a

Base

Mean-variance Estimator

μ_E

μ_E
σ_E

b

Local Chemical Environment

$\{|\boldsymbol{r}_{ij}|\}, \{Z_i, Z_j\}, \{\boldsymbol{r}_{ij}\}$

$\boldsymbol{R}_{ij}$

$\{Z_i\}$ $\{\boldsymbol{r}_{ij}\}$ $\{|\boldsymbol{r}_{ij}|\}$

1-Body Emb. | Angular Emb. | Radial Emb.

$a^{(1)}$

Linear $A^{(0)}$ e_{ij} $\tilde{e}_{ij}^{RBF}$

Layer 1

$A^{(1)}$ $E_i^{(2)}$

Layer 2

$A^{(2)}$ $E_i^{(3)}$

$A^{(\eta-1)}$ $E_i^{(\eta)}$

Layer η

$E_i^{(\eta+1)}$

c

$A^{(\eta-2)}$

Layer η-1

Residual Self-Interaction | Linear

e_{ij}

$\mathcal{M}(\tilde{e}_{ij}^{RBF})$

$a^{(1)}$

Σ **Aggregation**

Rotationally equivariant

$B_i^{(\eta-1)}$

Linear

Linear

Gate

Linear

$E_i^{(\eta)}$

$A^{(\eta-1)}$

$\otimes$: Tensor product
$||$: Concatenation
$\odot$: Multiplication
$+$: Sum

d

Deep Ensemble

Ensemble Combination

Stochastic Weight Averaging Gaussian

Training

Collecting Weights
$\theta_1, \theta_2, \theta_3, \cdots, \theta_T$

θ_s

Approximate Posterior distribution

Sampling

Improved Variational Online Newton

$q(\theta)$ $p(\theta)$

Kulback-Leibler divergence

$Loss$

$weight$

Second-order optimization

θ_s

Approximate Posterior distribution

Sampling

Laplace Approximation

$p(D|\theta)$

$p(\theta)$

θ_{MAP}

Hessian
$H = \nabla_\theta^2 \mathcal{L}(D;\theta)\big|_{\theta_{\text{MAP}}}$

θ_s

Approximate Posterior distribution

Sampling

e

Out-of-distribution Detection

ID

Training

ID
ID
OOD

Inference

Active Learning

Inference

Unlabeled Pool

Training

Low Uncertainty

High Uncertainty

Recalibration

Uncalibrated Confidence Intervals
True
Predicted

Calibrated Confidence Intervals
True
Predicted

Calibration Plot

Observed Confidence Level

Expected Confidence Level

Uncalibrated
Calibrated