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

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Introduction

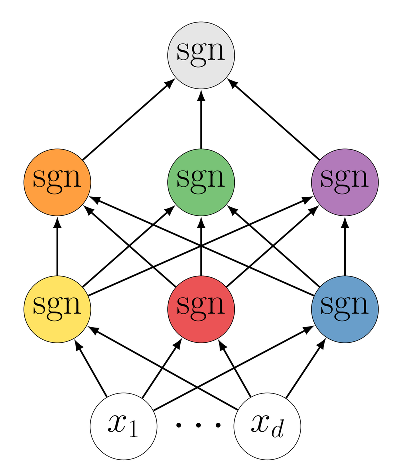
We present a comprehensive study of multilayer neural networks with binary activation, relying on the PAC-Bayesian theory.

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 k^{th} layer
- $\operatorname{sgn}(a) = 1$ if $a > 0$ and $\operatorname{sgn}(a) = -1$ otherwise
- Weights matrices : $\mathbf{W}_k \in \mathbb{R}^{d_k \times d_{k-1}}$, $\theta = \operatorname{vec}\big(\{\mathbf{W}_k\}_{k=1}^{L}\big) \in \mathbb{R}^D$



Prediction

$$f_\theta(\mathbf{x}) = \operatorname{sgn}\big(\mathbf{w}_L \operatorname{sgn}(\mathbf{W}_{L-1}\operatorname{sgn}(\ldots\operatorname{sgn}(\mathbf{W}_1\mathbf{x})))\big)$$

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 $f \in \mathcal{F}$:

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

$$\widehat{\mathcal{L}}_S(f) = \frac{1}{n}\sum_{i=1}^{n} \ell\big(f(\mathbf{x}_i), y_i\big) \quad \longleftarrow \boxed{\textit{empirical loss}}$$

PAC-Bayesian Theorem

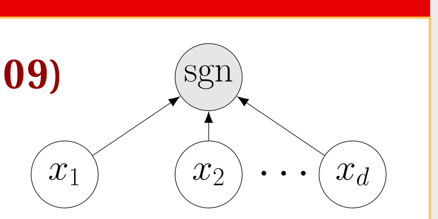
For any prior P on $\mathcal{F}$, with probability $1-\delta$ on the choice of $S\sim\mathcal{D}^n$, we have for all $C > 0$, and all posterior distribution Q on $\mathcal{F}$:

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

Linear Classifier

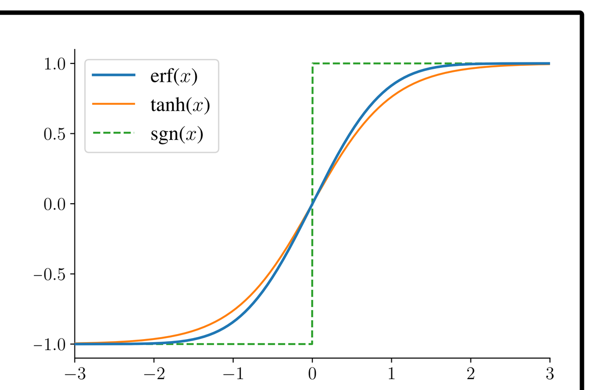
PAC-Bayesian Learning of Linear Classifiers **(Germain et al., 2009)**

$$f_{\mathbf{w}}(\mathbf{x}) := \operatorname{sgn}(\mathbf{w}\cdot\mathbf{x}), \text{ with } \mathbf{w} \in \mathbb{R}^d$$



PAC-Bayes analysis

- Space of all linear classifiers $\mathcal{F}_d := \{f_{\mathbf{v}} | \mathbf{v} \in \mathbb{R}^d\}$
- Gaussian posterior $Q_{\mathbf{w}} := \mathcal{N}(\mathbf{w}, I_d)$ over $\mathcal{F}_d$
- Gaussian prior $P_{\mathbf{u}} := \mathcal{N}(\mathbf{u}, I_d)$ over $\mathcal{F}_d$
- Predictor $F_{\mathbf{w}}(\mathbf{x}) := \mathbf{E}_{\mathbf{v}\sim Q_{\mathbf{w}}} f_{\mathbf{v}}(\mathbf{x}) = \operatorname{erf}\left(\frac{\mathbf{w}\cdot\mathbf{x}}{\sqrt{d}\|\mathbf{x}\|}\right)$
- Linear loss $\ell(f_{\mathbf{v}}(\mathbf{x}), y) := \frac{1}{2} - \frac{1}{2} y f_{\mathbf{v}}(\mathbf{x})$



Bound minimization

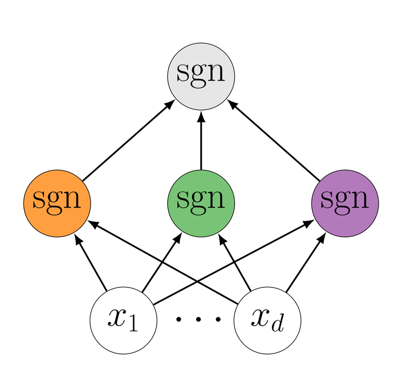
$$C\, n\, \widehat{\mathcal{L}}_S(F_{\mathbf{w}}) + \mathrm{KL}(Q_{\mathbf{w}}\|P_{\mathbf{u}}) = C\,\tfrac{1}{2}\textstyle\sum_{i=1}^{n} \operatorname{erf}\left(-y_i \frac{\mathbf{w}\cdot\mathbf{x}_i}{\sqrt{d}\|\mathbf{x}_i\|}\right) + \tfrac{1}{2}\|\mathbf{w} - \mathbf{u}\|^2$$

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

$$f_\theta(\mathbf{x}) = \operatorname{sgn}\big(\mathbf{w}_2 \cdot \operatorname{sgn}(\mathbf{W}_1\mathbf{x})\big)$$

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



PAC-Bayesian bound ingredients

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

Contact : gael.letarte.1@ulaval.ca **Code :** github.com/gletarte/dichotomize-and-generalize

Visualization

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

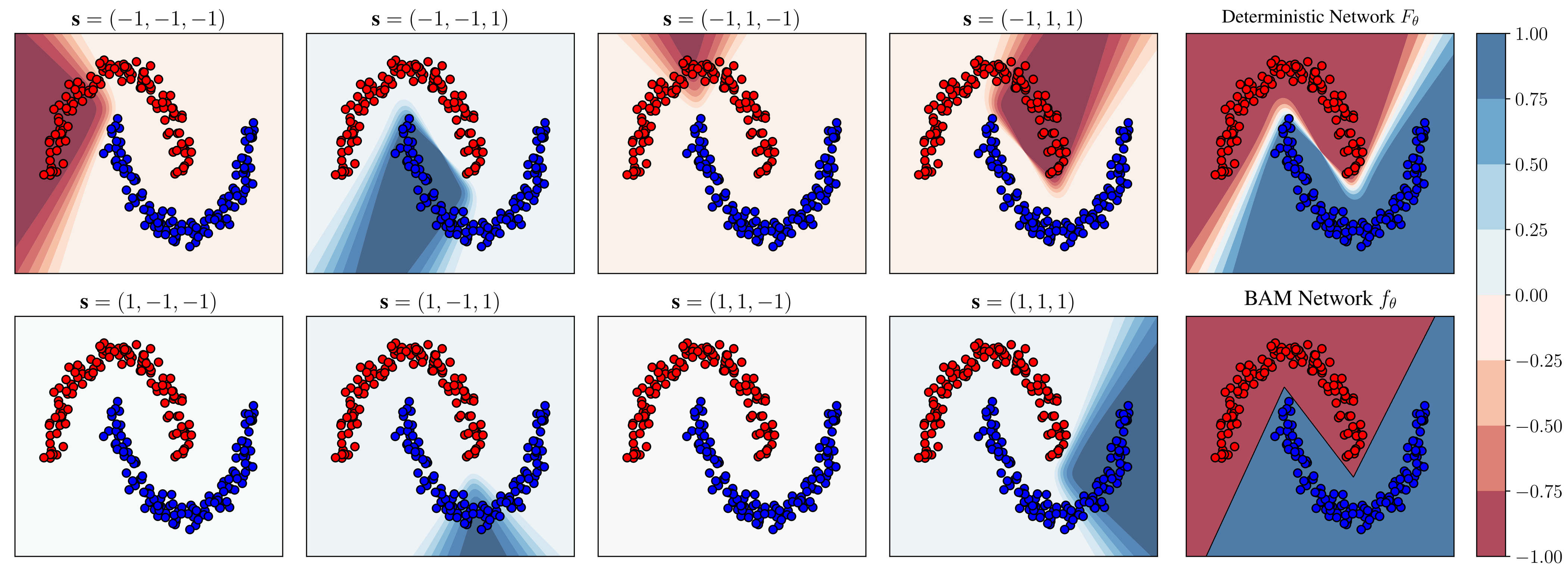


Figure 1: Illustration of the proposed method for a one hidden layer network of size d_1=3, interpreted as a majority vote over 8 binary representations $\mathbf{s} \in \{-1,1\}^3$. For each $\mathbf{s}$, a plot shows the values of $F_{\mathbf{w}_2}(\mathbf{s})\Pr(\mathbf{s}|\mathbf{x},\mathbf{W}_1)$.

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 $\operatorname{erf}'(x) := \frac{2}{\sqrt{\pi}}e^{-x^2}$.

$$\frac{\partial}{\partial \mathbf{w}_1^k}F_\theta(\mathbf{x}) = \frac{\mathbf{x}}{2^{\frac{3}{2}}\|\mathbf{x}\|}\operatorname{erf}'\left(\frac{\mathbf{w}_1^k\cdot\mathbf{x}}{\sqrt{2}\,\|\mathbf{x}\|}\right)\sum_{\mathbf{s}\in\{-1,1\}^{d_1}} s_k\, F_{\mathbf{w}_2}(\mathbf{s})\left[\frac{\Pr(\mathbf{s}|\mathbf{x},\mathbf{W}_1)}{\Pr(s_k|\mathbf{x},\mathbf{w}_1^k)}\right]$$

Monte Carlo sampling

We generate T random binary vectors $\{\mathbf{s}^t\}_{t=1}^{T}$ according to $\Pr(\mathbf{s}|\mathbf{x},\mathbf{W}_1)$.

$$F_\theta(\mathbf{x}) \approx \frac{1}{T}\sum_{t=1}^{T} F_{\mathbf{w}_2}(\mathbf{s}^t) \qquad \frac{\partial}{\partial \mathbf{w}_1^k}F_\theta(\mathbf{x}) \approx \frac{\mathbf{x}}{2^{\frac{3}{2}}\|\mathbf{x}\|}\operatorname{erf}'\left(\frac{\mathbf{w}_1^k\cdot\mathbf{x}}{\sqrt{2}\,\|\mathbf{x}\|}\right)\frac{1}{T}\sum_{t=1}^{T}\frac{s_k^t}{\Pr(s_k^t|\mathbf{x},\mathbf{w}_1^k)}F_{\mathbf{w}_2}(\mathbf{s}^t)$$

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

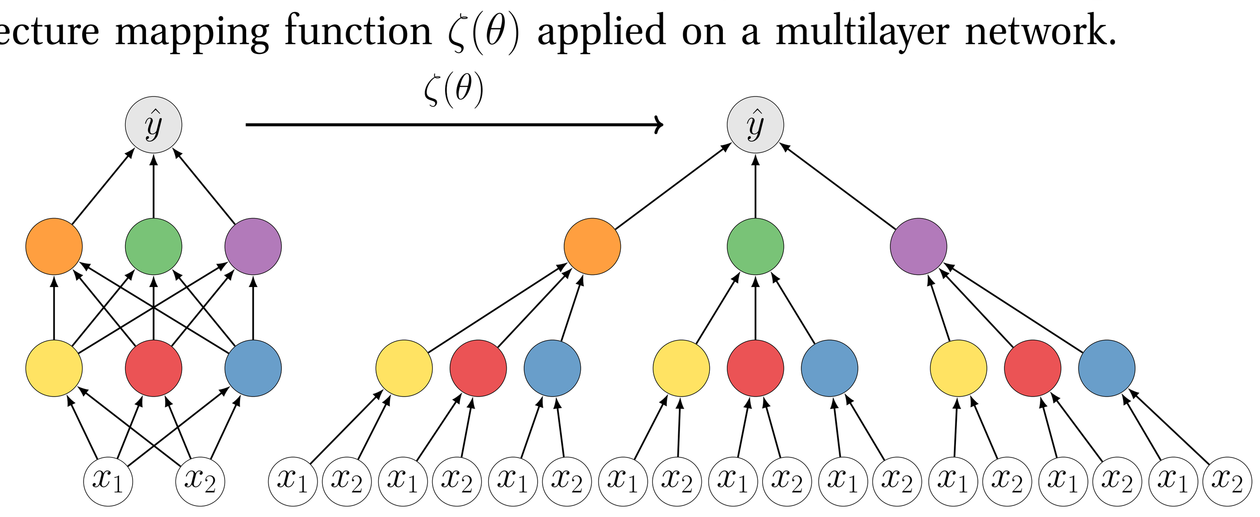
Deep Learning (PBGNet)

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 j^{th} neuron of the k^{th} hidden layer :

$$F_1^{(j)}(\mathbf{x}) = \operatorname{erf}\left(\tfrac{\mathbf{w}_1^j\cdot\mathbf{x}}{\sqrt{2}\|\mathbf{x}\|}\right) \quad \longleftarrow \boxed{\textit{first hidden layer}}$$

$$F_{k+1}^{(j)}(\mathbf{x}) = \sum_{\mathbf{s}\in\{-1,1\}^{d_k}} \operatorname{erf}\left(\tfrac{\mathbf{w}_{k+1}^j\cdot\mathbf{s}}{\sqrt{2d_k}}\right)\prod_{i=1}^{d_k}\left(\frac{1}{2} + \frac{1}{2}s_i \times F_k^{(i)}(\mathbf{x})\right)$$



Kullback-Leibler regularization

$$\mathrm{KL}\Big(Q_{\zeta(\theta)} \,\big\|\, P_{\zeta(\mu)}\Big) = \frac{1}{2}\left(\|\mathbf{w}_L - \mathbf{u}_L\|^2 + \sum_{i=1}^{L-1} d_{k+1}^{\dagger}\big\|\mathbf{W}_i - \mathbf{U}_i\big\|_F^2\right) \text{ for } d_k^{\dagger} := \textstyle\prod_{i=k}^{L} d_i\,.$$

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.

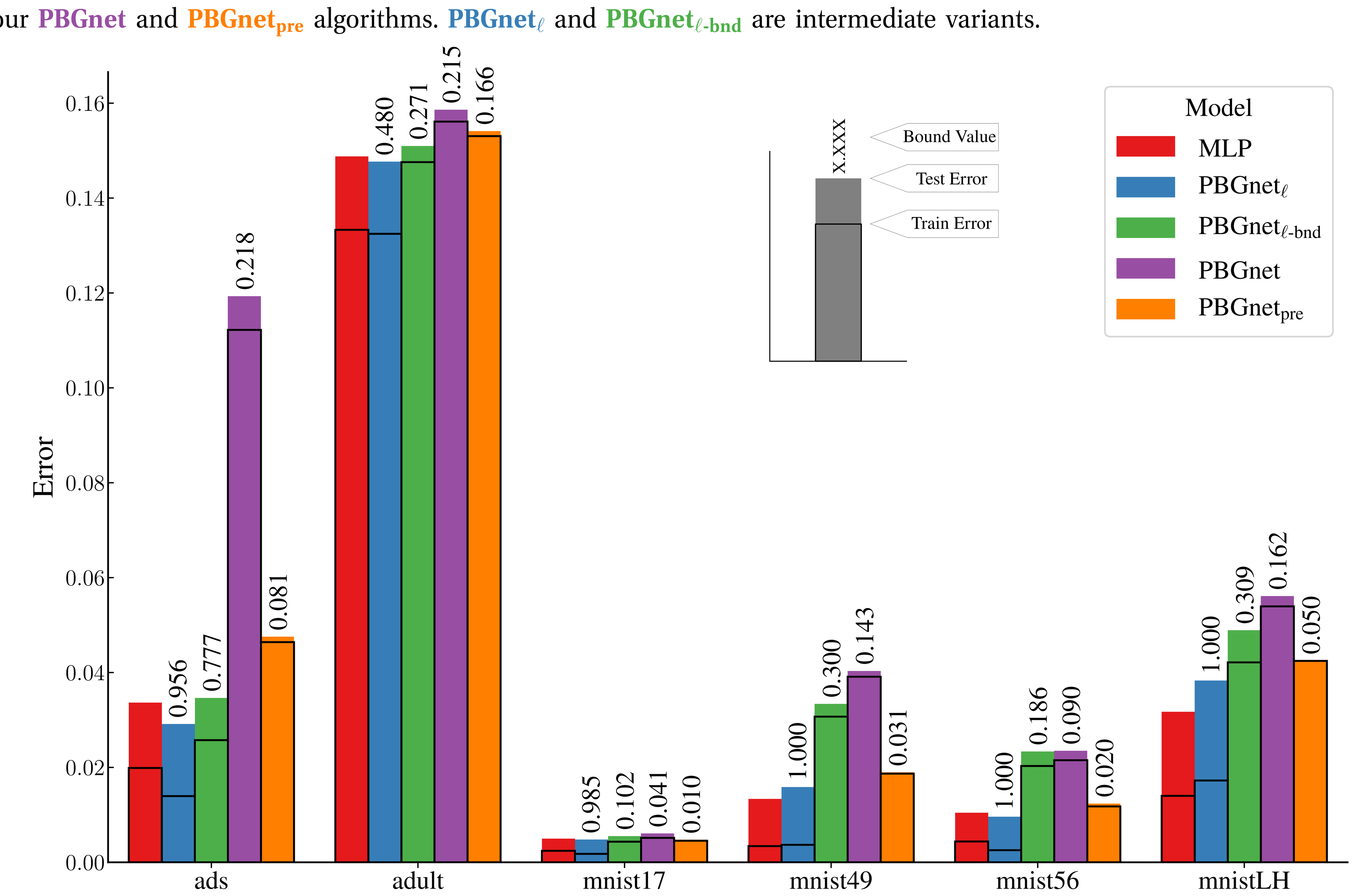


Figure 2: Experiment results for the considered models on the binary classification datasets. PAC-Bayesian bounds hold with probability 0.95.