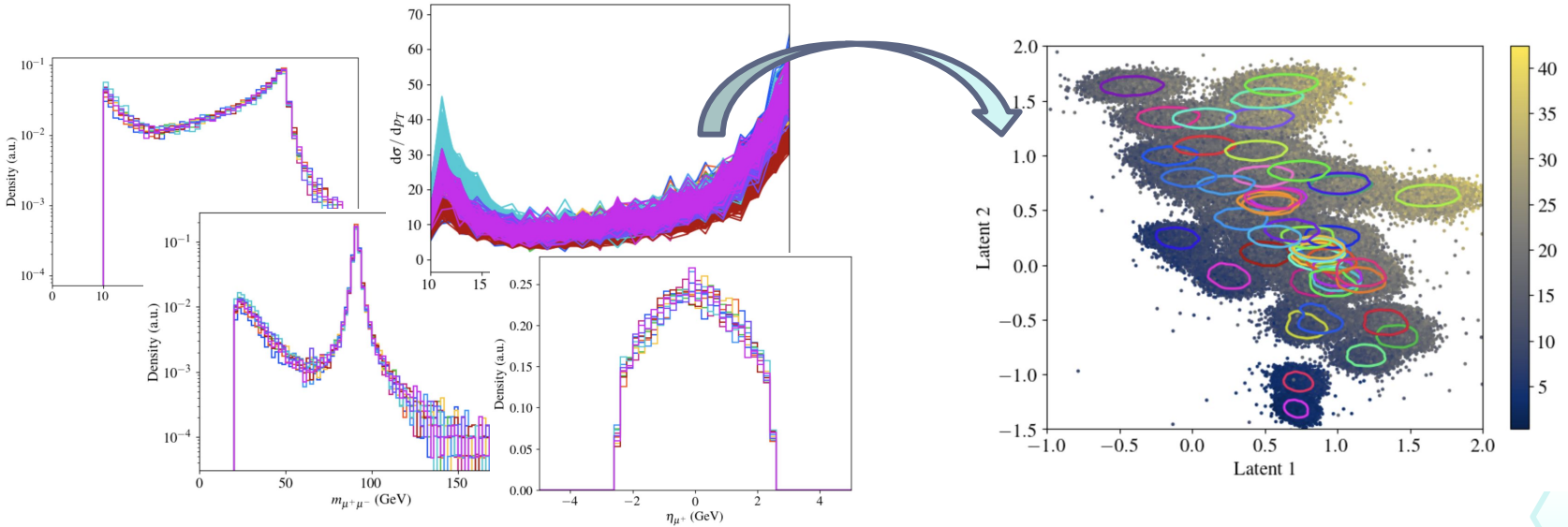
Bridging the Gap with AI/ML: Foundation models for fundamental physics

A foundation model = shared embedding space which can be used to perform specialized downstream tasks.



Foundational Embedding Space: Contrastive Learning

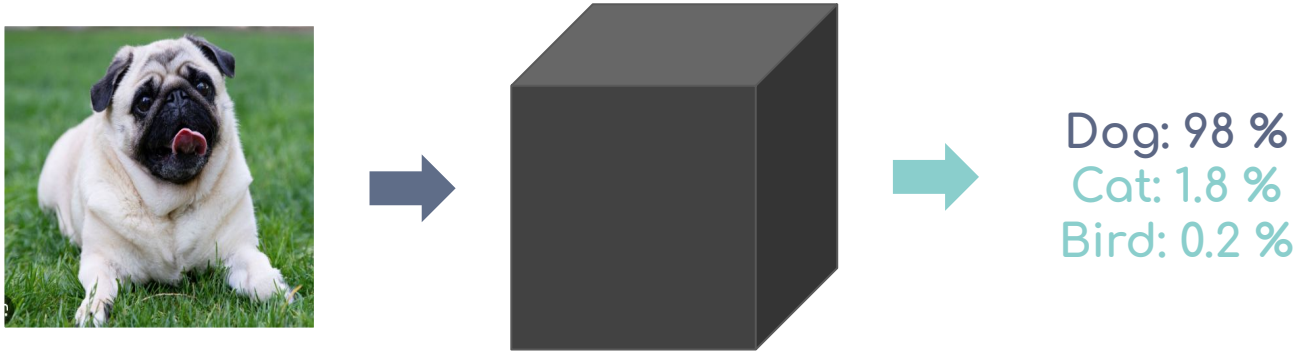
We generate training samples of NC DY data while varying the SMEFT Wilson coefficients which enter the process.



From this embedding, we can use plug-and-play models to perform various downstream tasks.
Classification: can we discriminate between these SMEFT scenarios with rigorous UQ?

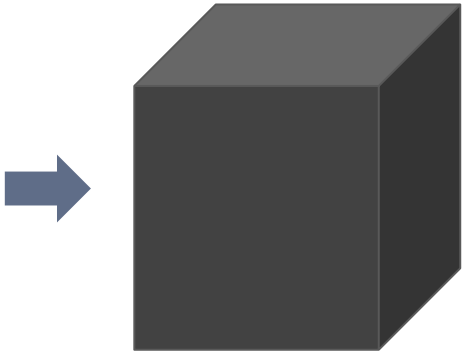
Probabilistic AI / ML

Probabilistic AI / ML is a mathematical paradigm of defining the outputs of algorithms in the language of probabilistic distributions. As an example, for classification algorithms the outputs are categorical distributions.



Uncertainty Quantification for Machine Learning

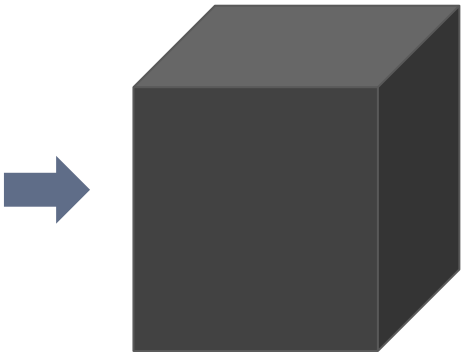
AI / ML algorithms can not only be wrong, but also be really confidently wrong!



Dog: 23 %
Cat: 65 %
Bird: 12 %

Uncertainty Quantification for Machine Learning

What we want is something like this, but how do we teach an ML algorithm to say 'I don't know?'



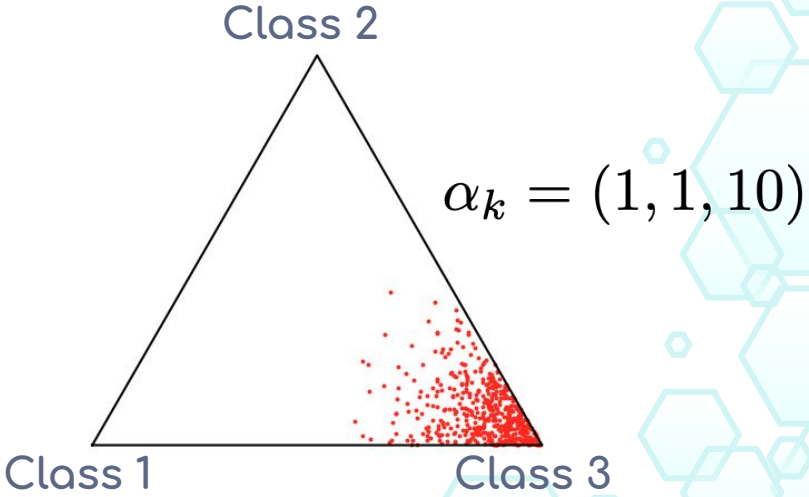
Dog: 0.3 %
Cat: 0.2 %
Bird: 0.5 %
Idk?: 99%

Dirichlet Prior Networks (DPNs)

A categorical distribution models individual probabilities of specific categories $(p_1, p_2, \ldots, p_k)$. The Dirichlet distribution models the prior beliefs over each category's probabilities, designated by parameters $(\alpha_1, \alpha_2, \ldots, \alpha_k)$

$$p(\mu; \alpha) = \frac{\Gamma(\alpha_o)}{\prod_{k=1}^{K} \Gamma(\alpha_k)} \prod_{k=1}^{K} p_k^{\alpha_k - 1}$$

So now we predict the alpha parameters and sample the Dirichlet to get as many categorical distributions as we want.



Malinin and Gales arXiv:1802.10501

Defining Aleatoric and Epistemic Uncertainty

Through training with maximum likelihood estimation (MLE) we can rework the expression to factorize into two distinct components. One is epistemic - the KL divergence term; and the other is aleatoric - the entropy term.

$$\mathbb{E}_{p_{true}(x,y)}\left[\mathcal{L}^{NLL}(y,x,\theta)\right] = \mathbb{E}_{p_{true}(x)}\left[D_{KL}\left(p_{true}(y|x)\|p(y|x,\theta)\right) + \mathbb{H}(p_{true}(y|x))\right]$$

Epistemic

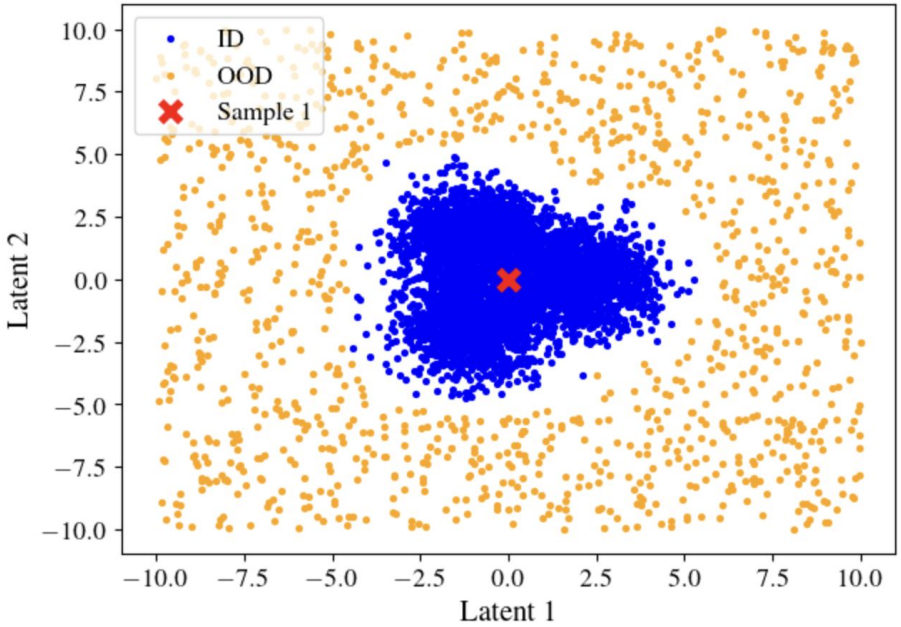
Epistemic uncertainty is reducible by training procedures or algorithmic development. Also can be influenced by choice of distribution to model the data.

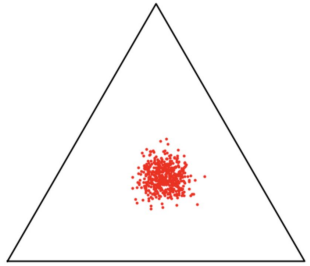
Aleatoric

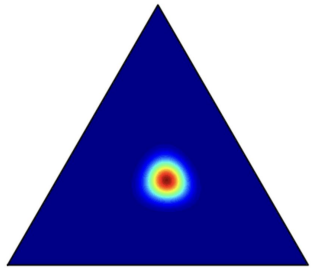
Aleatoric uncertainty is not reducible because it is related to the true underlying data distribution.

Malinin and Gales arXiv:1802.10501

Dirichlet Prior Networks - an example



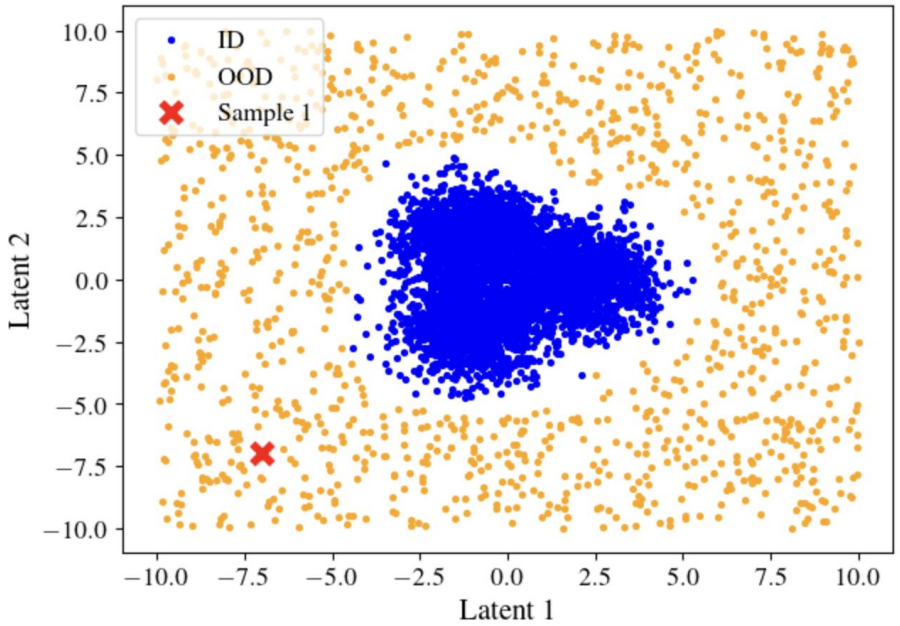


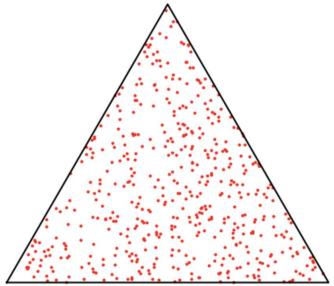


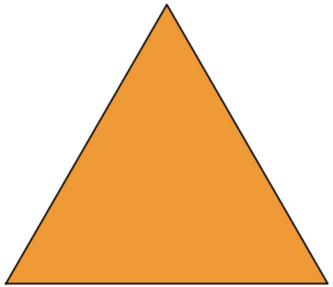
In-distribution sampling with high data uncertainty (samples are squeezed to the center of the simplex) with low knowledge uncertainty (high sample density).

$$\alpha_k = (8, 8, 8)$$

Dirichlet Prior Networks - an example



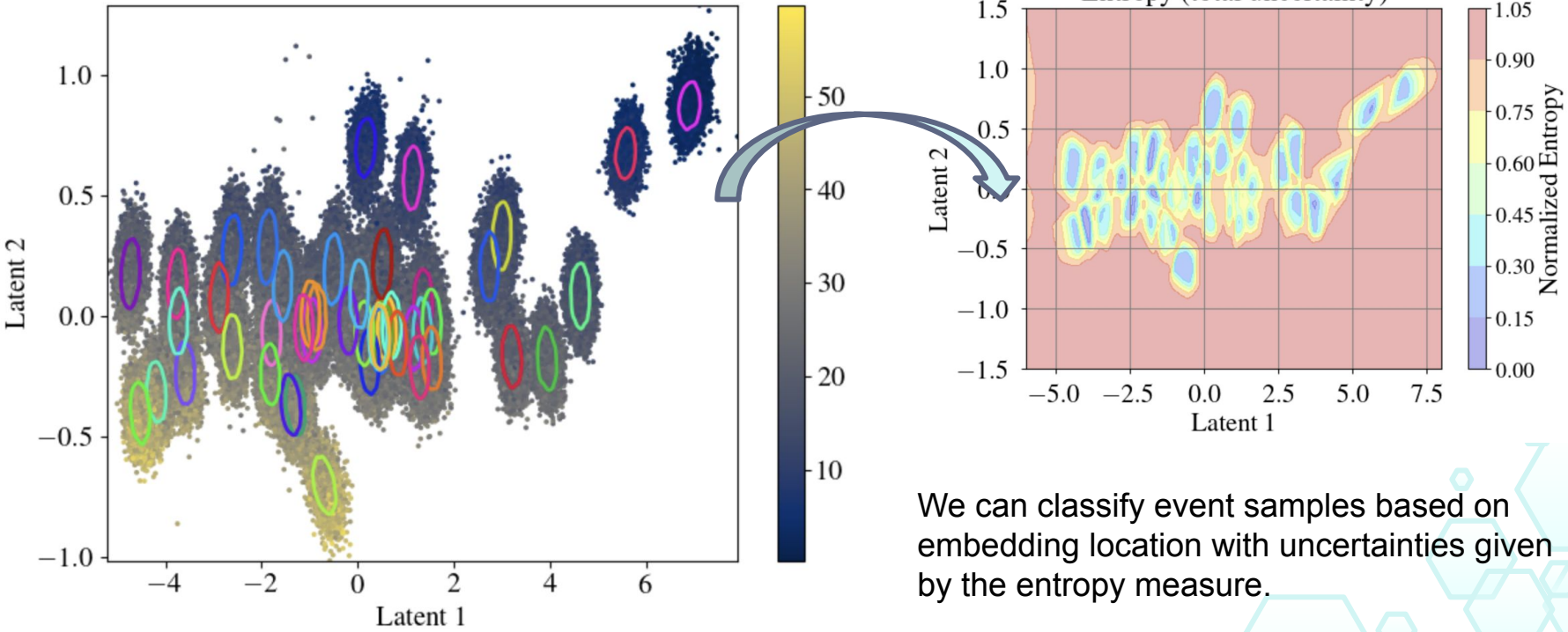




Out-of-distribution sampling with high data uncertainty (samples are not located at a specific corner) and high knowledge uncertainty (samples are diffuse).

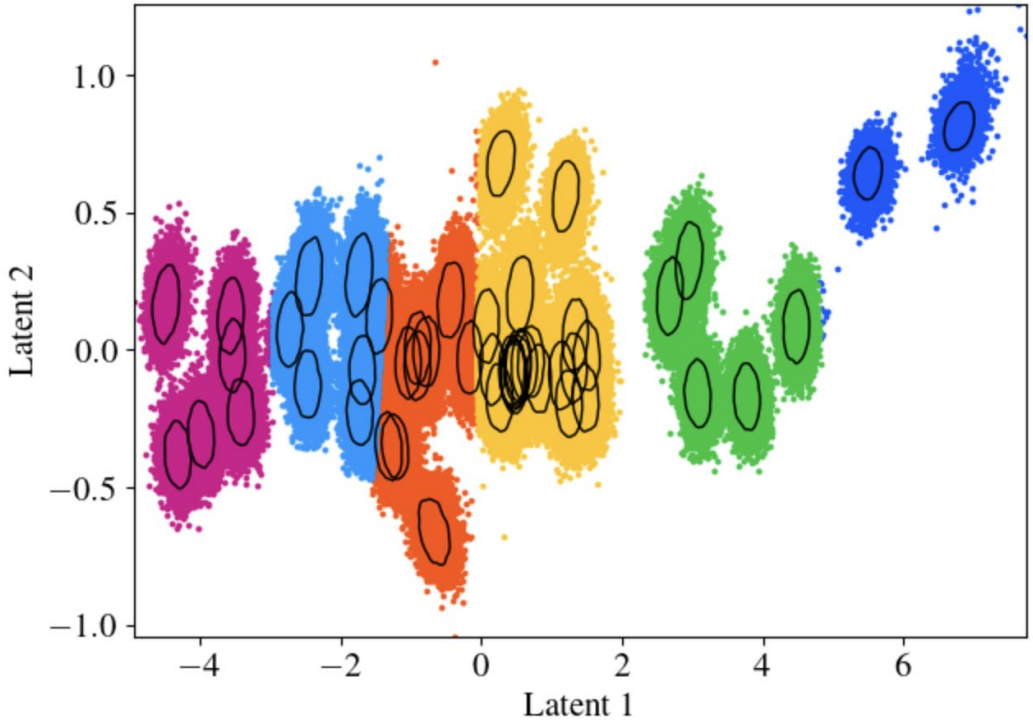
$$\alpha_k = (1, 1, 1)$$

Classifying SMEFT scenarios



We can classify event samples based on embedding location with uncertainties given by the entropy measure.

Identifying SMEFT “superclasses”



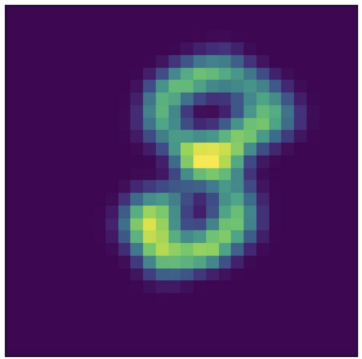
7-8 “superclasses” seem to emerge (using within-cluster sum of squares evaluation of cluster number).

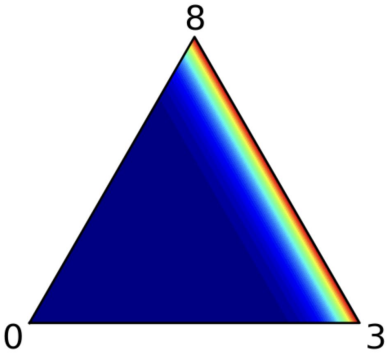
Can we identify within the theory why this specific number of clusters emerges phenomenologically:

$$X^3,\ \varphi^6,\ \varphi^4 D^2$$
$$\psi^2\varphi^3,\ X^2\varphi^2,\ \psi^2 X\varphi$$
$$\psi^2\varphi^2 D,\ \psi^4$$

Hyper Opinions and uncertainty on the ground truth

Consider a scenario where there exists an uncertainty on the ground truth label itself. How do we rule out classification labels?





Example: the above illustration with MNIST. It is uncertain whether the ground truth is 3 or 8 but it certainly isn't 0.

We can use a Grouped Dirichlet distribution to model not only the distribution over the priors of the categorical, but also the distribution over composite labels.

$$\mathrm{GDD}(p|\alpha, c) = Z^{-1} \prod_{k=1}^{K} p_k^{\alpha_k - 1} \prod_{j=1}^{\eta} \left(\sum_{\ell \in S_j} p_\ell \right)^{c_j}$$

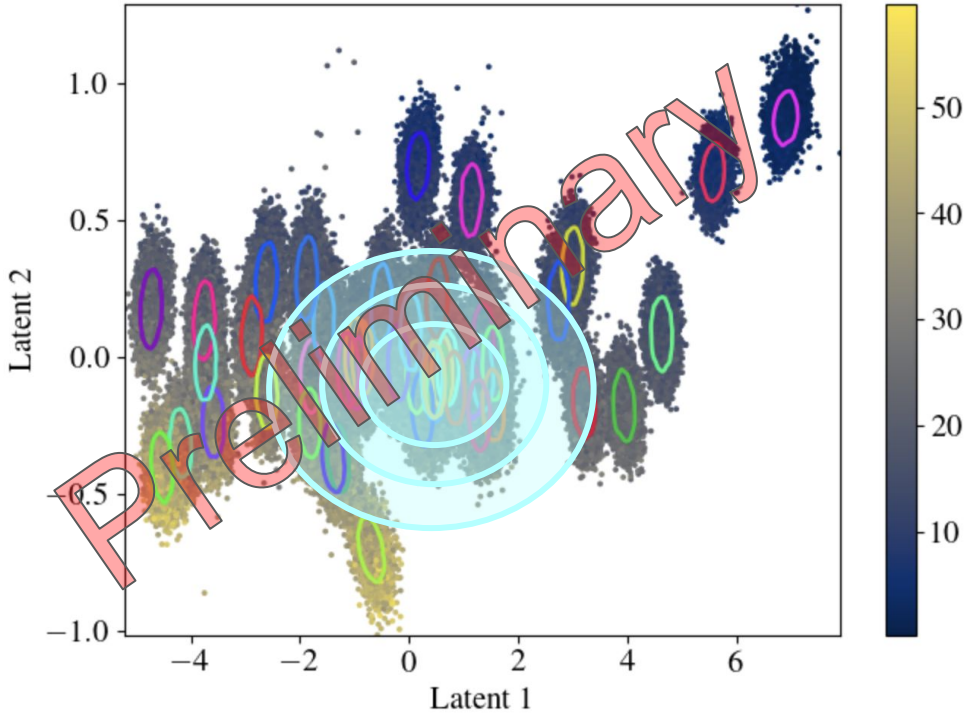
Extends physics use case to rule out models from classification.

BK, T.J. Hobbs **(in progress)**

Mapping PDF uncertainties: can we hide signatures of new physics?

Problem statement: PDF uncertainties can potentially hide model agnostic signatures of new physics. Can we measure this through our embedding space?

We can project the PDF uncertainties onto this embedding space to estimate how much coverage we can generate by rescaling the PDFs.



Conclusions / Outlooks

- We have constructed a ‘foundational’ embedding space through a single self-supervised pre-training workflow - more to come in testing different tasks.
- Uncertainty Quantification techniques through prior networks provide robust definitions of uncertainty which allow us to map the embedding space.
- We can use this embedding space with plug-and-play head models to perform a variety of downstream tasks.
- As the next generation of particle physics experiments come online (EIC, HL-LHC, etc), foundation models offer a route for robust, data-driven predictions for new physics observables - if we can benchmark these tools against known physics.

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Thank you for your attention!

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