Dichotomize and Generalize: PAC-Bayesian Binary Activated Deep Neural Networks

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Introduction

We present a comprehensive study of multilayer neural networks with binary activation, relying on the PAC-Bayesian theory.

Contributions
- An end-to-end framework to train a binary activated deep neural network (DNN).
- Nonvacuous PAC-Bayesian generalization bounds for binary activated DNNs.

Binary Activated Neural Networks

- L fully connected layers
- d_k denotes the number of neurons of the kth layer
- $\text{sgn}(a) = 1$ if $a > 0$ and $\text{sgn}(a) = -1$ otherwise
- Weights matrices : $\mathbf{W}_k \in \mathbb{R}^{d_k \times d_{k-1}}$, $\theta = \text{vec}\big(\{\mathbf{W}_k\}_{k=1}^L\big) \in \mathbb{R}^D$
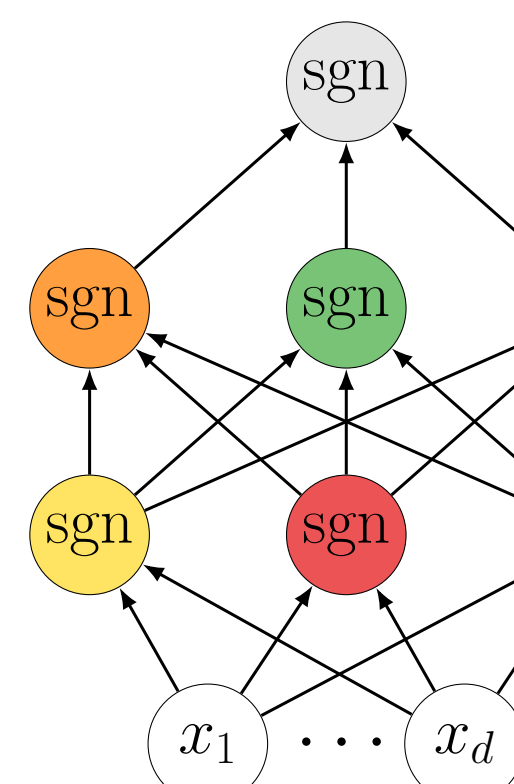
Prediction
$$f_\theta(\mathbf{x}) = \text{sgn}\big(\mathbf{w}_L \text{sgn}\big(\mathbf{W}_{L-1}\text{sgn}\big(\ldots \text{sgn}(\mathbf{W}_1\mathbf{x})\big)\big)\big)$$

PAC-Bayesian Theory

Given a data distribution $\mathcal{D}$, a training set $S = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)\} \sim \mathcal{D}^n$, with $\mathbf{x}_i \in \mathbb{R}^{d_0}$ and $y_i \in \{-1, 1\}$, a loss $\ell : [-1, 1]^2 \to [0, 1]$, a predictor $f \in \mathcal{F}$:

$$\mathcal{L}_\mathcal{D}(f) = \mathop{\mathbf{E}}_{(\mathbf{x},y)\sim\mathcal{D}} \ell\big(f(\mathbf{x}), y\big) \quad \leftarrow \boxed{generalization\ loss}$$

$$\widehat{\mathcal{L}}_S(f) = \frac{1}{n}\sum_{i=1}^n \ell\big(f(\mathbf{x}_i), y_i\big) \quad \leftarrow \boxed{empirical\ loss}$$
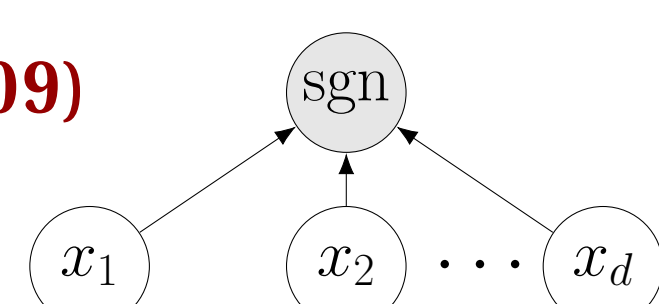
PAC-Bayesian Theorem
For any prior P on $\mathcal{F}$, with probability $1-\delta$ on the choice of $S\sim\mathcal{D}^n$, we have for all $C > 0$, and any posterior distribution Q on $\mathcal{F}$:

$$\mathop{\mathbf{E}}_{f\sim Q}\mathcal{L}_\mathcal{D}(f) \leq \frac{1}{1-e^{-C}}\left(1 - \exp\left(-C\mathop{\mathbf{E}}_{f\sim Q}\widehat{\mathcal{L}}_S(f) - \frac{1}{n}[\text{KL}(Q\|P) + \ln\frac{2\sqrt{n}}{\delta}]\right)\right)$$
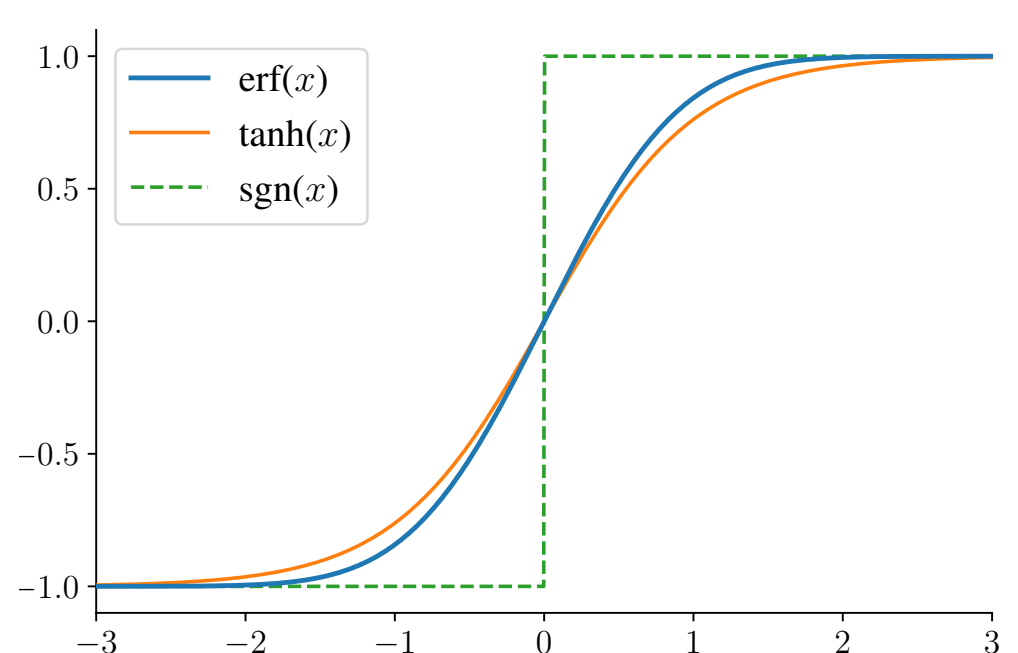
Linear Classifier

PAC-Bayesian Learning of Linear Classifiers **(Germain et al., 2009)**
$$f_\mathbf{w}(\mathbf{x}) := \text{sgn}(\mathbf{w} \cdot \mathbf{x}), \text{ with } \mathbf{w} \in \mathbb{R}^d$$

PAC-Bayesian analysis
- Space of all linear classifiers $\mathcal{F}_d := \{f_\mathbf{v}|\mathbf{v} \in \mathbb{R}^d\}$
- Gaussian prior $P_\mathbf{u} := \mathcal{N}(\mathbf{u}, I_d)$ over $\mathcal{F}_d$
- Gaussian posterior $Q_\mathbf{w} := \mathcal{N}(\mathbf{w}, I_d)$ over $\mathcal{F}_d$
- Predictor $F_\mathbf{w}(\mathbf{x}) := \mathbf{E}_{\mathbf{v}\sim Q_\mathbf{w}} f_\mathbf{v}(\mathbf{x}) = \text{erf}\left(\frac{\mathbf{w}\cdot\mathbf{x}}{\sqrt{2}\|\mathbf{x}\|}\right)$
- Linear loss $\ell(f_\mathbf{v}(\mathbf{x}), y) := \frac{1}{2} - \frac{1}{2}yf_\mathbf{v}(\mathbf{x})$
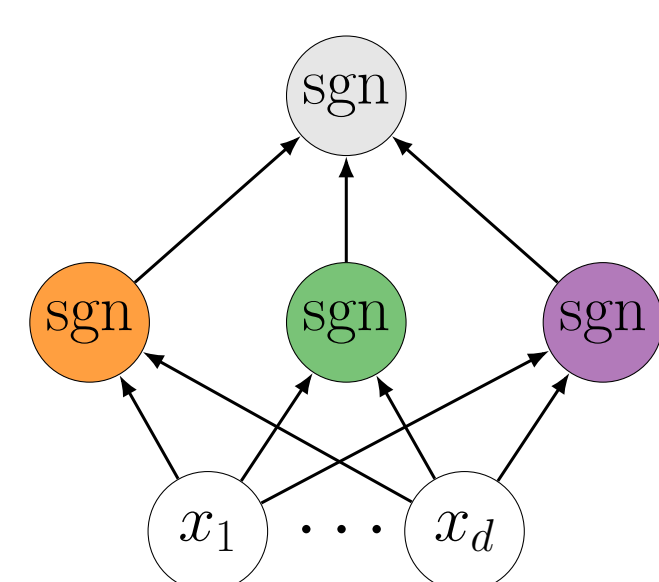
Bound minimization
$$C\,n\,\widehat{\mathcal{L}}_S(F_\mathbf{w}) + \text{KL}(Q_\mathbf{w}\|P_\mathbf{u}) = C\frac{1}{2}\sum_{i=1}^n \text{erf}\left(-y_i\frac{\mathbf{w}\cdot\mathbf{x}_i}{\sqrt{d}\|\mathbf{x}_i\|}\right) + \frac{1}{2}\|\mathbf{w} - \mathbf{u}\|^2$$

Shallow Learning

Posterior $Q_\theta = \mathcal{N}(\theta, I_D)$, over the family of all networks $\mathcal{F}_D = \{f_{\tilde\theta}\,|\,\tilde\theta \in \mathbb{R}^D\}$, where
$$f_\theta(\mathbf{x}) = \text{sgn}\big(\mathbf{w}_2 \cdot \text{sgn}(\mathbf{W}_1\mathbf{x})\big)$$

$$\begin{aligned}
F_\theta(\mathbf{x}) &= \mathop{\mathbf{E}}_{\tilde\theta\sim Q_\theta} f_{\tilde\theta}(\mathbf{x}) \\
&= \int_{\mathbb{R}^{d_1\times d_0}} Q_1(\mathbf{V}_1)\int_{\mathbb{R}^{d_1}} Q_2(\mathbf{v}_2)\text{sgn}(\mathbf{v}_2 \cdot \text{sgn}(\mathbf{V}_1\mathbf{x}))d\mathbf{v}_2 d\mathbf{V}_1 \\
&= \sum_{\mathbf{s}\in\{-1,1\}^{d_1}} \text{erf}\left(\frac{\mathbf{w}_2\cdot\mathbf{s}}{\sqrt{2d_1}}\right)\int_{\mathbb{R}^{d_1\times d_0}}\mathbb{1}[\mathbf{s} = \text{sgn}(\mathbf{V}_1\mathbf{x})]Q_1(\mathbf{V}_1)\,d\mathbf{V}_1 \\
&= \sum_{\mathbf{s}\in\{-1,1\}^{d_1}} \underbrace{\text{erf}\left(\frac{\mathbf{w}_2\cdot\mathbf{s}}{\sqrt{2d_1}}\right)}_{F_{\mathbf{w}_2}(\mathbf{s})}\underbrace{\prod_{i=1}^{d_1}\left[\frac{1}{2} + \frac{s_i}{2}\text{erf}\left(\frac{\mathbf{w}_1^i\cdot\mathbf{x}}{\sqrt{2}\|\mathbf{x}\|}\right)\right]}_{\Pr(\mathbf{s}|\mathbf{x},\mathbf{W}_1)}
\end{aligned}$$

PAC-Bayesian bound ingredients
- Empirical loss : $\widehat{\mathcal{L}}_S(F_\theta) = \mathbf{E}_{\theta'\sim Q_\theta}\widehat{\mathcal{L}}_S(f_{\theta'}) = \frac{1}{n}\sum_{i=1}^n\left[\frac{1}{2} - \frac{1}{2}y_iF_\theta(\mathbf{x}_i)\right]$
- Complexity term : $\text{KL}(Q_\theta\|P_\mu) = \frac{1}{2}\|\theta - \mu\|^2$, with $\mu \in \mathbb{R}^D$
- Generalization bound : $\frac{1}{1-e^{-C}}\left(1 - \exp\left(-C\widehat{\mathcal{L}}_S(F_\theta) - \frac{1}{n}[\text{KL}(Q_\theta\|P_\mu) + \ln\frac{2\sqrt{n}}{\delta}]\right)\right)$

Visualization

The proposed method can be interpreted as a majority vote of hidden layer representations.
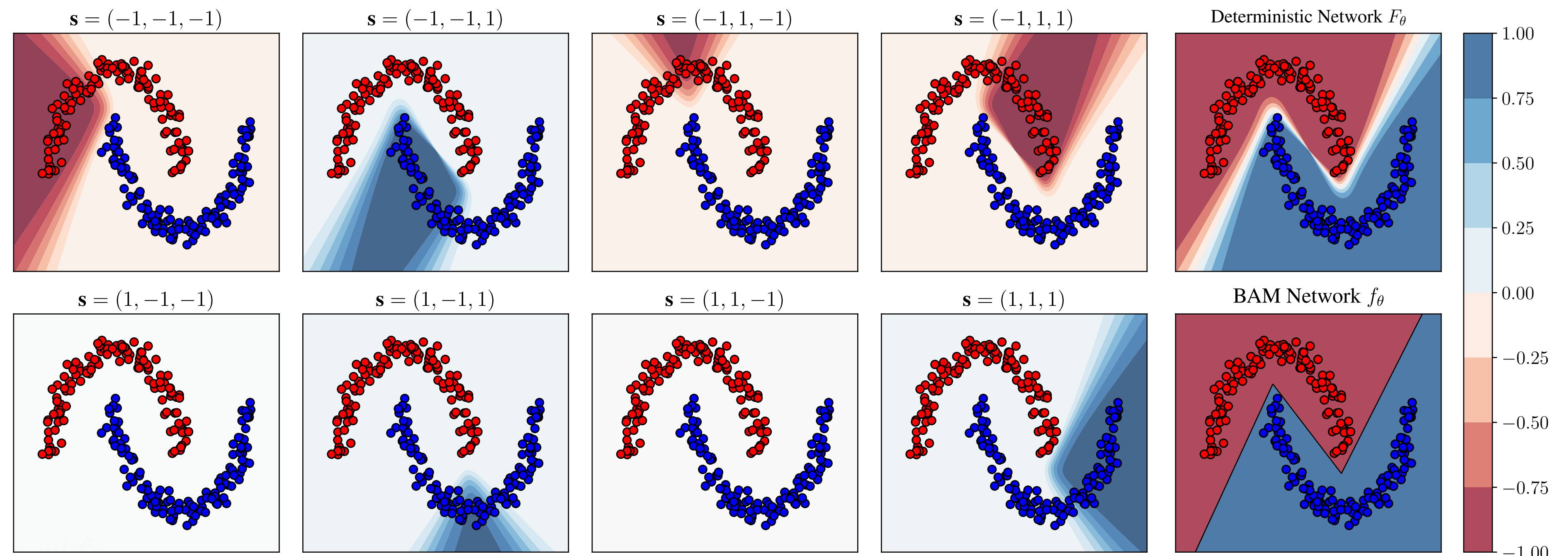

Figure 1: Illustration of the proposed method for a one hidden layer network of size $d_1=3$, interpreted as a majority vote over 8 binary representations $\mathbf{s} \in \{-1, 1\}^3$. For each $\mathbf{s}$, a plot shows the values of $F_{\mathbf{w}_2}(\mathbf{s})\Pr(\mathbf{s}|\mathbf{x},\mathbf{W}_1)$.

Stochastic Approximation

Prediction.
$$F_\theta(\mathbf{x}) = \sum_{\mathbf{s}\in\{-1,1\}^{d_1}} F_{\mathbf{w}_2}(\mathbf{s})\Pr(\mathbf{s}|\mathbf{x},\mathbf{W}_1)$$

Hidden layer partial derivatives, with $\text{erf}'(x) := \frac{2}{\sqrt{\pi}}e^{-x^2}$.
$$\frac{\partial}{\partial\mathbf{w}_1^k}F_\theta(\mathbf{x}) = \frac{\mathbf{x}}{2^{\frac{3}{2}}\|\mathbf{x}\|}\text{erf}'\left(\frac{\mathbf{w}_1^k\cdot\mathbf{x}}{\sqrt{2}\|\mathbf{x}\|}\right)\sum_{\mathbf{s}\in\{-1,1\}^{d_1}} s_k F_{\mathbf{w}_2}(\mathbf{s})\left[\frac{\Pr(\mathbf{s}|\mathbf{x},\mathbf{W}_1)}{\Pr(s_k|\mathbf{x},\mathbf{w}_1^k)}\right]$$

Monte Carlo sampling
We generate T random binary vectors $\{\mathbf{s}^t\}_{t=1}^T$ according to $\Pr(\mathbf{s}|\mathbf{x},\mathbf{W}_1)$.
$$F_\theta(\mathbf{x}) \approx \frac{1}{T}\sum_{t=1}^T F_{\mathbf{w}_2}(\mathbf{s}^t) \qquad \frac{\partial}{\partial\mathbf{w}_1^k}F_\theta(\mathbf{x}) \approx \frac{\mathbf{x}}{2^{\frac{3}{2}}\|\mathbf{x}\|}\text{erf}'\left(\frac{\mathbf{w}_1^k\cdot\mathbf{x}}{\sqrt{2}\|\mathbf{x}\|}\right)\frac{1}{T}\sum_{t=1}^T\frac{s_k^t}{\Pr(s_k^t|\mathbf{x},\mathbf{w}_1^k)}F_{\mathbf{w}_2}(\mathbf{s}^t)$$

This turns out to be a variant of the REINFORCE algorithm **(Williams, 1992)**.

Deep Learning (PBGNet)

To enable a layer-by-layer computation of the prediction function, we want the neurons of a given layer to be independent of each other. This is achieved with the tree architecture mapping function $\zeta(\theta)$ applied on a multilayer network.

Recursive definition. $F_k^{(j)}$ denotes the output of the jth neuron of the kth hidden layer :
$$F_1^{(j)}(\mathbf{x}) = \text{erf}\left(\frac{\mathbf{w}_1^j\cdot\mathbf{x}}{\sqrt{2}\|\mathbf{x}\|}\right) \quad \leftarrow \boxed{first\ hidden\ layer}$$
$$F_{k+1}^{(j)}(\mathbf{x}) = \sum_{\mathbf{s}\in\{-1,1\}^{d_k}}\text{erf}\left(\frac{\mathbf{w}_{k+1}^j\cdot\mathbf{s}}{\sqrt{2d_k}}\right)\prod_{i=1}^{d_k}\left(\frac{1}{2} + \frac{1}{2}s_i \times F_k^{(i)}(\mathbf{x})\right)$$
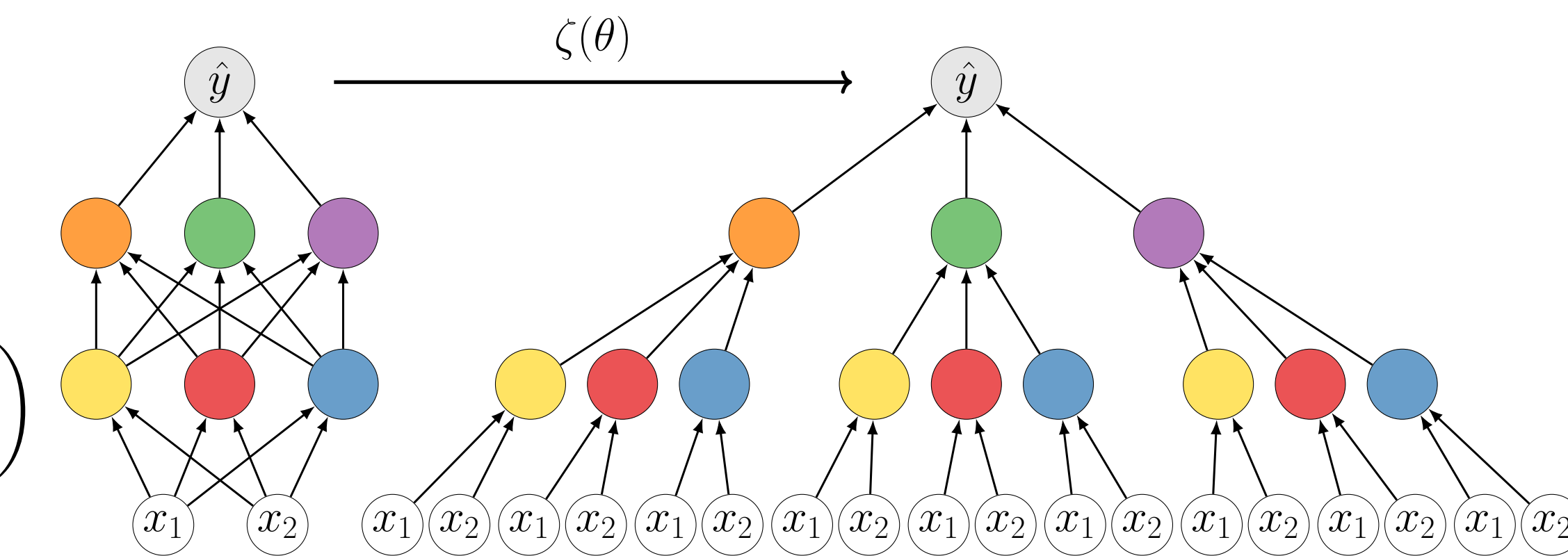
Kullback-Leibler regularization
$$\text{KL}\big(Q_{\zeta(\theta)}\,\|\,P_{\zeta(\mu)}\big) = \frac{1}{2}\left(\|\mathbf{w}_L - \mathbf{u}_L\|^2 + \sum_{i=1}^{L-1}d_{k+1}^\dagger\|\mathbf{W}_i - \mathbf{U}_i\|_F^2\right)\text{ for }d_k^\dagger := \prod_{i=k}^L d_i.$$

Experiment

We perform model selection using a validation set for a **MLP with tanh activations**, and using the PAC-Bayes bound for our **PBGnet** and **PBGnet$_\text{pre}$** algorithms. **PBGnet$_\ell$** and **PBGnet$_{\ell\text{-bnd}}$** are intermediate variants.
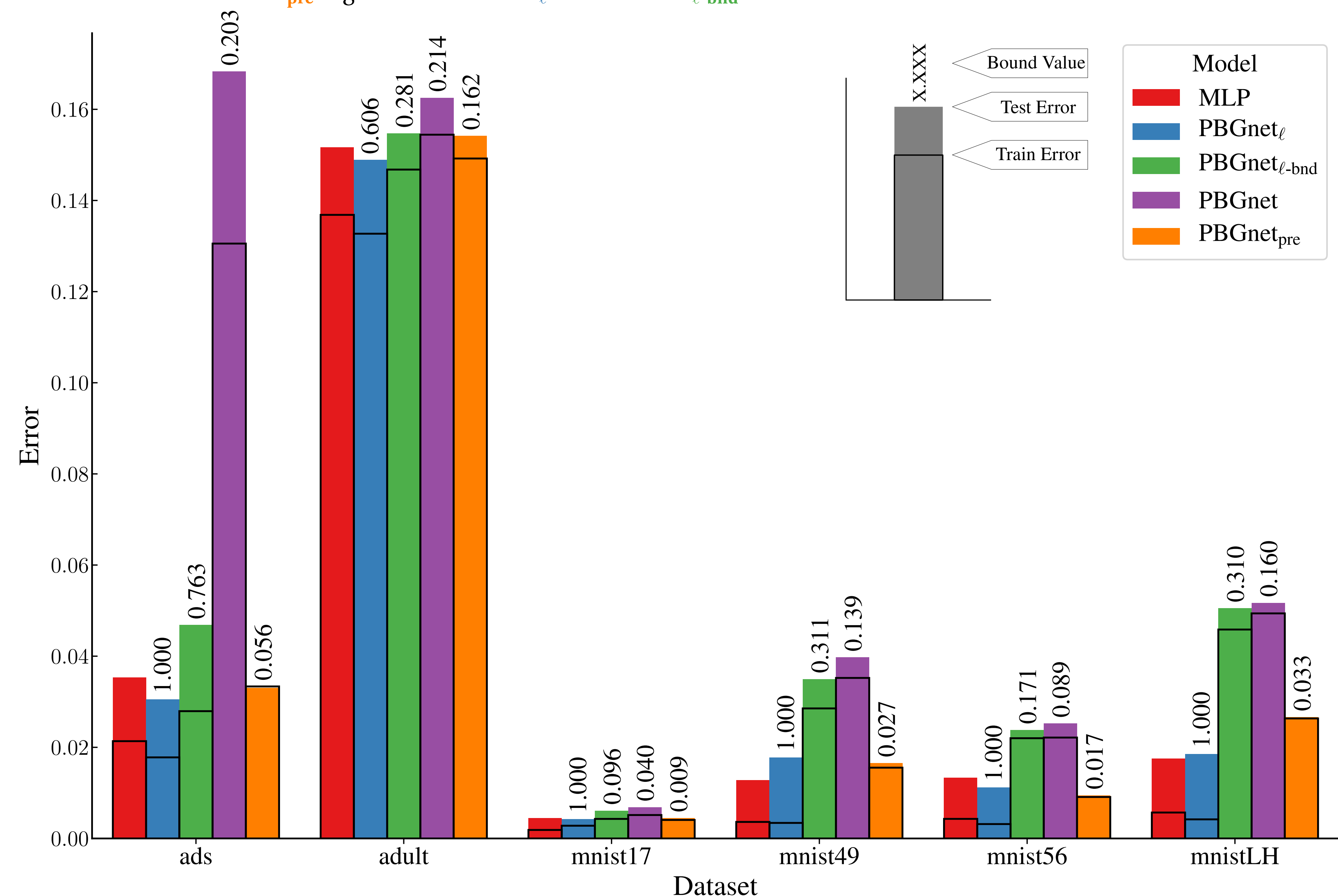

Figure 2: Experiment results for the considered models on the binary classification datasets. PAC-Bayesian bounds hold with probability 0.95.