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

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Introduction

We present a comprehensive study of multifactor 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
- \( d_j \) denotes the number of neurons of the \( k \)-th layer
- \( \text{sgn}(a) = 1 \) if \( a > 0 \) and \( \text{sgn}(a) = -1 \) otherwise
- Weights matrices: \( W \in \mathbb{R}^{k \times k} \), \( \theta = \text{vec}(W) \in \mathbb{R}^{k} \)

Prediction

\[ f(x) = \text{sgn}(W_{L}(\ldots \text{sgn}(W_{1}x))) \]

PAC-Bayesian Theory

Given a data distribution \( D \), a training set \( S = \{(x_i, y_i)\}_{i=1}^{n} \sim D^n \), with \( x_i \in \mathbb{R}^d \) and \( y_i \in \{-1, 1\} \), a loss \( L : [-1, 1] \rightarrow [0, 1] \), a predictor \( f \in \mathcal{F} \):

\[ L(f) = \mathbb{E}_{(x,y) \sim D^n} L(f(x), y) \]

\[ \bar{L}(f) = \frac{1}{n} \sum_{i=1}^{n} L(f(x_i), y_i) \]

PAC-Bayesian Theorem

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

\[ C \bar{L}(P) + \text{KL}(Q||P) \leq -\log \left( 1 - \text{Pr}(L(f) \leq C) \right) \]

Linear Classifier

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

\[ f_N(x) = \text{sgn}(w^T x) \]

PAC-Bayesian analysis

- Space of all linear classifiers: \( \mathcal{F}_N = \{ f_N \mid w \in \mathbb{R}^d \} \)
- Gaussian prior \( P_0 = N(0, I_2) \) over \( \mathcal{F}_N \)
- Gaussian posterior \( Q = N(\mu, \sigma) \) over \( \mathcal{F} \)
- Predictor \( f_N = \text{vec}(Q \mid \mu, \sigma) \)
- Linear loss \( L(f(x), y) = \frac{1}{2} - y f(x) \)

Bound minimization

\[ C \bar{L}(P) + \text{KL}(Q||P) = C \frac{1}{n} \sum_{i=1}^{n} \text{sgn}(y_i, w^T x_i) + \frac{1}{2}||w||^2 \]

Shallow Learning

Posterior \( Q_0 = N(\theta, I_0) \), over the family of all networks \( \mathcal{F}_D = \{ f_\theta \mid \theta \in \mathbb{R}^q \} \), where \( f_\theta(x) = \text{sgn}(w_{\theta}) \cdot \text{sgn}(W(x)) \)

\[ f_\theta(x) = \mathbb{E}_{\theta \sim Q_0} f_\theta(x) \]

\[ = \int_{\theta \sim Q_0} Q_0(\theta) \text{sgn}(w_{\theta}) \cdot \text{sgn}(V(x)) d\theta \]

\[ = \int_{\theta \sim Q_0} \text{sgn}(w_{\theta}) \cdot \text{sgn}(V(x)) Q_0(\theta) d\theta \]

\[ = \int_{\theta \sim Q_0} \text{sgn}(w_{\theta}) \prod_{x \sim \mathcal{D}} \left( \frac{1}{2} - y f_\theta(x) \right) d\theta \]

PAC-Bayesian bound ingredients

- Empirical loss: \( \bar{L}(f_\theta) = \mathbb{E}_{x \sim \mathcal{D}} \bar{L}(f_\theta) = \frac{1}{n} \sum_{x \sim \mathcal{D}} \left( \frac{1}{2} - y f_\theta(x) \right) \)
- Complexity term: \( \text{KL}(Q_0||P_0) = \frac{1}{n} \mu^2 ||\mu||^2 \), with \( \mu \in \mathbb{R}^q \)
- Generalization bound: \( 1 - \exp\left( -C \bar{L}(f_\theta) - \frac{1}{2} \text{KL}(Q_0||P_0) + \text{KL}(Q_0||P) \right) \)

Stochastic Approximation

Prediction.

\[ F_\theta(x) = \sum_{s \sim \{1, -1\}} F_{\theta}(s|x, W_i) \]

Hidden layer partial derivatives, with \( \text{erf} \):

\[ \frac{\partial F_\theta(x)}{\partial W_{ij}} = \frac{x_i}{\sqrt{2\pi}} \text{erf} \left( \frac{x_i}{\sqrt{2}} \right) \sum_{s \sim \{1, -1\}} s_j F_{\theta}(s|x, W_i) \]

Monte Carlo sampling

We generate \( T \) random binary vectors \( s_i \sim \{1, -1\} \), according to \( P(s|x, W_i) \):

\[ F_\theta(x) \approx \frac{1}{T} \sum_{t=1}^{T} F_\theta(s_i|x, W_i) \]

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. \( F^{(i)}_\theta \) denotes the output of the \( j^{th} \) neuron of the \( k^{th} \) hidden layer:

\[ F^{(i)}_\theta(x) = \text{erf} \left( \frac{x_i}{\sqrt{2}} \right) \sum_{s \sim \{1, -1\}} s_j F^{(i-1)}_\theta(x) \]

Kullback-Leibler regularization

\[ \text{KL}(Q_0||P_0) = \frac{1}{2} \left( ||w||^2 + \sum_{i=1}^{n} d_i ||w_i - U||^2 \right) \]

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_{max} algorithms. PBGNet and PBGNet_{max} are intermediate variants.

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Code: github.com/gael/laviolette/dichotomize-and-generalize

Figure 1: Illustration of the proposed method for a one hidden layer network of size \( d_0=1 \), interpreted as a majority vote over 8 binary representations \( s \in \{-1,1\}^8 \). For each \( s \), a plot shows the values of \( F_{\theta}(s)|P(w_i, W_i)\).

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