ICCUB Winter Meeting 2025

# Improving Statistical Analyses in Particle Physics Phenomenology

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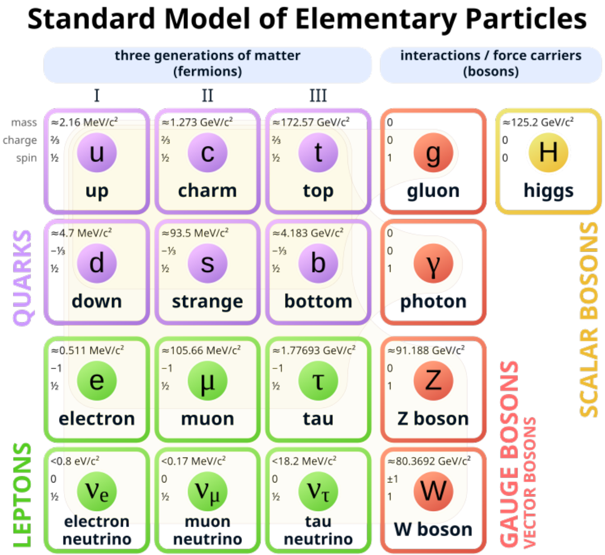
European Commission

*In collaboration with:*

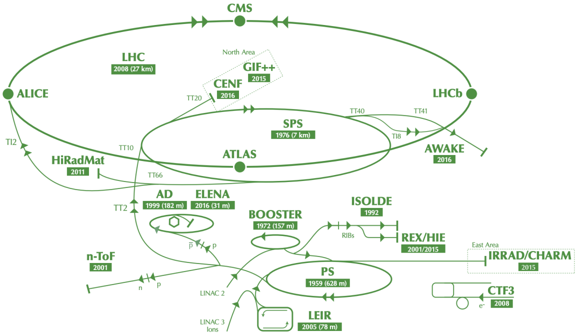
**A. Scaffidi; arXiv:250x.xxxx**

# Outline

# Basic Ideas in Particle Physics Phenomenology


Standard Model of Elementary Particles
three generations of matter (fermions)
interactions / force carriers (bosons)
I
II
III
mass
charge
spin
≈2.16 MeV/c²
⅔
½
u
up
≈1.273 GeV/c²
⅔
½
c
charm
≈172.57 GeV/c²
⅔
½
t
top
0
0
1
g
gluon
≈125.2 GeV/c²
0
0
H
higgs
≈4.7 MeV/c²
−⅓
½
d
down
≈93.5 MeV/c²
−⅓
½
s
strange
≈4.183 GeV/c²
−⅓
½
b
bottom
0
0
1
γ
photon
≈0.511 MeV/c²
−1
½
e
electron
≈105.66 MeV/c²
−1
½
μ
muon
≈1.77693 GeV/c²
−1
½
τ
tau
≈91.188 GeV/c²
0
1
Z
Z boson
<0.8 eV/c²
0
½
νe
electron neutrino
<0.17 MeV/c²
0
½
νμ
muon neutrino
<18.2 MeV/c²
0
½
ντ
tau neutrino
≈80.3692 GeV/c²
±1
1
W
W boson
QUARKS
LEPTONS
GAUGE BOSONS
VECTOR BOSONS
SCALAR BOSONS

# The LHC Era of Particle Physics



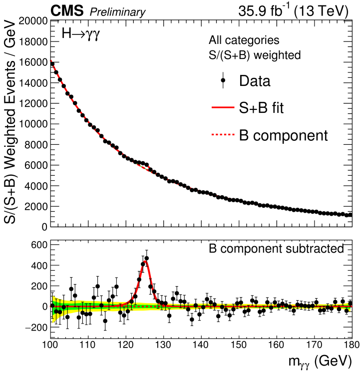

⇒ We explore this theory (and potentially others) using **Particle Colliders**

⇒ The current era of Particle Physics is shaped significantly by the LHC, the world's **largest** and **most powerful** collider ever built

⇒ Several other colliders and accelerators are operational, fulfilling more specialised roles

- ⇒ SuperKEKB (Belle / Belle II)
- ⇒ The Relativistic Heavy Ion Collider (RHIC) at Brookhaven National Laboratory
- ⇒ Many others, including dedicated accelerator experiments, beam experiments, . . .

# The Higgs Boson Discovery




CMS, CMS-PAS-HIG-17-015

⇒ The discovery of the **Higgs boson** in 2012 stands as the crowning achievement of the LHC era

⇒ We usually say that *this discovery marked the completion of the Standard Model*, but did it?

- ⇒ The precise nature of the Higgs boson remains an open question
- ⇒ With a large portion of the Higgs potential parameter space still unexplored

# The Current Paradigm

$$\begin{aligned}\mathcal{L}_{\rm SM} = i\left(\bar{\ell}_L \not{D} \ell_L + \bar{e}_R \not{D} e_R + \overline{Q}_L \not{D} Q_L + \bar{u}_R \not{D} u_R + \bar{d}_R \not{D} d_R\right) \\ - \frac{1}{4} G^A_{\mu\nu} G^{A\mu\nu} - \frac{1}{4} W^I_{\mu\nu} W^{I\mu\nu} - \frac{1}{4} B_{\mu\nu} B^{\mu\nu} \\ + \left(D_\mu \phi\right)^\dagger \left(D^\mu \phi\right) - \mu^2 \phi^\dagger \phi - \lambda \left(\phi^\dagger \phi\right)^2 \\ - \left(\bar{\ell}_L Y^\ell \phi e_R + \overline{Q}_L Y^u \epsilon \phi^* u_R + \overline{Q}_L Y^d \phi d_R + \text{h.c.}\right)\end{aligned}$$

- ⇒ The Standard Model is arguably the *most successful* theory of fundamental physics
- ⇒ **However**, it is clear that it remains incomplete ...
  - ⇒ **Gravity**, **Dark Matter**, and **Dark Energy** are not accounted for within the SM

... and it presents several unresolved questions, often referred to as *problems* or *puzzles*:

- ⇒ *Hierarchy Problem*: stabilising the Higgs boson requires **large cancellations** of **quantum corrections**
- ⇒ *Strong CP Problem*: the CP-violating term $\mathcal{L}_{SM} \supset \theta \frac{g_s^2}{32\pi^2} G_{\mu\nu} \tilde{G}^{\mu\nu}$ allowed, yet experimentally $\theta \sim 0$
- ⇒ *Flavour Puzzle*: why are there **three families** of **quarks** and **leptons**?
- ⇒ *Neutrino masses*: not incorporated in the SM
- ⇒ *Baryon Asymmetry Problem*: the CP-violation present in $\mathcal{L}_{\rm SM}$ is insufficient to explain the observed matter-antimatter asymmetry
- ⇒ ...

# Towards a Deeper Understanding of the SM and Beyond

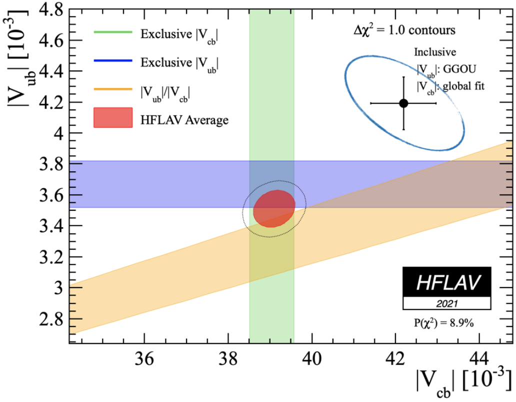
$$
\begin{aligned}
\mathcal{L}_{\text{BSM}} \supset\, & i\left(\bar{\ell}_L \not{D} \ell_L + \bar{e}_R \not{D} e_R + \overline{Q}_L \not{D} Q_L + \bar{u}_R \not{D} u_R + \bar{d}_R \not{D} d_R\right) \\
& - \frac{1}{4} G^A_{\mu\nu} G^{A\mu\nu} - \frac{1}{4} W^I_{\mu\nu} W^{I\mu\nu} - \frac{1}{4} B_{\mu\nu} B^{\mu\nu} \\
& + \left(D_\mu \phi\right)^\dagger \left(D^\mu \phi\right) - \mu^2 \phi^\dagger \phi - \lambda \left(\phi^\dagger \phi\right)^2 \\
& - \left(\bar{\ell}_L Y^\ell \phi e_R + \overline{Q}_L Y^u \epsilon \phi^* u_R + \overline{Q}_L Y^d \phi d_R + \text{h.c.}\right) + \ldots
\end{aligned}
$$

⇒ Despite the many **indications of potential shortcomings** in the SM, no **conclusive evidence** against it has been found in current data

⇒ The unresolved puzzles and missing elements necessitate **further investigation**

- ⇒ **Mathematical approach**: Quantum Gravity, extended symmetries (model building), formal QFT, . . .
- ⇒ **Phenomenological approach**: understanding how data aligns with the SM (**anomaly detection**), refining SM predictions, exploring extended symmetries (model building), determining SM fundamental parameters, . . .

# Determinations of $V_{cb}$ and $V_{ub}$



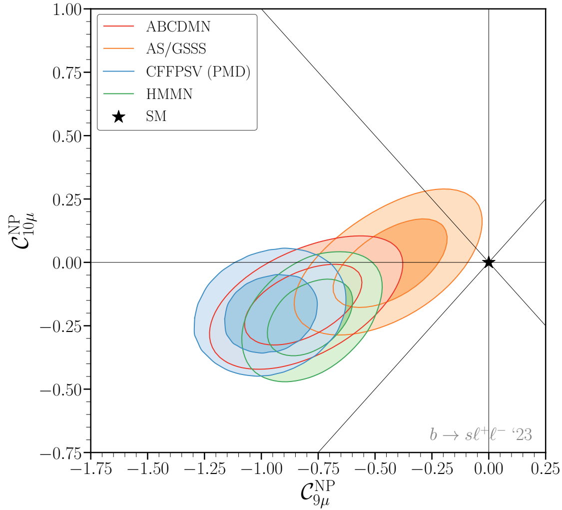

BC, Gambino, Nandi; **JHEP 04 (2021) 137** [arXiv:2102.03343]
Bordone, BC, Gambino; **Phys. Lett. B 822 (2021) 136679** [arXiv:2107.00604]

⇒ $V_{ub}$ and $V_{cb}$ are two elements of the **CKM matrix** that governs *quark-level transitions*

⇒ These elements arise from the diagonalisation of the *quark mass matrix*

$$u_L^i \to U_u^{ij} u_L^j, \quad d_L^i \to U_d^{ij} d_L^j, \quad V_{\text{CKM}} = U_u^\dagger U_d$$

# Anomaly Detection and Characterisation



# Anomaly Detection

# Anomalies in Particle Physics

⇒ The term **anomaly** has different meanings in the context of Particle Physics

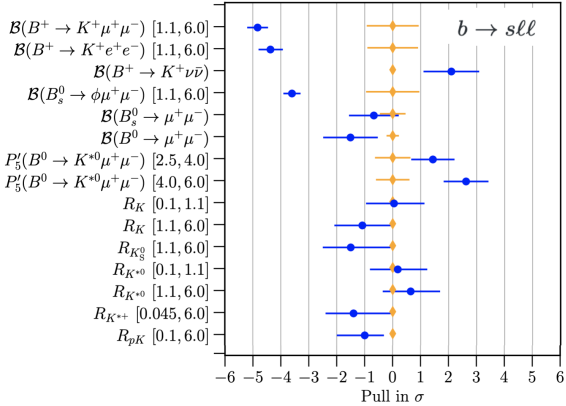
⇒ In QFT, an anomaly is a *symmetry* of the *classical theory* that is *broken* by *quantum corrections*

⇒ In the context of *phenomenology*, anomalies refer to **deviations** between **experimental data** and **theoretical predictions** under a given **null hypothesis**

⇒ **Goal:** to *properly* quantify the **statistical significance** of observed anomalies

# Recent Anomalies in Particle Physics

- ⇒ $B$-meson[1] anomalies ($b \to s\ell^+\ell^-$, $b \to c\ell\nu$)
- ⇒ $(g-2)_\mu$
- ⇒ $V_{cb}$, $V_{ub}$ puzzle
- ⇒ ...




[1] A $B$-meson is a $b$-quark and a light-quark bound state, i.e. $B^0$ ($\bar{b}d$), $B^+$ ($\bar{b}u$), $B_s$ ($\bar{b}s$), $B_c$ ($\bar{b}c$), ...

# Traditional Frequentist Analyses

⇒ In **conventional analyses**, Gaussian likelihoods are assumed

$$p(\boldsymbol{x}|H_i) = \mathcal{N}(\boldsymbol{x}; \boldsymbol{x}_{H_i}, \boldsymbol{\Lambda}_{H_i}) = \frac{1}{\sqrt{(2\pi)^n |\boldsymbol{\Lambda}_{H_i}|}} \exp\left(-\frac{1}{2}(\boldsymbol{x} - \boldsymbol{x}_{H_i})^T \boldsymbol{\Lambda}_{H_i}^{-1} (\boldsymbol{x} - \boldsymbol{x}_{H_i})\right)$$

- ⇒ $\boldsymbol{\Lambda}_{H_i}$ is the **sum of theoretical and experimental covariances**

$$\boldsymbol{\Lambda}_{H_i} = \boldsymbol{\Lambda}_{H_i}^{\text{th}} + \boldsymbol{\Lambda}^{\text{exp}}$$

⇒ Measuring goodness-of-fit

- ⇒ Use $-\log p(\boldsymbol{x}|H_i)$ as a **statistic** to measure **agreement between data and hypothesis** $H_i$
- ⇒ If **theoretical predictions** and **experimental data** are **normally distributed**, $-\log p(\boldsymbol{x}|H_i)$ follows a $\chi^2$-distribution with $n_{\text{dof}} = n_{\text{obs}}$ in the analysis
- ⇒ If **not normally distributed**, $-\log p(\boldsymbol{x}|H_i)$ is **only asymptotically** $\chi^2$ due to the central limit theorem
- ⇒ Assuming $\chi^2$-distribution when it is not **creates biases** in calculating $p$-values from $-\log p(\boldsymbol{x}_{\text{exp}}|H_i)$

# Experimental Data in Phenomenological Analyses

- ⇒ Experimental data:
  - ⇒ Released from the experiments as a **vector of means** $\mu^{\text{exp}}$ and a **covariance matrix** $\Lambda^{\text{exp}}$
- ⇒ **Implicitly assumes a Gaussian distribution** for the experimental measurements

$$p(\boldsymbol{x}^{\text{exp}}) = \mathcal{N}(\boldsymbol{x}^{\text{exp}}; \boldsymbol{\mu}^{\text{exp}}, \boldsymbol{\Lambda}^{\text{exp}})$$

| | $4.0 < q^2 < 6.0\,\text{GeV}^2/c^4$ |
|---|---|
| $P_1$ | $0.088 \pm 0.235 \pm 0.029$ |
| $P_2$ | $0.105 \pm 0.068 \pm 0.009$ |
| $P_3$ | $-0.090 \pm 0.139 \pm 0.006$ |
| $P_4'$ | $-0.312 \pm 0.115 \pm 0.013$ |
| $P_5'$ | $-0.439 \pm 0.111 \pm 0.036$ |
| $P_6'$ | $-0.293 \pm 0.117 \pm 0.004$ |
| $P_8'$ | $0.166 \pm 0.127 \pm 0.004$ |

| | $F_L$ | $P_1$ | $P_2$ | $P_3$ | $P_4'$ | $P_5'$ | $P_6'$ | $P_8'$ |
|---|---|---|---|---|---|---|---|---|
| $F_L$ | 1.00 | 0.04 | 0.05 | −0.10 | −0.04 | −0.14 | −0.17 | 0.14 |
| $P_1$ | | 1.00 | 0.06 | 0.07 | −0.06 | −0.10 | −0.03 | 0.02 |
| $P_2$ | | | 1.00 | −0.02 | −0.14 | −0.09 | −0.03 | −0.01 |
| $P_3$ | | | | 1.00 | −0.01 | 0.07 | 0.19 | −0.01 |
| $P_4'$ | | | | | 1.00 | 0.02 | 0.04 | 0.01 |
| $P_5'$ | | | | | | 1.00 | 0.09 | 0.00 |
| $P_6'$ | | | | | | | 1.00 | 0.02 |
| $P_8'$ | | | | | | | | 1.00 |

LHCb, arXiv:2003.04831

# Theoretical Predictions in Phenomenological Analyses

⇒ Theoretical predictions

- ⇒ For the observables in the analysis $\boldsymbol{x} = (x_1, \ldots, x_n)$, we have functions representing their **theoretical predictions** in terms of several **input parameters** $\boldsymbol{\nu} = (\nu_1, \ldots, \nu_m)$

$$x_i = x_i(\nu_1, \ldots, \nu_m)$$

- ⇒ The **input parameters** are distributed according to some distribution, usually Gaussian

$$\boldsymbol{\nu} \sim \mathcal{N}(\boldsymbol{\nu}; \boldsymbol{\mu}_\nu, \boldsymbol{\Lambda}_\nu)$$

where $\boldsymbol{\mu}_\nu$ and $\boldsymbol{\Lambda}_\nu$ means and covariance of the distribution of underlying parameters

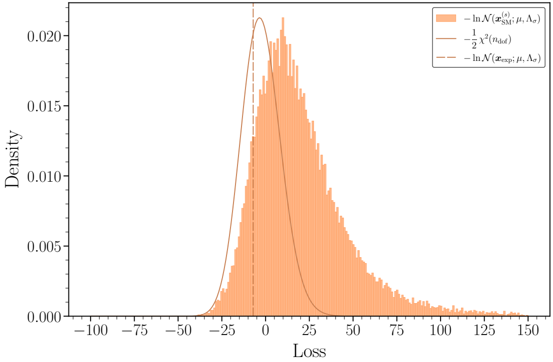
⇒ Implications

- ⇒ Even if the distribution of parameters is Gaussian, observables with complex structures **do not distribute normally**
- ⇒ **Only** observables with a **linear dependence** on the underlying parameters
- ⇒ The **likelihood** $p(\boldsymbol{x}|H_i)$ will generally be distributed under a **non-Gaussian distribution**

# Distribution of $-\log p(\boldsymbol{x}|H_i)$ vs Asymptotic $\chi^2$

⇒ Using samples $x_{\text{SM}}^{(s)}$ of SM predictions for the $b \to s\ell\ell$ observables dataset, we calculated $-\log p(\boldsymbol{x}|H_0)$ for each sample ⇒ log-likelihood distribution

⇒ Sizeable difference between the $-\log p(\boldsymbol{x}|H_i)$ and the asymptotic $\chi^2$ distribution with corresponding degrees of freedom



# Estimating Likelihoods with Full Generality

- ⇒ Goal: determine the full likelihood $p(\boldsymbol{x}|H_i) = p(\boldsymbol{x})$ **without introducing bias**
- ⇒ Known: distribution of underlying inputs $p(\boldsymbol{\nu})$ (model parameters)
- ⇒ Computable: $p(\boldsymbol{x}|\boldsymbol{\nu})$, achievable by simulating observables $\boldsymbol{x}$ using sampled parameters $\boldsymbol{\nu}$ from their known distributions
- ⇒ Explicitly calculate $p(\boldsymbol{x})$ as a marginal likelihood

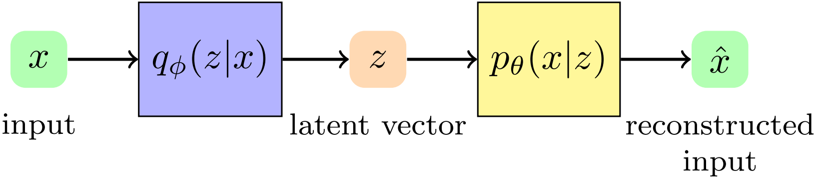
$$p(\boldsymbol{x}) = \int d\boldsymbol{\nu}\; p(\boldsymbol{x}|\boldsymbol{\nu})p(\boldsymbol{\nu})$$

  - ⇒ The **curse of dimensionality**: in most real-life applications $\boldsymbol{\nu}$ is usually high-dimensional
  - ⇒ Challenge: a direct computation the $d\boldsymbol{\nu}$ integral is generally **intractable** or **computationally very expensive**

- ⇒ Using **Machine Learning** techniques to learn the full likelihood function
  - ⇒ Using **Normalising Flows** to encode the densities $p(x_i|H_0)$
  - ⇒ **Variational Autoencoders** (VAEs) provide a feasible approach to approximate $p(\boldsymbol{x})$ with **arbitrary precision**

# Anomaly Detection with VAEs

# Introducing Variational Autoencoders




- ⇒ VAE framework
  - ⇒ **Model**: Pairs a probabilistic decoder $p_\theta(\boldsymbol{x}|\boldsymbol{z})$ with a probabilistic encoder $q_\phi(\boldsymbol{z}|\boldsymbol{x})$
  - ⇒ **Latent variable $\boldsymbol{z}$** approximates underlying parameters $\boldsymbol{\nu}$
  - ⇒ VAEs **do not** map inputs to a deterministic latent variable, but to a **probability space** $p(\boldsymbol{z})$
  - ⇒ $\theta$: parameters of the decoder
  - ⇒ $\phi$: parameters of the decoder

# The Variational Lower Bound

- ⇒ The Variational Lower Bound (ELBO) relates to two joint probability density functions: $p_\theta$ and $q_\phi$

$$\mathcal{L}(\theta, \phi; \boldsymbol{x}) = \mathbb{E}_{q_\phi(\boldsymbol{z}|\boldsymbol{x})}\left[\log \frac{p_\theta(\boldsymbol{x}, \boldsymbol{z})}{q_\phi(\boldsymbol{z}|\boldsymbol{x})}\right]$$

  - ⇒ $p_\theta(\boldsymbol{x}, \boldsymbol{z})$: joint distribution of $\boldsymbol{x}$ and $\boldsymbol{z}$
  - ⇒ $q_\phi(\boldsymbol{z}|\boldsymbol{x})$: approximate encoder posterior
  - ⇒ Simplifies to

$$\mathcal{L}(\theta, \phi; \boldsymbol{x}) = \mathbb{E}_{q_\phi(\boldsymbol{z}|\boldsymbol{x})}\left[\log p_\theta(\boldsymbol{x}|\boldsymbol{z})\right] - D_{KL}(q_\phi(\boldsymbol{z}|\boldsymbol{x})||p_\theta(\boldsymbol{z}))$$

- ⇒ Includes Kullback-Leibler divergence (KL-div) which is a distance in distribution space

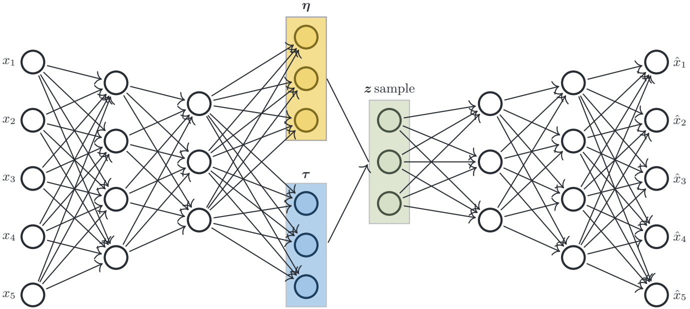
$$D_{KL}(q_\phi(w)||p_\theta(w)) = \mathbb{E}_{q_\phi(w)}\left[\log \frac{q_\phi(w)}{p_\theta(w)}\right]$$

- ⇒ ELBO and VAE objective function
  - ⇒ Log-likelihood relation

$$\log p_\theta(\boldsymbol{x}) \geq \mathcal{L}(\theta, \phi; \boldsymbol{x})$$

  - ⇒ Maximize ELBO to approximate the true log-likelihood

# Deep Learning Implementation of Variational Autoencoders




⇒ Implementation and parametrisation

- ⇒ **Neural Networks as parametrisers**
- ⇒ $p_\theta(\boldsymbol{x}|\boldsymbol{z})$ and $q_\phi(\boldsymbol{z}|\boldsymbol{x})$ parameterised using deep neural networks

$$\theta = \{W_{l_1}, \ldots, W_{l_L}, b_{l_1}, \ldots, b_{l_L}\}$$
$$\phi = \{V_{l_1}, \ldots, V_{l_L}, c_{l_1}, \ldots, c_{l_L}\}$$

where $W_l$ $(V_l)$, $b_l$ $(c_l)$ are the weights and biases of the encoder (decoder) network

- ⇒ This setup enables the modeling of complex, non-linear relationships between observed data and latent variables

# Training the VAE with Theoretical and Experimental Inputs

⇒ Generating Theoretical Predictions

- ⇒ Start by sampling the distribution of underlying inputs under hypothesis $H_0$, $p(\boldsymbol{\nu}|H_0)$
- ⇒ Compute the vector of observables $\boldsymbol{x}^s$ for these values to obtain a sample of theoretical predictions: $\boldsymbol{x}^s = (\boldsymbol{x}^1, \ldots, \boldsymbol{x}^{n_{\text{sample}}})$

⇒ Incorporating Experimental Uncertainties

- ⇒ Smear the samples with experimental uncertainties to simulate realistic observational data

$$\boldsymbol{x}'^s = \boldsymbol{x}^s + \boldsymbol{L}_{\boldsymbol{\Lambda}^{\text{exp}}} \boldsymbol{w}$$

- ⇒ $\boldsymbol{L}_{\boldsymbol{\Lambda}^{\text{exp}}}$: Cholesky decomposition of the experimental covariance matrix $\boldsymbol{\Lambda}^{\text{exp}}$
- ⇒ $\boldsymbol{w} \sim \mathcal{N}(w; \mathbf{0}, \mathbf{1})$: Normal noise vector simulating experimental noise

⇒ Training the VAE

- ⇒ Divide the smeared dataset into **training and testing datasets**
- ⇒ Use the training dataset to **optimise the parameters** of the VAE, **minimising** the -ELBO

$$\mathcal{L}(\theta, \phi; \boldsymbol{x}) = \mathbb{E}_{q_\phi(\boldsymbol{z}|\boldsymbol{x})} \left[\log p_\theta(\boldsymbol{x}|\boldsymbol{z})\right] - \beta D_{KL}(q_\phi(\boldsymbol{z}|\boldsymbol{x}) || p_\theta(\boldsymbol{z}))$$

- ⇒ Objective: **approximate the full log-likelihood distribution** of the observables under $H_0$ as closely as possible

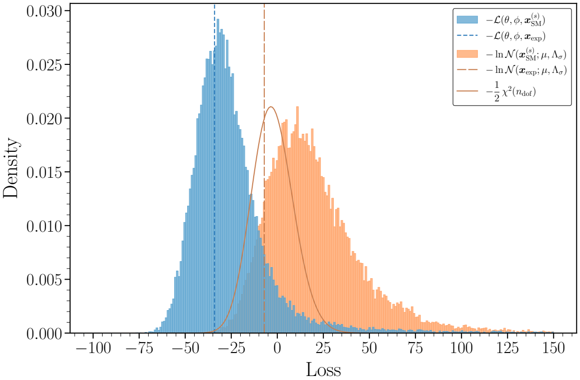
# Statistical Analysis Using Trained VAE for $b \to s\ell^+\ell^-$

⇒ Analysing the test dataset

⇒ Compute the -ELBO distribution using the test dataset, approximating the full -log-likelihood under hypothesis $H_0$.

⇒ Evaluate -ELBO for the experimental data to compute the $p$-value

⇒ Preliminary results for the $b \to s\ell\ell$ dataset



# Outlook

# Outlook and Continued Research

- ⇒ Deepening understanding of VAE parameters
  - ⇒ Exploring how different parameters influence the anomaly score and VAE's generative properties
- ⇒ Ongoing hyperparameter optimisation
  - ⇒ Continuously refining the model to enhance its predictive accuracy and anomaly detection
- ⇒ Addressing sparse covariance matrices
  - ⇒ Using random matrix theory techniques to sample observables and covariance matrices at the same time (LKJ distribution, Wishart distribution)
  - ⇒ Will allow us to quantify the uncertainty attached to many unnatural zeros in the experimental covariance matrix
- ⇒ Expanding application scope
  - ⇒ Applying methodologies to SMEFT fits beyond $b \to s\ell\ell$

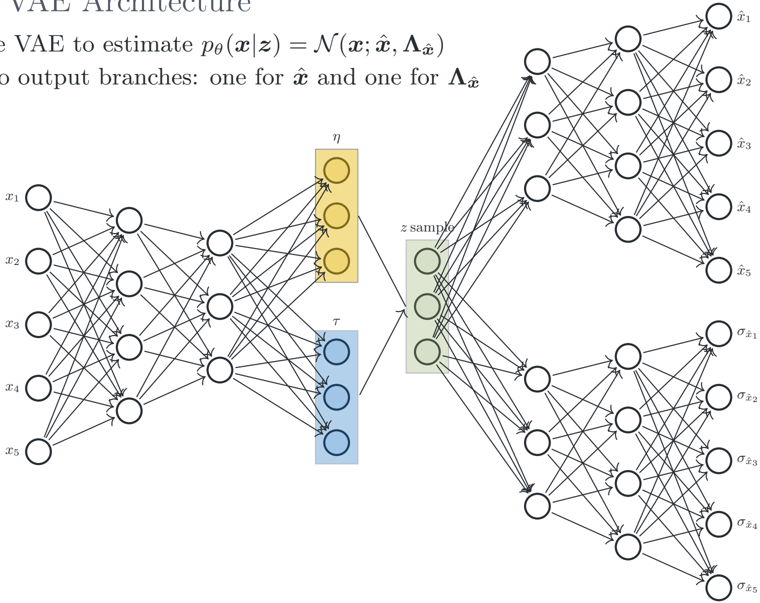
Thank You!

# Backup Slides

# Dual-Branch VAE Architecture

⇒ We need the VAE to estimate $p_\theta(\boldsymbol{x}|\boldsymbol{z}) = \mathcal{N}(\boldsymbol{x}; \hat{\boldsymbol{x}}, \boldsymbol{\Lambda}_{\hat{\boldsymbol{x}}})$

⇒ We need two output branches: one for $\hat{\boldsymbol{x}}$ and one for $\boldsymbol{\Lambda}_{\hat{\boldsymbol{x}}}$



# Refining Model Tuning and Validity in VAE Training

- Challenges in Model Tuning
  - ⇒ How do we determine the optimal dimensionality for the DNNs of the encoder and decoder, or the correct value of $\beta$?
  - ⇒ Could these choices bias the $p$-value?
  - ⇒ The choice of neural networks' architecture and $\beta$ significantly affects the model's performance and the fidelity of the statistical results
- Testing and Validating Model Parameters
  - ⇒ Ongoing research and empirical testing are essential to optimise these parameters while minimising biases
- Strategies for Validation and Hyperparameter Optimisation
  - ⇒ Employ validation techniques to ensure model outputs are stable and reliable across various parameter configurations
  - ⇒ Use synthetic datasets to evaluate the impact of hyperparameter adjustments on model performance

# Optimising Hyperparameters

- Generating artificially anomalous data
  - ⇒ Used to train the VAE across different configurations to optimise anomaly detection
- Tuning $\beta$ in the ELBO
  - ⇒ Exploring the impact of $\beta$ on anomaly detection and VAE's generative accuracy
- Pre-experimental blind analysis
  - ⇒ Ensures that the final measurement of experimental data is unbiased