Bayes Theorem:

$$\underbrace{p(\mathbf{W_i},\mathbf{b_i}|D,M)}_{\text{Posterior}} \propto \underbrace{p(D|\mathbf{W_i},\mathbf{b_i},M)}_{\text{Likelihood}}\underbrace{p(\mathbf{W_i},\mathbf{b_i}|M)}_{\text{Prior}}$$

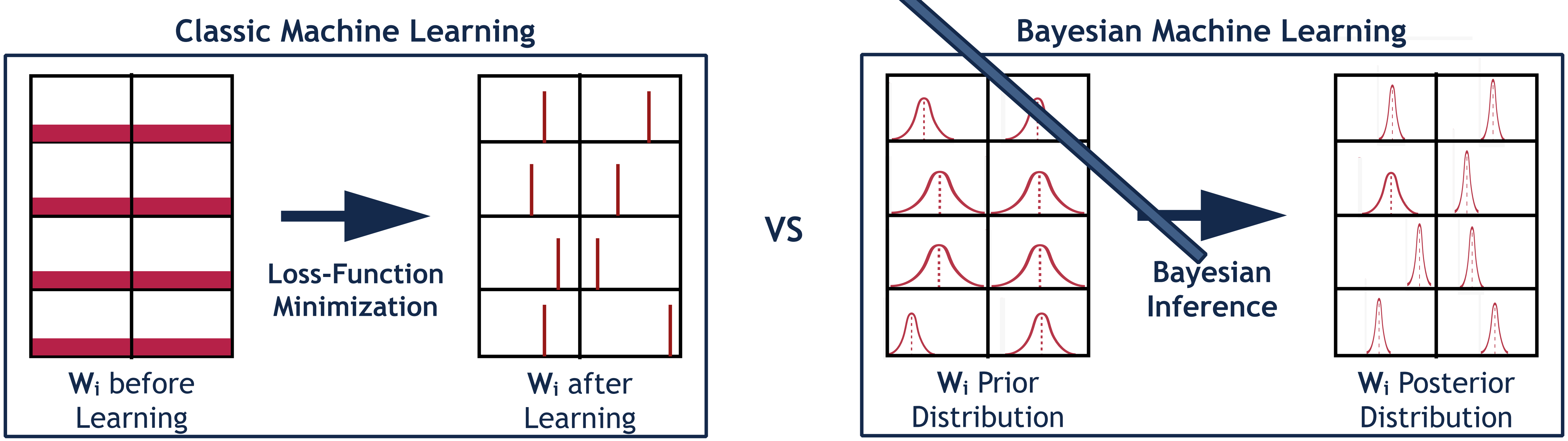
Prior: $p(\mathbf{W_i},\mathbf{b_i}|\mathbf{M}) \sim \mathcal{N}(\mu = ..., \sigma = ...)$

Likelihood: $p(\mathbf{D}|\mathbf{W_i},\mathbf{b_i},\mathbf{M}) = \dfrac{\mathbf{1}}{\sqrt{\mathbf{2}\pi\sigma_{\mathbf{L}}^{\mathbf{2}}}} \exp\left(\sum_{\mathbf{j}}^{\mathbf{N_D}} \dfrac{(\log(\mathbf{V_j}) - \log(\mathbf{D_j}))^{\mathbf{2}}}{\mathbf{2}\sigma_{\mathbf{L}}}\right)$

Posterior distributions have been computed through the **Automatic Differentiation Variational Inference** (ADVI) algorithm.

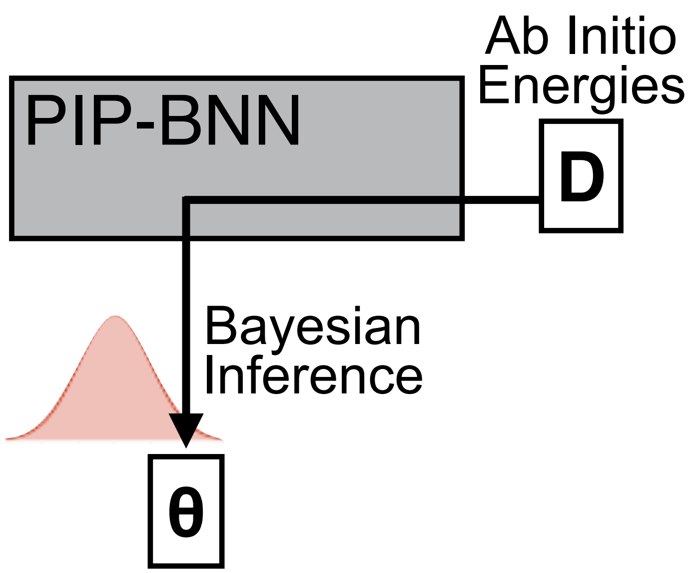
Non-Deterministic attribute of BNNs is a consequence of:

- Functional **parameters treated as random variables** (parameter uncertainty):

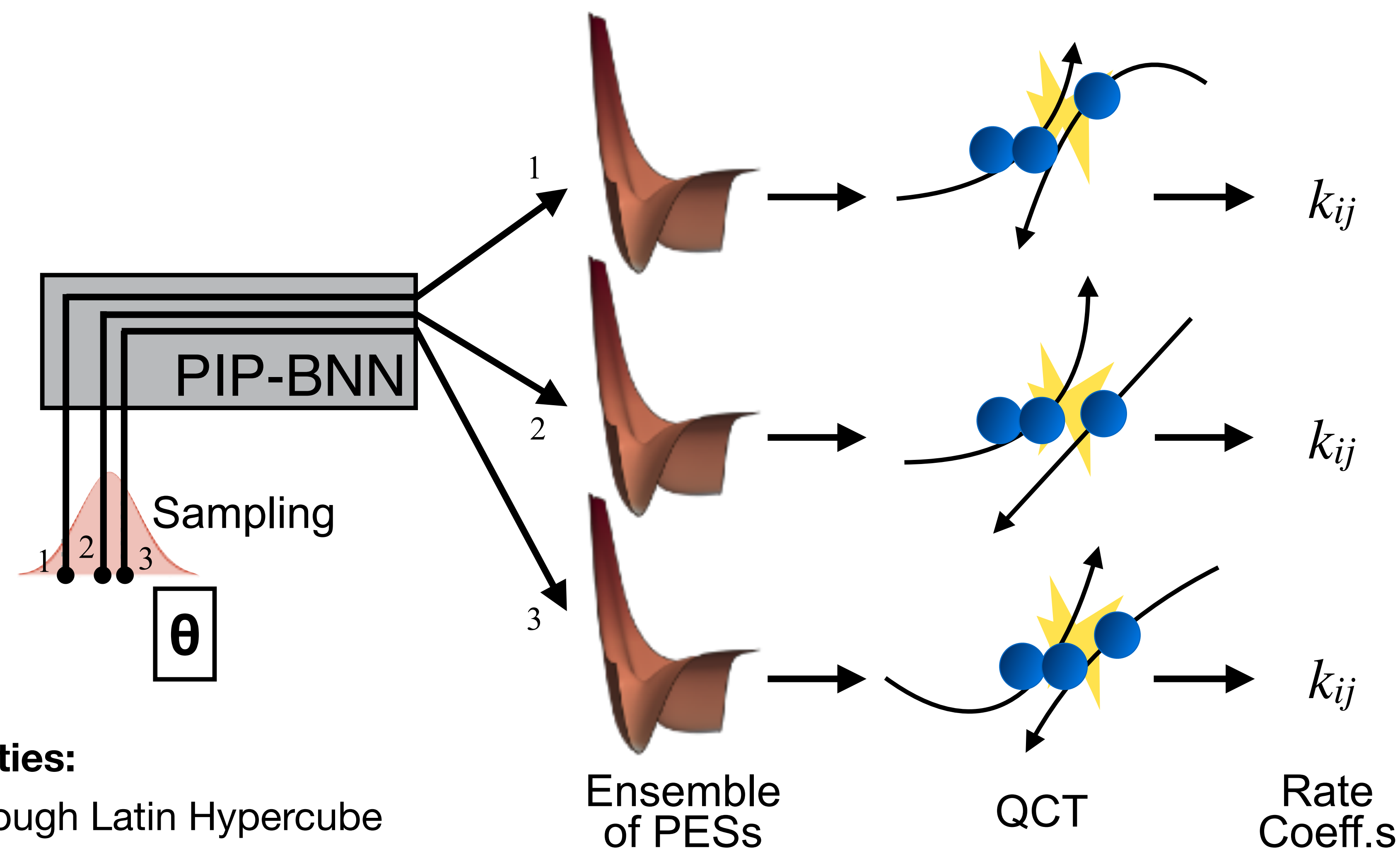


- Some **noise superimposed** to the functional form (model uncertainty).

PES UQ: Methodology



Solution of the inverse problem:
The optimal PDFs characterizing the PIP-BNN parameters are learnt through Bayesian variational inference from the ab initio data points.



Forward propagation of the Uncertainties:
The posterior distribution is sampled through Latin Hypercube Sampling, an ensemble of PESs is computed through the PIP-BNN, and the surfaces are used for simulating collisions.