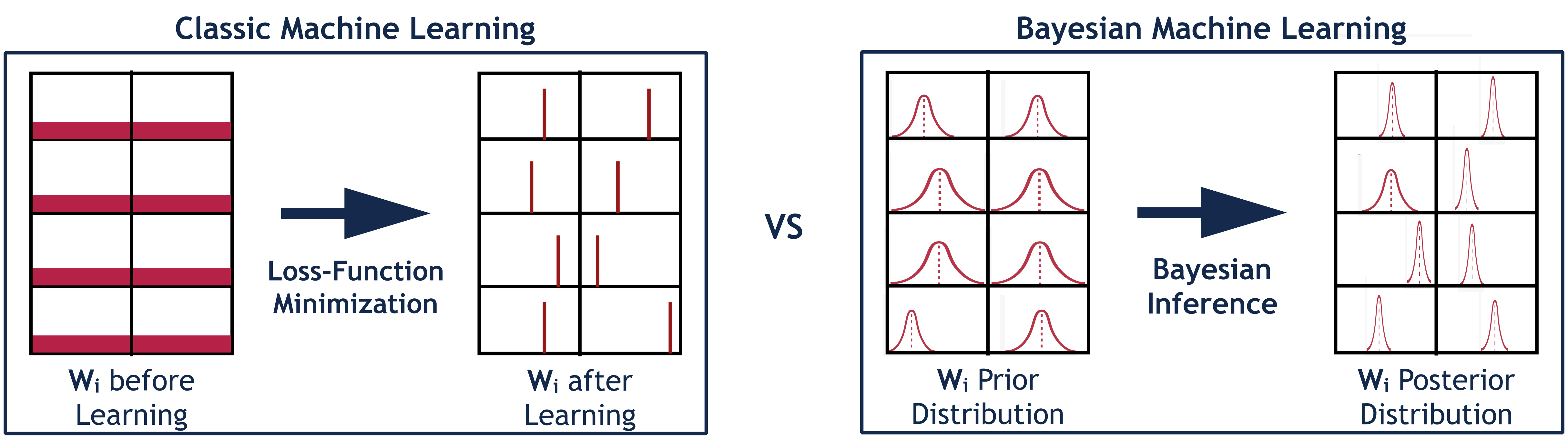
From Deterministic To Stochastic

We propose the construction of a **stochastic PES**, which condenses the inaccuracy content related to both the grid of atom configuration chosen and the fitting function adopted.

Thus, we extend the ANN to **Bayesian Neural Networks** (BNNs), following the work initiated by R. Neal and recently pursued by C. Blundell *et al*.

Non-Deterministic attribute of BNNs is a consequence of:

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



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

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

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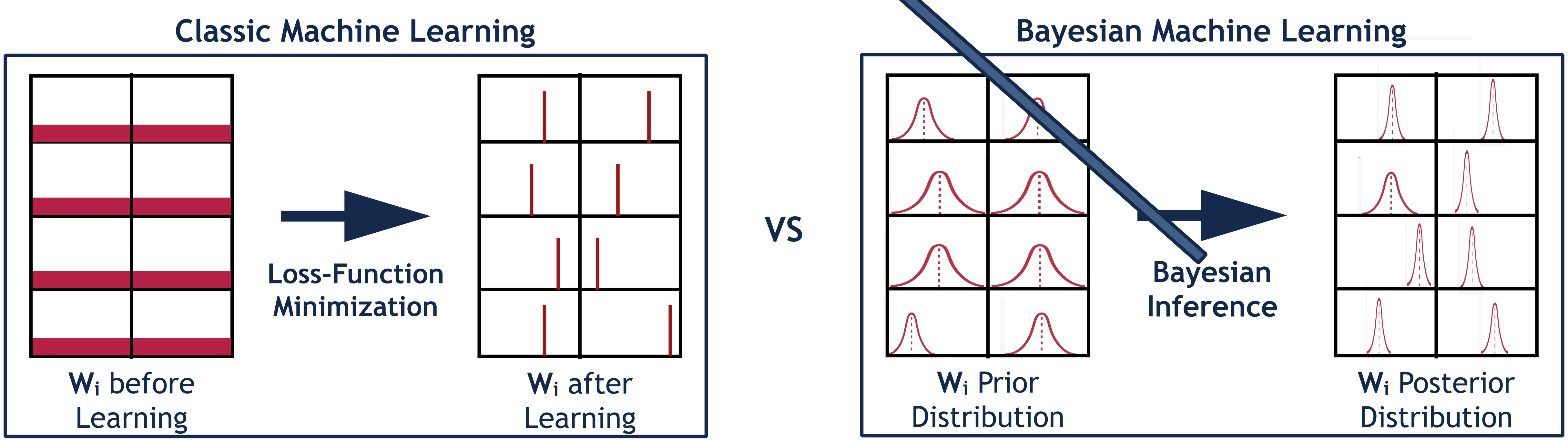

- Some **noise superimposed** to the functional form (model uncertainty).