Spectral-Pruning: Compressing deep neural network via spectral analysis

Abstract

The model size of deep neural network is getting larger and larger to realize superior performance in complicated tasks. This makes it difficult to implement deep neural network in small edge-computing devices. To overcome this problem, model compression methods have been gathering much attention. However, there have been only few theoretical back-grounds that explain what kind of quantity determines the compression ability. To resolve this issue, we develop a new theoretical frame-work for model compression, and propose a new method called Spectral-Pruning based on the theory. Our theoretical analysis is based on the observation such that the eigenvalues of the covariance matrix of the output from nodes in the internal layers often shows rapid decay. We define “degree of freedom” to quantify an intrinsic dimensionality of the model by using the eigenvalue distribution and show that the compression ability is essentially controlled by this quantity. Along with this, we give a generalization error bound of the compressed model. Our proposed method is applicable to wide range of models, unlike the existing methods, e.g., ones possess complicated branches as implemented in SegNet and ResNet. Our method makes use of both “input” and “output” in each layer and is easy to implement. We apply our method to several datasets to justify our theoretical analyses and show that the proposed method achieves the state-of-the-art performance.

1 Introduction

Currently, deep learning is the most promising approach adopted by various machine learning applications, such as computer vision, natural language processing, and audio processing. Along with the rapid development of the deep learning techniques, its network structure is getting extensively complicated. For example, SegNet [4] has skip connections, ResNet [20] and its variants [23, 10] also possess several skip connections. In addition to the model structure, the model size is getting
larger, which prevents us from implementing deep neural networks in edge-computing devices for such applications as smart phone services, autonomous vehicle driving and drone control.

To overcome this difficulty, model compression techniques have been studied extensively in the literature. One approach is pruning by an explicit regularization, such as $\ell_1$ and $\ell_2$ penalization during training \cite{50, 53, 50, 21}. A similar effect can be realized by an implicit randomized regularization, such as DropConnect \cite{49}, which randomly removes connections during the training phase. The factorization method performs a matrix/tensor decomposition of the weight matrices to reduce the number of parameters \cite{13, 14}. Information redundancy can be reduced by a quantization technique that expresses the network by smaller bit variable type or hash tables \cite{9, 18}. More closely related ones are ThinNet \cite{33} and Net-Trim \cite{1} which prune the network weight so that the behaviors of the internal layers of the pruned network are as close as possible to those of the original network. \cite{12} is quite close to ours, but its theoretical support is not satisfactory. In particular, the suggested way of the best subset selection is just a random choice. \cite{51} proposed parameter sharing technique to reduce redundant parameters based on similarity between the weights. Another big issue is that only few of them (e.g., Net-Trim \cite{1}) are supported by statistical learning theory. In particular, it has been unclear what kind of quantity controls the compression ability. Another big issue is that the above mentioned methods can not be trivially applied to the recently developed networks with complicated structures such as skip connections like ResNet and SegNet.

In this paper, we develop a new simple network compression method that is applicable to networks with complicated structures, and give theoretical support to explain what quantity controls the compression ability. The theoretical analysis is applicable not only to our method but also to the existing methods. Almost all of the existing methods try to find a smaller network structure that approximates only the “output” from each layer as well as possible. In contrast, our method also deals with the “input” to each layer. The information of the input is exploited as a covariance matrix, and redundant nodes are discarded on the basis of that information. It can be applied even if the “outputs” are split into several branches. Moreover, by combining the information of both input and output, it achieves better accuracy.

We also develop a theoretical analysis to characterize the compression error by using the notion of degree of freedom. The degree of freedom represents a kind of intrinsic dimensionality of the model. This quantity is determined by the eigenvalues of the covariance matrix calculated in each layer. Usually, we observe that the eigenvalue drops rapidly (Figs. 1 and 2a), which means that important information processed in each layer is not large. In particular, rapid decay of eigenvalues leads to low degree of freedom. Because of this, we can compress the network effectively though explicit number of parameters of the original network is large. Behind the theory, there is essentially a connection to the kernel quadrature rule \cite{3}. In addition to the model compression ability analysis, we also develop a generalization error analysis. Our analysis is categorized to so called fast learning rate that achieves $O(1/n)$ convergence rate for sample size $n$ unlike such theories as \cite{44, 40, 7, 41} showing $O(1/\sqrt{n})$ convergence. Fast learning rate has been also studied in deep learning, e.g., \cite{28, 5, 36, 6, 26, 27, 42, 25, 46}, but they are not about model compression. According to our generalization error bound, we see that there appears bias and variance trade-off where bias is induced by the network compression and variance is induced by the training data variation. Finally, we conduct extensive numerical experiments to show the superiority of our method and give experimental verification of our theory. Our contributions are summarized as follows:

- We propose a new simple method for compressing the trained network that can be executed by simply observing the covariance matrix in the internal layers. Unlike existing methods, the proposed method can easily be implemented and applied to any type of network structure.
- We give a theoretical guarantee of the model compression ability by utilizing the notion of degree of freedom which represents an intrinsic dimensionality of the model. We reveal that the covariance between nodes affects the compression ability. We also give a generalization error analysis and derive the bias-variance trade-off induced by the model compression.

\section{Model compression problem and its algorithm}

Let the input domain be $\mathcal{X} = \mathbb{R}^d$, and the output domain be $\mathcal{Y}$ where $\mathcal{Y}$ could be the set of real numbers $\mathbb{R}$ for regression and be a binary label $\{\pm 1\}$ for binary classification. Suppose that there
exists a probability measure $P$ defined on a measurable space $(\Omega, \mathcal{B})$, and there is a Borel measurable random variable $(X, Y) : \Omega \to (\mathcal{X}, \mathcal{Y})$. The training data $D_\ell = \{(x_i, y_i)\}_{i=1}^{m_\ell} \subset \mathcal{X} \times \mathcal{Y}$ are i.i.d. realizations of $(X, Y)$ obeying the distribution $P$. The marginal distribution of $X$ is denoted by $P_X$.

To train the appropriate relationship between $x$ and $y$, we construct a deep neural network model as

$$f(x) = (W^{(L)} \eta(\cdot) + b^{(L)}) \circ \cdots \circ (W^{(1)} x + b^{(1)}),$$

where $W^{(\ell)} \in \mathbb{R}^{m_{\ell+1} \times m_{\ell}}$, $b^{(\ell)} \in \mathbb{R}^{m_{\ell+1}}$ ($\ell = 1, \ldots, L$), and $\eta : \mathbb{R} \to \mathbb{R}$ is an activation function (here, the activation function is applied in an element-wise manner; for a vector $x \in \mathbb{R}^d$, $\eta(x) = (\eta(x_1), \ldots, \eta(x_d))^T$). Furthermore, $m_\ell$ is the width of the $\ell$-th layer such that $m_{L+1} = 1$ (output) and $m_1 = d_x$ (input). Let $\hat{f}$ be a trained network obtained from a training data $D_\ell = \{(x_i, y_i)\}_{i=1}^{m_\ell}$. Accordingly, its parameters are denoted by $(\hat{W}^{(\ell)}, \hat{b}^{(\ell)})_{\ell=1}^L$, i.e., $\hat{f}(x) = (\hat{W}^{(L)} \eta(\cdot) + \hat{b}^{(L)}) \circ \cdots \circ (\hat{W}^{(1)} x + \hat{b}^{(1)})$, and the output of its internal layer (before activation) is denoted by

$$\hat{F}_\ell(x) = (\hat{W}^{(\ell)} \eta(\cdot) + \hat{b}^{(\ell)}) \circ \cdots \circ (\hat{W}^{(1)} x + \hat{b}^{(1)}).$$

Here, we do not specify how to train the network $\hat{f}$. Any learning method for training $\hat{f}$ is valid for the following argument to be true. It might be the empirical risk minimizer, the Bayes estimator, or another estimator. We want to compress the trained network $\hat{f}$ to another smaller network $f^*$ having widths $(m_\ell^*)_{\ell=1}^L$ which are as small as possible.

### 2.1 New model compression algorithm

To compress the trained network $\hat{f}$, we propose a simple strategy called Spectral-Pruning. The method works in a layer-wise manner. The main idea of the method is to find the most informative subset of the nodes where the amount of information is measured by how the selected nodes can explain the other nodes in the layer. If some nodes are heavily correlated to each other, then only one of them should be selected. The information redundancy can be computed by solving a simple regression problem, and requires only a covariance matrix. We do not need to solve some specific nonlinear optimization problem as in [30, 53, 50, 1]. Our method can be executed by only using the input to the layer. We call such an approach input aware one. On the other hand, it can also make use of the output from the layer as in the most existing methods. We call such approaches output aware ones. Another important characteristics of our method is to incorporate the distribution of the data while some existing pruning techniques try to approximate the parameter itself and is independent from the data distribution.

### 2.2 Algorithm description

Let $\phi(x) = \eta(\hat{F}_{\ell-1}(x)) \in \mathbb{R}^{m_\ell}$ be the input to the $\ell$-th layer, and let $\phi_J(x) = (\phi_J(x))_{j \in J} \in \mathbb{R}^{|J|}$ be a subvector of $\phi(x)$ corresponding to an index set $J \in [m_\ell]^{[J]}$ where $[m] := \{1, \ldots, m\}$. Basically,
the strategy is to recover \( \phi(x) \) from \( \phi_J(x) \) as accurately as possible. To do so, we solve the following optimization problem:

\[
\hat{A}_J = \arg\min_{A \in \mathbb{R}^{m \times |J|}} \hat{E}[\|\phi - A \phi_J\|^2] + \|A\|_w^2, \quad (1)
\]

where \( \hat{E}[\cdot] \) is the expectation with respect to the empirical distribution (\( \hat{E}[f] = \frac{1}{n} \sum_{i=1}^{n} f(x_i) \)) and \( \|A\|_w = \text{Tr}[A\Sigma A^\top] \) for a regularization parameter \( w \in \mathbb{R}^{|J|} \) and \( I_w = \text{diag}(w) \). The optimal solution \( \hat{A}_J \) can be explicitly expressed by utilizing the (non-centered) covariance matrix in the \( \ell \)-th layer of the trained network \( \hat{f} \) which is defined as

\[
\hat{\Sigma} := \hat{\Sigma}(\ell) = \frac{1}{n} \sum_{i=1}^{n} \eta(\hat{F}_{\ell-1}(x_i))\eta(\hat{F}_{\ell-1}(x_i))^\top, 
\]
defined on the empirical distribution (here, we omit the layer index \( \ell \) for notational simplicity).

Accordingly, let \( \hat{\Sigma}_{I,J} \in \mathbb{R}^{|I| \times |J|} \) be the submatrix of \( \hat{\Sigma} \) for index sets \( I \subset [m]|J| \), \( J \subset [m]|J| \) such that \( \hat{\Sigma}_{I,J} = (\hat{\Sigma}_{i,j})_{i \in I, j \in J} \). Let \( F = \{1, \ldots, m\} \) be the full index set. By noting that \( \hat{E}[\phi \phi^\top] = \hat{\Sigma} \) due to its definition, we can easily check that

\[
\hat{A}_J = \hat{\Sigma}_{F,J}(\hat{\Sigma}_{J,J} + I_w)^{-1}. 
\]

Hence, we can decode the full vector \( \phi(x) \) from \( \phi_J(x) \) as \( \phi(x) \approx \hat{A}_J \phi_J(X) = \hat{\Sigma}_{F,J}(\hat{\Sigma}_{J,J} + I_w)^{-1} \phi_J(X) \). Another approach is to directly approximate a specific “output” \( z^\top \phi \) for a specific \( z \in \mathbb{R}^m \) instead of approximating the “input” \( \phi \) as Eq. (1). This can be realized by solving the following regression problem which we call an “output-aware” approach:

\[
\hat{a}_J = \arg\min_{a \in \mathbb{R}^{|J|}} \hat{E}[\|z^\top \phi - a^\top \phi_J\|^2] + \|a\|_w^2. 
\]

It can be easily checked that the optimal solution \( \hat{a}_J \) is given as \( \hat{a}_J = \hat{A}_J^\top z \). Therefore, an output aware compression can be recovered from the input aware method (1). In particular, the output to the next layer \( \hat{W}^{(\ell)} \phi(x) = (\hat{W}^{(\ell)} \eta(\hat{F}_{\ell-1}(x))) \) can be approximated by \( \hat{W}^{(\ell)} \hat{A}_J \phi_J(x) \).

**Selecting optimal subindices** Next, we aim to optimize \( J \). Since the output to the next layer is multi-variate and we need to bound the approximation error of multiple outputs uniformly to reduce the approximation error in the entire network, we minimize the following quantity with respect to \( J \):

\[
L_w^{(A)}(J) = \max_{z \in \mathbb{R}^m : \|z\|_2 \leq 1} \min_{a \in \mathbb{R}^{|J|}} \hat{E}[\|z^\top \phi - a^\top \phi_J\|^2] + \|a\|_w^2. 
\]

By considering this, our method works no matter what branches there exist. The right hand side is equivalent to \( \|\hat{E}[(\phi - \hat{A}_J \phi_J)(\phi - \hat{A}_J \phi_J)^\top]\| + \hat{A}_J I_w \hat{A}_J^\top \|_{\text{op}} \), where \( \|\cdot\|_{\text{op}} \) is the spectral norm (the maximum singular value of the matrix). By substituting the explicit formula of \( \hat{A}_J \), this is further simplified as

\[
L_w^{(A)}(J) = \|\hat{\Sigma}_{F,F} - \hat{\Sigma}_{F,J}(\hat{\Sigma}_{J,J} + I_w)^{-1} \hat{\Sigma}_{J,F}\|_{\text{op}}. 
\]

To obtain the optimal \( J \) under a cardinality constraint \( |J| \leq m_2 \) for a pre-specified width \( m_2 \) of the compressed network, we propose to solve the following sparse subset selection problem:

\[
\min_J L_w^{(A)}(J) \quad \text{s.t.} \quad |J| \in [m_2]^{m_1}. 
\quad (2)
\]

Let \( \hat{J} \) be the optimal \( J \) that minimizes the objective. This optimization problem is NP-hard, but an approximate solution is obtained by the greedy algorithm since it is reduced to monotone submodular function maximization [29]. That is, we start from \( J = \emptyset \), sequentially choose an element \( j^* \in [m_1] \) that maximally reduces the objective \( L_w^{(A)} \), and add this element \( j^* \) to \( J (J \leftarrow J \cup \{j^*\}) \) until \( |J| = m_2 \) is satisfied.

An advantage of this approach is that it requires only the covariance matrix, and it is accomplished by purely linear algebraic procedures. Moreover, our method can be applied to a complicated network structure in which there are recurrent structures, several branches, or outputs from the internal layers that are widely distributed to several other units (e.g., skip connections).
Output aware method  Suppose that there is an “important” subset of weight vectors, say $Z_\ell \subset \mathbb{R}^{m_\ell}$, such that the output $z^T \phi$ corresponding to $z \in Z_\ell$ should be well approximated. Then it would be more effective to focus on approximating $z^T \phi (z \in Z_\ell)$ instead of all $z^T \phi (z \in \mathbb{R}^{m_\ell})$. Here, suppose that $Z_\ell$ is a finite set, and let the weight matrix $Z \in \mathbb{R}^{m_\ell \times m_\ell}$ be the one each row which corresponds to each distinguish element in $Z_\ell$: $Z_\ell = [z_1, \ldots, z_{|Z_\ell|}]^T$ for $z_j \in Z_\ell$. If $Z_\ell$ is not a finite set, we may set $Z_\ell$ as a projection matrix to the span of $Z_\ell$. Then, we consider an objective $L_w^{(B)} := \max_{\|u\| \leq 1} \min_{a \in \mathbb{R}^{m_\ell}} \mathbb{E}[\{u^TZ\ell \phi - a^T \phi_j\}^2] + \|a\|_2^2$, which is equivalent to $L_w^{(B)}(J) = \|Z_\ell[\Sigma_{F,F} - \Sigma_{J,F}^{-1}\Sigma_{J,F}]Z_\ell\|_{op}$. A typical situation is to approximate the output $\hat{W}^{(f)} \phi$. In that situation, we may set $Z_\ell = \hat{W}^{(f)}$ which corresponds to $Z_\ell = \{(\hat{W}^{(f)}_j)^\top \mid j = 1, \ldots, m_{\ell+1}\}$.

Combination of input aware and output aware methods  In our numerical experiments, we have found that only one of either input or output aware method does not give the best performance, but the combination of them achieved the best performance (see Fig. 3). Moreover, if the network has several branches, then it is not trivial which branches should be included in $Z_\ell$ for the output aware method. In that situation, it is preferable to combine input aware and output aware methods instead of using only the output aware method. Therefore, we propose to take the convex combination of the both criteria given for a parameter $0 \leq \theta \leq 1$ as

$$\begin{align*}
\text{(Spectral-Pruning)} \quad & \min_{J} L_w^{(\theta)}(J) = \theta L_w^{(A)}(J) + (1 - \theta)L_w^{(B)}(J) \quad \text{s.t.} \quad J \in [m_\ell]^{m_\ell}.
\end{align*}$$

2.3 Practical algorithm

Calculating the exact value of $L_w^{(\theta)}$ is computationally demanding for a large network because we need to specify the spectral norm. However, we do not need to obtain the exact solution for the problem \(3\) in practice, because, if we obtain a reasonable candidate that approximately achieves the optimal, then additional fine-tuning gives a much better network. Hence, instead of solving \(3\) directly, we upper bound $L_w^{(A)}$ and $L_w^{(B)}$ by replacing the operator norm in their definitions with trace, and minimize it as a practical variant of our method. By setting $w = 0$, the objective of the variational method is reduced to $\text{Tr}[\{\theta I + (1 - \theta)R_Z\}(\Sigma_{F,F} - \Sigma_{J,F}^{-1}\Sigma_{J,F})]$. Then, the proposed optimization problem can be rearranged to the following problem:

$$\begin{align*}
\text{(Spectral-Pruning-2)} \quad & \min_{J \subset \{1, \ldots, m_\ell\}} |J| \quad \text{s.t.} \quad \frac{\text{Tr}[\{\theta I + (1 - \theta)Z_\ell^\top Z_\ell\}\Sigma_{F,F}^{-1}\Sigma_{J,F}]}{\text{Tr}[\{\theta I + (1 - \theta)Z_\ell^\top Z_\ell\}]} \geq \alpha
\end{align*}$$

for a pre-specified $\alpha > 0$. Here, since the denominator in the constraint is the best achievable objective value of the numerator without cardinality constrain, $\alpha$ represents “information loss ratio.” The index set $J$ is restricted to a subset of $\{1, \ldots, m_\ell\}$ that has no duplication. This problem is not only much simpler but also easier to implement than the original one \(3\). In our numerical experiments, we employed this simpler problem.

An extension of our method to convolutional layers is a bit tricky. There are several options, but to perform channel-wise pruning, we used the following “covariance matrix” between channels in the experiments. Suppose that a channel $k$ receives the input $\phi_{k;u,v}(x)$ where $1 \leq u \leq I_w$, $1 \leq v \leq I_h$ indicate the spatial index, then “covariance” between the channels $k$ and $k'$ can be formulated as $\Sigma_{k,k'} = \frac{1}{n_{tr}} \sum_{i=1}^{n_{tr}} (\Psi_{w,k} \sum_{u,v} \phi_{k;u,v}(x_i)\phi_{k';u,v}(x_i))$. As for the covariance between an output channel $k'$ and an input channel $k$ (which corresponds to the $(k,k')$-th element of $Z_\ell \Sigma_{F,F}$), we can calculate as $\Sigma_{k,k'} = \frac{1}{n_{tr}} \sum_{i=1}^{n_{tr}} (\Psi_{w,k} \sum_{u,v} \phi_{k;u,v}(x_i)\phi_{k';u,v}(x_i))$, where $\text{Res}(u',v')$ is the receptive field of the location $u',v'$ in the output channel $k'$, and $I'_{(u,v)}$ are the number of locations $(u',v')$ that contain $(u,v)$ in their receptive fields.

3 Compression accuracy analysis and generalization error bound

In this section, we give a theoretical guarantee of our model compression method. More specifically, we introduce a quantity called degree of freedom and show that it determines the approximation
accuracy. The degree of freedom is defined by the spectrum of the covariance matrix between the nodes in an internal layer. In practice, we observe that a trained network typically shows a rapid decay of its spectrum (see Fig. 2a), which results in a small degree of freedom. For the theoretical analysis, we define a neural network model with norm constraints on the parameters \( W^{(\ell)} \) and \( \hat{b}^{(\ell)} \) (\( \ell = 1, \ldots, L \)). Let \( R > 0 \) and \( R_0 > 0 \) be upper bounds of the parameters, and define the norm constraint model as

\[
\mathcal{F} := \{ (W^{(L)}\eta(\cdot) + b^{(L)}) \circ \cdots \circ (W^{(1)}x + b^{(1)}) \mid \max_{j} \| W^{(\ell)}_{j,\cdot} \| \leq R / \sqrt{m_{\ell}}, \| \hat{b}^{(\ell)} \|_{\infty} \leq R_0 \},
\]

where \( W^{(\ell)}_{j,\cdot} \) means the \( j \)-th column of the matrix \( W^{(\ell)} \), \( \| \cdot \| \) is the Euclidean norm and \( \| \cdot \|_{\infty} \) is the \( \ell_{\infty} \)-norm. Here, we bound the approximation error induced by compressing the trained network \( \hat{f} \in \mathcal{F} \) into a smaller one \( f^{\sharp} \). First, we make the following assumption.

**Assumption 1.** We assume the following conditions on the activation function \( \eta \).

- \( \eta \) is scale invariant: \( \eta(ax) = a\eta(x) \) for all \( a > 0 \) and \( x \in \mathbb{R}^d \) (for arbitrary \( d \)).
- \( \eta \) is \( 1 \)-Lipschitz continuous: \( |\eta(x) - \eta(x')| \leq \|x - x'\| \) for all \( x, x' \in \mathbb{R} \) (for arbitrary \( d \)).

These conditions are satisfied by ReLU activation \( [38, 17] \) and leaky ReLU (LReLU) \([34]\). The first condition reduces the model complexity because some networks with different scales can be identified as a function. The second condition ensures that the approximation error in each layer is not amplified through signal propagation to the last layer.

### 3.1 Approximation error analysis

Recall that the empirical covariance matrix in the \( \ell \)-th layer is denoted as \( \hat{\Sigma}_{(\ell)} \). Then, the degree of freedom is defined by

\[
\hat{N}_{\ell}(\lambda) := \text{Tr}[\hat{\Sigma}_{(\ell)}(\hat{\Sigma}_{(\ell)} + \lambda I)^{-1}] = \sum_{j=1}^{m_{\ell}} \frac{\hat{\mu}_{j}^{(\ell)}}{\hat{\mu}_{j}^{(\ell)} + \lambda}
\]

where \( (\hat{\mu}_{j}^{(\ell)})_{j=1}^{m_{\ell}} \) are the eigenvalues of \( \hat{\Sigma}_{(\ell)} \). Let \( (m_{\ell}^{(\ell)})_{\ell=1}^{L} \) denote the width of the \( \ell \)-th layer. The next theorem characterizes the approximation accuracy between \( f^{\sharp} \) and \( \hat{f} \) on the basis of the degree of freedom with respect to the empirical \( L_2 \)-norm \( \|g\|_{2} := \frac{1}{m_{\ell}} \sum_{i=1}^{m_{\ell}} \|g(x_i)\|_{2} \) for a vector valued function \( g \).

**Theorem 1** (Compression rate via degree of freedom). Suppose that there exists \( \bar{J}_{\ell} \subset [m_{\ell+1}] \) such that \( \mathcal{Z}_{\ell} = \{ \hat{W}_{j,\cdot}^{(\ell)} / \max_{j' \notin \bar{J}_{\ell}} \| \hat{W}_{j',\cdot}^{(\ell)} \| : j \in \bar{J}_{\ell} \} \). Let \( \lambda_{\ell} > 0 \) be

\[
\lambda_{\ell} = \inf \{ \lambda \geq 0 \mid m_{\ell}^{(\ell)} \geq 5\hat{N}_{\ell}(\lambda) \log(80\hat{N}_{\ell}(\lambda)) \} \tag{5}
\]

and the weight vector \( w \) for the regularization is defined by the “leverage score”; that is, \( w_{j} = \frac{m_{\ell}^{(\ell)}\lambda_{\ell} \hat{\Sigma}_{(\ell)}^{1/2}}{\hat{N}_{(\ell)}(\lambda_{\ell})} \sum_{k=1}^{m_{\ell}} U_{j,k}^{(\ell)} (\hat{\mu}_{k}^{(\ell)} + \lambda_{\ell}) \) where \( U_{(\ell)} = (U_{\ell,k})_{j,k} \) is the orthogonal matrix that diagonalizes \( \hat{\Sigma}_{(\ell)} \). Let

\[
\alpha_{j,\ell} = \begin{cases} \theta^{-1} \max_{j' \notin \bar{J}_{\ell}} \| \hat{W}_{j',\cdot}^{(\ell)} \|^2 & (j \notin \bar{J}_{\ell}), \\ \max_{j' \in [m_{\ell+1}]} \| \hat{W}_{j',\cdot}^{(\ell)} \|^2 & (\text{otherwise}), \end{cases}
\]

and \( \zeta_{\ell,\theta} = \theta + (1 - \theta) \| Z_{\ell} \tilde{\Sigma}_{(\ell)}^{1/2} + \lambda_{\ell} I \|_{op} \). Then, the solution \( \hat{A}_{j} \) obtained by Spectral-Pruning \([3]\) satisfies

\[
\max_{1 \leq j \leq m_{\ell+1}} \frac{\| \hat{W}_{j,\cdot}^{(\ell)} - \hat{W}_{j,\cdot}^{(\ell)} \hat{A}_{j}(\hat{\phi}_{j}) \|_{n}}{\alpha_{j,\ell}} \leq 4\zeta_{\ell,\theta} \lambda_{\ell} m_{\ell} R^{2}. \tag{6}
\]

Moreover, there exists a universal constant \( \hat{c} > 0 \) such that the parameter of the compressed network satisfies the following norm bound:

\[
\| \hat{W}_{j,\cdot}^{(\ell)} \hat{A}_{j} \hat{\phi}_{j} \|_{1/2} \leq \hat{c} \lambda_{\ell} R^{2} \tag{7}
\]
Moreover, if we solve the optimization problem \([3]\) with an additional constraint \(\sum_{j \in J} w_j^{-1} \leq \frac{2}{m} m_\ell \lambda_\ell^{-1}\) for all \(1 \leq \ell \leq L\), then the optimization problem is feasible and, the overall approximation error is bounded as

\[
\| \hat{f} - f^2 \|_n \leq \sum_{\ell=2}^{L} \left( \prod_{\ell' = \ell+1}^{L} \frac{\max\{\alpha_{j,\ell'}\}}{\sqrt{\ell' - \ell + 1}} \right) \sqrt{\ell' - \ell + 1} R^{L - \ell + 1} \sqrt{\max\{\alpha_{j,\ell}\} \lambda_\ell},
\]

for a compressed network \(f^2\) given by our algorithm; in particular, if we set \(\alpha_{\text{max}} = \max_{j,\ell} \{\alpha_{j,\ell}\}\) and \(R = \sqrt{\alpha_{\text{max}} R}\), then it holds that

\[
\| \hat{f} - f^2 \|_n \leq \sum_{\ell=2}^{L} R^{L - \ell + 1} \sqrt{\alpha_{\text{max}} \lambda_\ell}. \tag{8}
\]

The proof is given in Appendix A. It is basically proven using the techniques developed by [46] in which theories of the kernel quadrature rule developed by [3] are used for deep learning analysis. This theorem indicates that the approximation error induced by the compression is directly controlled by the degree of freedom. Since the degree of freedom \(N_\ell(\lambda_\ell)\) is a monotonically decreasing function with respect to \(\lambda_\ell\), it becomes large as \(\lambda_\ell\) is decreased to 0. The behavior of the eigenvalues determines how rapidly \(N_\ell(\lambda_\ell)\) increases as \(\lambda_\ell \to 0\). We can see that if the eigenvalues \(\hat{\mu}_1^{(\ell)} \geq \mu_2^{(\ell)} \geq \ldots\) decrease rapidly, then \(\lambda_\ell\) becomes small for a specific network size \(m_\ell\). In other words, \(\hat{f}\) can be much smaller under a specific approximation error constraint if a network \(\hat{f}\) has many small eigenvalues. Another important aspect of the theorem is that the norms of the parameters are bounded properly (Eq. (7)). This bound is not trivial. Therefore, the effects of the approximation errors in the internal layers on the entire function are well regulated.

The quantity \(\alpha_{j,\ell}\) appearing in the bound represents the effect of misspecification of \(Z_\ell\) for the output aware method. For \(j \notin J_\ell\), \(\theta^{-1} \geq 1\) appears in the definition of \(\alpha_{j,\ell}\), but its effect could be canceled out if the norm \(\|\hat{W}_{j'}(\ell)\|\ (j' \notin J_\ell)\) is small. This means that, if we want to use the output aware method, it is recommended to include \(\hat{W}_{j'}(\ell)\) with large norm into the range of \(Z_\ell\). If we do so, the effect of misspecification is negligible. Otherwise,

**Kernel method perspective** The compression method can be viewed from the kernel method point of view. Here, we define the kernel function in the \(\ell\)-th layer as

\[
k_\ell(x, x') = \eta(F_{\ell-1}(x))^T \eta(F_{\ell-1}(x')) \in \mathbb{R}.
\]

The kernel function, \(k_\ell\), has a decomposition in \(L_2(P_n)\) (where \(P_n\) is the empirical distribution) as

\[
k_\ell(x, x') = \sum_{j=1}^{m_\ell} \mu_j^{(\ell)} \phi_j^{(\ell)}(x) \phi_j^{(\ell)}(x'),
\]

where \((\phi_j^{(\ell)})_{j=1}^{m_\ell}\) is an orthonormal system in \(L_2(P_n)\) \(\frac{1}{n} \sum_{i=1}^{n} \phi_j^{(\ell)}(x_i) \phi_j^{(\ell)}(x_i) = \delta_{j,j'}\) and \(\mu_j^{(\ell)} \geq 0\) is an eigenvalue. The kernel decomposition and the covariance matrix have connection, i.e., for a decomposition \(\Sigma(\ell) = U_\ell S_\ell U_\ell^T\), where \(U_\ell\) is an orthogonal matrix and \(S_\ell\) is a positive-semidefinite diagonal matrix, it holds that \(S_\ell = \text{diag}(\mu_1^{(\ell)}, \ldots, \mu_{m_\ell}^{(\ell)})\), and \(\eta(F_{\ell-1}(x)) = U_\ell \sqrt{S_\ell} (\phi_1^{(\ell)}(x), \ldots, \phi_{m_\ell}^{(\ell)}(x))^T\). In particular, the eigenvalues of the kernel and the covariance matrix are identical. This can be checked as follows. First, note that \(\eta(F_{\ell-1}(x))\) can be represented as \(\eta(F_{\ell-1}(x)) = B(\phi_1^{(\ell)}(x), \ldots, \phi_{m_\ell}^{(\ell)}(x))^T\) for a matrix \(B \in \mathbb{R}^{m_\ell \times m_\ell}\) because \(\eta(F_{\ell-1}(\cdot))\) is included in the RKHS (reproducing kernel Hilbert space) defined by the kernel \(k_\ell\). Then, from the definition of the kernel, \(B^T B = S_\ell\). On the other hand, by the definition of the covariance matrix, it holds that \(\Sigma(\ell) = BB^T\). Therefore, \((U_\ell^T B)(U_\ell^T B)^T = (U_\ell^T B)^T (U_\ell^T B) = S_\ell\) which indicates that \(U_\ell^T B\) is a normal matrix and \(B = U_\ell \sqrt{S_\ell}\) must be satisfied.

The RKHS \(\mathcal{H}_\ell\), which is associated with the kernel function \(k_\ell\), is uniquely defined, and its unit ball \(B(\mathcal{H}_\ell)\) is given by

\[
B(\mathcal{H}_\ell) = \{ f(x) = \sum_{j=1}^{m_\ell} \alpha_j \sqrt{\mu_j^{(\ell)}} \phi_j^{(\ell)}(x) \ | \ ||\alpha|| \leq 1 \} = \{ f(x) = \sum_{j=1}^{m_\ell} \alpha_j \eta(F_{\ell-1}(x))_j \ | \ ||\alpha|| \leq 1 \}.
\]
In particular, the output to the next layer $\hat{W}^{(t)}_j \eta(H_{\hat{f}}_t(x))$ is an element in the RKHS. Thus, choosing a subset $\hat{J} \subset \{1, \ldots, m_2\}$ of nodes can be seen as choosing a lower dimensional subspace in $H_\ell$ that approximates the original RKHS as accurately as possible. The kernel quadrature rule enables this by choosing $\hat{J}$ so that an alternative kernel defined as

$$\hat{k}_\ell(x, x') = \sum_{j \in \hat{J}} \mu_\ell_j \phi_\ell_j(x) \phi_\ell_j(x')$$

approximates the original kernel $k_\ell(x, x')$ as well as possible.

### 3.2 Generalization error analysis

So far, we have developed an approximation error bound with respect to the “empirical” $L_2$-distance. Here, we derive a generalization error bound for the compressed network, which is defined by the population $L_2$ distance. We see that there appears bias-variance trade-off induced by the network compression. The bound we derive is so called fast learning rate meaning that it is $O(1/n)$ with respect to the sample size $n$ rather than $O(1/\sqrt{n})$ as in the usual Rademacher complexity analysis. For this purpose, we specify the data generation model. First, we consider a simple regression model:

$$y_i = f^\ast(x_i) + \xi_i \ (i = 1, \ldots, n_tr),$$

where $f^\ast : \mathbb{R}^{d_x} \rightarrow \mathbb{R}$ is the true function that we want to estimate, $(x_i)^{n_{tr}}_{i=1}$ is independently identically distributed from $P_X$, and $(\xi_i)^{n_{tr}}_{i=1}$ is i.i.d. Gaussian noise with mean 0 and variance $\sigma^2$. A regression problem is considered for theoretical simplicity. Nearly the same discussion is applicable to classification problems with margin conditions such as Tsybakov’s noise condition \cite{35}. The relative generalization error of $f$ is evaluated as $E_{X,Y}[(Y - f(X))^2] - E_{X,Y}[(Y - f^\ast(X))^2] = E[(f(X) - f^\ast(X))^2] = \|f - f^\ast\|_{L_2}$ where $\|\cdot\|_{L_2}$ is defined as $\|f\|_{L_2} = \sqrt{E[f(X)^2]}$. Hence, we aim to bound $\|f^\ast - f^\ast\|^2_{L_2}$. The training error is denoted by $\hat{L}(f) := \frac{1}{n_tr} \sum_{i=1}^{n_{tr}} (y_i - f(x_i))^2$. We assume (approximately) optimality of the trained network $\hat{f}$ as follows.

**Assumption 2** (Optimality). There exists a constant $\hat{\zeta} \geq 0$ such that the following inequality holds almost surely: $\hat{L}(\hat{f}) \leq \min_{f \in \mathcal{F}} \hat{L}(f) + \hat{\zeta}$.

In practice, it is difficult to assume that the global optimal solution is attained because of the non-convexity of the deep learning problem. This assumption ensures that the optimization error is bounded by $\hat{\zeta}$. This can be relaxed to $\hat{L}(\hat{f}) \leq \hat{L}(f^\ast) + \hat{\zeta}$ where $f^\ast = \arg\min_{f \in \mathcal{F}} \|f - f^\ast\|_{L_2}$. However, we use Assumption 2 just for simplicity. Next, we assume the following bound on the input data.

**Assumption 3.** The support of $P_X$ is compact and its $\ell_\infty$-norm is bounded as $\|x\|_\infty \leq D_x \ (\forall x \in \text{supp}(P_X))$.

Then, under the same setting as Theorem 1 we define the following constants corresponding to the norm bounds:

$$\hat{R}_\infty := \max\{R^L D_x + \sum_{\ell=1}^L R^{L-\ell} R_b, \|f^\ast\|_\infty\}, \hat{\zeta} := L \hat{R}^{L-1} D_x + \sum_{\ell=1}^L R^{L-\ell},$$

where $\hat{R} = \sqrt{\alpha_{\text{max}} R}$ and $\hat{R}_b = \sqrt{\epsilon} R_b$ for the constants $\epsilon$ and $\alpha_{\text{max}}$ introduced in Theorem 1.

To bound the generalization error, we define $\delta_1$ and $\delta_2$ for $\lambda = (\lambda_1, \ldots, \lambda_L) \in \mathbb{R}_+^L$ and $m' = (m'_1, \ldots, m'_L) \in \{m_1\} \times \cdots \times \{m_L\}$ as\footnote{$\log_+(x) = \max\{1, \log(x)\}$}:

$$\delta_1(\lambda) = \sum_{\ell=2}^L \hat{R}^{L-\ell+1} \sqrt{\alpha_{\text{max}} \hat{\zeta}_\ell \lambda_\ell},$$

$$\delta_2(m') = \frac{1}{n} \sum_{\ell=1}^L m'_\ell \log_+ \left(1 + \frac{4\sqrt{2} \hat{\zeta} \max\{R, R_b\}}{\sigma \sqrt{n}} \right).$$

Under these notations, we obtain the following generalization error bound for the compressed network $f^\ast$ with respect to the population $L_2$-norm $\|f^\ast - f^\ast\|^2_{L_2}$.
Theorem 2 (Generalization error bound of the compressed network). Suppose that Assumptions 1, 2 are satisfied. Consider a setting where \( \theta = 1 \) or \( z_\ell = \frac{w(\ell)}{\max_{1 \leq j' \leq m_{\ell+1}} \|w(\ell,j')\|} \) for \( \ell = 1, \ldots, L \).

Let \( \lambda_\ell > 0 \) (\( \ell = 2, \ldots, L \)) are the variables satisfying the condition (5):

\[
\lambda_\ell = \inf \{ \lambda \geq 0 \mid m_\ell^2 \geq 5N_\ell(\lambda) \log(80N_\ell(\lambda)) \},
\]

and assume that \( f^* \) satisfy the approximation error bound (3) with the norm bound (7) as given in Theorem 1. Let \( R_{n,t} = (\sqrt{\hat{R}_\ell^2 + \sigma^2} \delta_2(m^\sharp) + \sigma \delta_2(m) + \min_{f \in \mathcal{F}} \| f - f^0 \|_{L_2} + \zeta + R_{n,t}) \).

Then, there exists a constant \( C_1 > 0 \) such that for all \( t > 0 \),

\[
\| f^t - f^0 \|_{L_2}^2 \leq C_1 \{ \delta_1^2 + (\sigma^2 + \hat{R}_\ell^2) \delta_2^2(m^\sharp) + \sigma \delta_2(m) + \min_{f \in \mathcal{F}} \| f - f^0 \|_{L_2}^2 + \zeta + R_{n,t} \}
\]

uniformly over all choices of \( m^\sharp = (m_1^\sharp, \ldots, m_L^\sharp) \) with probability \( 1 - 5e^{-t} \).

The proof is given in Appendix B.2. In a small noise situation \( \sigma \approx 0 \), the main term becomes

\[
\| f^t - f^0 \|_{L_2}^2 \leq \delta_1^2 + \delta_2^2(m^\sharp) \approx \left( \sum_{\ell=2}^L \sqrt{\lambda_\ell} \right)^2 + \frac{1}{n} \sum_{\ell=1}^L m_\ell^4 m_\ell^2 \log(n).
\]

The remaining terms are just residual terms. Actually, \( R_{n,t} \) is basically \( O(\sum_{\ell=1}^L \log(m_{\ell+1}) / n) \), which is much smaller than \( \delta_1^2 + \delta_2^2 \) and is thus negligible. By Theorem 1, \( \delta_1 \) represents the approximation error between \( \hat{f} \) and \( f^* \); hence, it can be regarded as a bias. The second term \( \delta_2(m^\sharp) \) is the variance term that is induced by the sample deviation. Here, it should be noted that the variance term \( \delta_2(m^\sharp) \) depends only on the size of the compressed network rather than the original network size. On the other hand, a naive application of the theorem implies that \( \| f^t - f^0 \|_{L_2}^2 \leq \delta_2^2(m) = O\left(\frac{1}{n} \sum_{\ell=1}^L m_{\ell+1} m_\ell \log(n)\right) \) (here, the residual terms are omitted) which is much larger than \( \delta_2^2(m^\sharp) \) when \( m_\ell^4 \ll m_\ell \). Therefore, the variance is reduced significantly by the model compression resulting in a much improved generalization error. Note that there appears bias-variance trade-off between \( \delta_1 \) and \( \delta_2(m^\sharp) \). Actually, when \( m_\ell^4 \) is large, the bias \( \delta_1 \) becomes small due to the monotonicity of the degree of freedom but the variance \( \delta_2(m^\sharp) \) will be large. Hence, we need to tune the size \( m_\ell^\sharp \) to obtain the best generalization error by balancing the bias \( \delta_1 \) and variance \( \delta_2 \).

The generalization error bound is uniform over the choice of \( m^\sharp \) (to ensure this, there appears \( \sum_{\ell=1}^L \log(m_{\ell+1}) \) in \( R_{n,t} \)). Thus \( m^\sharp \) can be arbitrary and be chosen in a data dependent way. This means that the bound is a posteriori one, and achieves a tight bound than a simple application of the VC-dimension analysis in which the complexity of the model is fixed a priori. Actually, the best choice of \( m^\sharp \) depends on the trained network, and the bound claims that if the trained network has rapidly decaying eigenvalues, then we can obtain a compressed network with preferable generalization error from the trained one. In other words, the degree of freedom gives a data dependent intrinsic “complexity” of the trained network. This is beneficial from the practical point of view because the degree of freedom can be computed empirically. In particular, the width of the network can be estimated in a data dependent way by looking at the degree of freedom unlike the previous approaches in which we determined that in a trial-and-error manner involving combinatorial computational cost.

Generalization error of the original network. The bound obtained above is just for the compressed network \( f^\sharp \), which is not for the original network \( \hat{f} \). It is difficult to convert the bound to that of \( \hat{f} \) naively, because the deviation between the empirical covariance matrix and the population covariance matrix depends on the size of the original network size instead of the compressed one.

This difficulty essentially comes from the difficulty to bound the empirical \( L_2 \)-norm and the population one by using the data dependent quantity such as the degree of freedom \( N_\ell \). However, if we suppose that the validation error for \( \hat{f} \) is better than that for \( f^\sharp \) (which is a strong assumption), then the generalization error for the original network \( \hat{f} \) is also easily guaranteed. Let \( \{(x_i', y_i')\}_{i=1}^{n_{val}} \) be \( n_{val} \)-copies of the training observation; that is, each observation \( (x_i', y_i') \) obeys the same distribution as \( (X, Y) \) and independently identically distributed.

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Proposition 1. Suppose that, for a given constant $q_n > 0$, the validation error for $\hat{f}$ is smaller than that for $f^\#$ up to $q_n \geq 0$:

$$\frac{1}{n_{val}} \sum_{i=1}^{n_{val}} (y'_i - \hat{f}(x'_i))^2 \leq \frac{1}{n_{val}} \sum_{i=1}^{n_{val}} (y'_i - f^\#(x'_i))^2 + q_n,$$

for a validation data $(x'_i, y'_i)_{i=1}^{n_{val}}$. Then, there exists a universal constant $C_2$ such that

$\|\hat{f} - f^o\|_{L_2} \leq C_2 \left( \|f^\# - f^o\|_{L_2} + \frac{\sigma^2 + \hat{R}_\infty^2}{n_{val}} t \right) + q_n$

with probability $1 - 3 \exp(-t)$ for $t > 0$. Here, the probability is taken for the choice of the validation error.

The proof is given in Appendix C. Combining Theorem 2 with Proposition 1 indicates that, if the network can be compressed into a smaller one and the validation error is not much improved by compression, then the trained network $\hat{f}$ possesses a good generalization error. This clearly explains the practically observed phenomenon that a massive network with numerous parameters achieves good generalization performance. Actually, we observed that a compressed network of VGG-16 with 1/17 of its original size achieves a comparable performance to the original one.

4 Relation to existing work

Here, we describe the relation between our method and the most relevant existing methods. ThiNet [33] finds the subset $J \subset \{1, \ldots, m\}$ such that it minimizes the approximation to the next output. In that sense, it is close to our output aware method. Since ThiNet should specify the output value exactly, it is not trivial to directly apply this method to other networks having complicated structures such as skip connections and recurrence. Net-Trim [1] is similar to ThiNet, but it minimizes the approximation error of the output after nonlinear activation. It requires a nonlinear optimization program, such as the alternating direction method of multipliers, whereas ThiNet and ours do not. Moreover, Net-Trim also needs to specify the output exactly. Net-Trim is supported by a theoretical analysis for approximation error bounds, but what kind of factors affect its compression rate was still not analyzed. [12] also proposed a method essentially same as our input aware method [1]. However, the best subset selection scheme and combination with the output aware method are not well exploited in a theoretically guaranteed way. Our analysis is also applicable to this work and our method improves the accuracy by taking the combination of input and output aware methods. Recently, [51] also proposed to pruning correlated weights. However, they measure the information redundancy via correlation between parameters which is not the statistical correlation. Therefore, our method is more effective to capture the property of the distribution. Recently, independent to our analysis, [2] showed a generalization error bound based based on how the network can be compressed. Their analysis is not directly connected to our analysis. In particular, their analysis does not explain pruning performance. However, the concept behind their analysis is that the important information is included in a small subspace in each layer, which shares a similar consideration with ours. Moreover, their bound is not a fast learning rate. It would be an interesting future work to see connection between our investigation and their analysis.

5 Numerical experiments

In this section, we conduct numerical experiments to show the effectiveness of the proposed method, and justify our theoretical analysis. As for our method, all experiments have been conducted by the practical variant (Spectral-Pruning-2 (Eq. (4))).

5.1 Relation between eigenvalue distribution and compression ability

We show how the decreasing rate of eigenvalues affect the compression accuracy to justify our theoretical analysis. We constructed a network (namely NN3) consisting of 3 hidden fully connected layers with width $(300, 1000, 300)$ following the setting of [1], and trained it by 60,000 images in MNIST and 50,000 images in CIFAR-10. Figure 2a shows magnitudes of the eigenvalues of
the 2nd and 3rd hidden layers of the networks trained in each dataset (plotted in semi-log scale). The eigenvalues are sorted in decreasing order, and they are normalized by being divided by the maximum eigenvalue. We see that eigenvalues for MNIST decrease much more rapidly than those in CIFAR-10. This indicates that MINST is “easier” than CIFAR-10 because the degree of freedom (an intrinsic dimensionality) of the network trained on MNIST is relatively smaller than that on CIFAR-10. Actually, Figure 2b presenting the test accuracy without fine tuning against the compression rate (the ratio between the numbers of parameters of the compressed network and the original network) shows rapid drop of accuracy at relatively larger compression rate in CIFAR-10 than MNIST.

Figure 3 shows relation between the test classification accuracy and the hyper parameter $\theta$. It is plotted for VGG-13 network trained on CIFAR-10. We can see that the best accuracy is achieved around $\theta = 0.3$ through the whole compression rate, which indicates superiority of “combination” of input aware and output aware approaches.

Next, we compare our method with two existing methods, HPTD [19] and Net-Trim [1] for NN3 network, in MNIST data. Table 1 shows the result. The accuracies for HPTD and Net-Trim are taken from [1]. We see that our method is comparable (and even favorable) to the other methods (HPTD for 70% compression rate is trapped in a bad local minimum over three repetition). Especially, our method shows better performance before fine tuning. Note that our method requires only linear algebraic computation and do not require a nonlinear optimization procedure unlike Net-Trim.

5.2 ImageNet

We apply our method to the ImageNet dataset [11]. We used the ILSVRC2012 dataset in ImageNet consisting of 1.3M training data and 50,000 validation data. Each image is annotated into one of 1,000 categories. We used a publicly available VGG-16 network [43] as the original network. We
Table 1: Comparison with existing methods for NN3 network on MNIST dataset. The accuracy after fine tuning is presented and that without fine tuning is shown inside bracket.

| Compression rate (%) | 22.5 | 40  | 50  | 70  |
|----------------------|------|-----|-----|-----|
| HPTD [19]            | 97.96 (8.92) | –   | –   | < 98 (8.92) |
| Net-Trim [11]        | 98.19 (97.35) | –   | –   | 98.12 (98.10) |
| Spec-Prun (θ = 0)    | 98.26 (98.14) | 98.32 (98.31) | 98.34 (98.33) | 98.34 (98.35) |
| Spec-Prun (θ = 1)    | 98.24 (98.09) | 98.32 (98.30) | 98.33 (98.34) | 98.33 (98.36) |

Table 2: Performance comparison on ImageNet dataset. Our proposed method is compared with APoZ-2 [22], SqueezeNet [24], and ThiNet [33]. Our method is indicated as “Spec-(type).”

| Model               | Top-1 | Top-5 | # Param | FLOPs   |
|---------------------|-------|-------|---------|---------|
| Original VGG [43]   | 68.34%| 88.44%| 138.34M | 30.94B  |
| APoZ-2 [22]         | 70.15%| 89.69%| 51.24M  | 30.94B  |
| SqueezeNet [24]     | 57.67%| 80.39%| 1.24M   | 1.72B   |
| ThiNet-Conv [33]    | 69.80%| 89.53%| 131.44M | 9.58B   |
| ThiNet-GAP [33]     | 67.34%| 87.92%| 8.32M   | 9.34B   |
| ThiNet-Tiny [33]    | 59.34%| 81.97%| 1.32M   | 2.01B   |
| Spec-Conv (θ = 0)   | 71.39%| 90.63%| 114.62M | 20.02B  |
| Spec-Conv (θ = 0.5) | 72.15%| 91.06%| 131.44M | 22.13B  |
| Spec-Conv (θ = 1)   | 71.86%| 90.88%| 130.37M | 18.73B  |
| Spec-Conv-FC (θ = 1)| 70.09%| 89.82%| 131.44M | 9.58B   |
| Spec-GAP (θ = 0.5)  | 67.55%| 88.27%| 8.31M   | 11.21B  |
| Spec-GAP (θ = 1)    | 60.10%| 82.89%| 2.31M   | 2.07B   |
| Spec-GAP2 (θ = 0.5) | 67.33%| 87.99%| 8.32M   | 9.34B   |
| Spec-GAPe (θ = 0.5) | 67.78%| 88.52%| 8.25M   | 14.77B  |

applied our method to this network and compared it with existing state-of-the-art methods, namely APoZ [22], SqueezeNet [24], and ThiNet [33]. For fair comparison, we followed the same experimental settings as [33]: the way of training data generation, data augmentation, performance evaluation schemes and so on. The results are summarized in Table 2. It summarizes the Top-1/Top-5 classification accuracies, the number of parameters (#Param), and the float point operations (FLOPs) to classify a single image. Our method is indicated by “Spec-(type).” In Spec-Conv, we applied our method only to the convolutional layers (it is not applied to the fully connected layers (FC)). The conv-layers are compressed gradually by solving Eq. (4) with \( \alpha = 0.99 \) a few times until the #Param becomes comparable to ThiNet-Conv which also applies the ThiNet method only to conv-layers. After each compression operation, we applied fine tuning. In our experiments, one or two iteration was sufficient to reach the comparable compression rate. For each \( \theta \), we selected the weight decay parameter of fine tuning from \( 10^{-4} \) and 0. Spec-Conv-FC compresses the FC layers as well as the conv-layers, whereas it is difficult to apply ThiNet to the FC layers because it is computationally too demanding. We employed \( \theta = 1 \) for Spec-Conv-FC. Spec-GAP is a method that replaces the FC layers of Spec-Conv with a global average pooling (GAP) layer [32, 52]. We chose \( \alpha \) so that one time application of the compression achieves the same #Param as ThiNet-GAP which is also a method utilizing the GAP layer as the fully connected layer. We employed \( \theta = 0.5 \) for Spec-GAP. Spec-GAPe sets the parameter \( \alpha \) in each layer as \( \alpha_\ell = 0.9944^{\ell} \) for the \( \ell \)-th layer. The other setting of Spec-GAPe is same as Spec-GAP. Spec-Tiny is a method where Eq. (4) with \( \alpha = 0.97 \) is performed to conv-layers several times until the #Params and FLOPs becomes comparable to that of ThiNet-Tiny. We employed \( \theta = 1 \) for Spec-Tiny. As for Spec-Conv2, we set the number of channels in each layer to be same as that of ThiNet-Conv. Similarly, in Spec-GAP2, we set the number of channels in each layer to be same as that of ThiNet-GAP.

APoZ shows favorable accuracy but this method can reduce the parameters in only non-convolutional layers. Thus, its applicability is limited; consequently, it does not reduce the FLOPs significantly. ThiNet is the most comparable method, but if the number of parameters is set to be equal, our method (especially Spec-Conv) yields much better performance than it. We would like to remark that ThiNet (and existing methods) does not have a criterion to automatically determine the shape of compressed network. On the other hand, our method may determine that through the
degree of freedom or the formula (4). From computational viewpoint, Spec-GAP is obtained by one compression and one fine-tuning, which is much faster than ThiNet which executed layer by layer pruning and fine-tuning. Our method is also useful to compress the fully connected layers as performed by Spec-Conv-FC. Interestingly, Spec-Conv-FC show even better classification accuracy than the original VGG network while it has 3 times smaller number of parameters.

5.3 Compression of SegNet

Here, we conduct an experiment on SegNet-Basic-EncoderAddition [4] (with a slight modification) for segmentation of street scenes. We abbreviate “SegNet-Basic-EncoderAddition” to “SegNet-Basic” for simplicity. Since SegNet-Basic is equipped with skip connections, the output from each layer in the down-sampling layers consists of two parts: the output to the next layer through standard convolution and that to the corresponding up-sampling layer through skip connections. Therefore, ThiNet and Net-Trim are not trivially applied. We adopted our method with $\theta = 1$ to compress SegNet-Basic and investigated how the compression rate affects the test error. We compressed the network gradually, i.e., in each stage, we solved Eq. (4) with $\alpha = 0.95$ and applied fine-tuning.

SegNet-Basic is trained on the Mapillary Vistas Dataset [39], which consists of 18,000 training data and 2,000 validation data. Each data is provided with pixel-wise annotations into 66 categories, such as “pedestrians” and “bicycle.” We converted the 66-class classification task into a 22-class classification task by appropriately grouping the 66 categories. The test accuracy of SegNet-Basic...
on this dataset is of two types: **global accuracy** and **mean class accuracy**. Global accuracy is the average segmentation accuracy over all pixels. Mean class accuracy is the average class-wise segmentation accuracy over all classes. Figure 4 shows the test accuracy (global accuracy and mean class accuracy) versus the compression rate (number of parameters of the original network /that of compressed one) and the speed up rate for processing one image for several epochs in fine tuning procedure after compression. We can see that even if the number of parameters is nearly half of that in the original network, good generalization performance is achieved.

Figure 5 shows the segmentation results for the original network and the compressed network. The results appear to be nearly the same, which indicates that the compression is performed adequately.

### 6 Conclusion

In this paper, we proposed a new model compression frame-work that utilizes both of “input” and “output”, and showed that the **degree of freedom** characterizes the extent to which a trained network can be compressed. The algorithm is easily implemented and can be run in a layer-wise manner. Moreover, we connected the compression ability to the generalization ability. There appeared bias and variance trade-off according to compression rate. The numerical experiments showed a favorable performance to the existing state-of-the-art methods despite its algorithmic simplicity.

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### A Proof of Theorem 1

#### A.1 Preparation of lemmas

To derive the approximation error bound, we utilize the following proposition that was essentially proven by Bach [3].

**Proposition 2.** There exists a probability measure \( q_\ell \) on \( \{1, \ldots, m_\ell \} \) such that for any \( \delta \in (0, 1) \) and \( \lambda > 0 \), i.i.d. sample \( v_1, \ldots, v_m \in \{1, \ldots, m_\ell \} \) from \( q_\ell \) satisfies, with probability \( 1 - \delta \), that

\[
\inf_{\beta \in \mathbb{R}^{m_\ell} : \|\beta\|_2^2 \leq \frac{4m_\ell^2}{m}} \left\{ \left\| \eta(\hat{F}_{\ell-1}(\cdot)) - \sum_{j=1}^m \beta_j q_\ell(v_j) \right\|_{\mathbb{F}}^2 \right\} + m\lambda \|\beta\|^2 \leq 4\lambda \alpha^\top \hat{\Sigma}_\ell (\hat{\Sigma}_\ell + \lambda I)^{-1} \alpha,
\]

for every \( \alpha \in \mathbb{R}^{m_\ell} \), if

\[
m \geq 5\tilde{N}_\ell(\lambda) \log(16\tilde{N}_\ell(\lambda)/\delta).
\]

**Proof.** This is basically a direct consequence from Proposition 1 in Bach [3] and its discussions. The original statement does not include the regularization term \( m\lambda \|\beta\|^2 \) in the left hand side and \( \alpha^\top \hat{\Sigma}_\ell (\hat{\Sigma}_\ell + \lambda I)^{-1} \alpha \) in the right hand side. However, by carefully following the proof, the bound including these additional factors is indeed proven.

By the scale invariance of \( \eta, \eta(ax) = a\eta(x) (a > 0) \), we have the following proposition based on Proposition 2.

**Lemma 1.** Suppose that

\[
w_j' = \frac{1}{\tilde{N}_\ell(\lambda)} \sum_{i=1}^{m_\ell} U_{j,\ell}^2 \frac{\hat{\mu}_j^{(\ell)}}{\hat{\mu}_i^{(\ell)} + \lambda} (j \in \{1, \ldots, m_\ell \}), \quad (9)
\]
where \( U = (U_{j,t})_{j,t} \) is the orthogonal matrix that diagonalizes \( \hat{\Sigma}_t \), that is, \( \hat{\Sigma}_t = U \text{diag} \left( \hat{\mu}_1^{(t)}, \ldots, \hat{\mu}_m^{(t)} \right) U^\top \). For \( \lambda > 0 \), and any \( 1/2 > \delta > 0 \), if

\[
m \geq 5\hat{N}_t(\lambda) \log(16\hat{N}_t(\lambda)/\delta),
\]
then there exist \( v_1, \ldots, v_m \in \{1, \ldots, m_\ell\} \) such that, for every \( \alpha \in \mathbb{R}^{m_\ell} \),

\[
\inf_{\beta \in \mathbb{R}^m : \|\beta\|_2 \leq \frac{2\alpha_n}{m}} \left\{ \left\| \alpha^\top \eta(\hat{F}_{\ell-1}(\cdot)) - \sum_{j=1}^m \beta_j w_j^{-1/2}\eta(\hat{F}_{\ell-1}(\cdot)) \right\|_n^2 + m\lambda \|\beta\|^2 \right\} \leq 4\lambda \alpha^\top \hat{\Sigma}_t(\hat{\Sigma}_t + \lambda I)^{-1}\alpha,
\]

and

\[
\sum_{j=1}^m w_j^{-1} \leq (1 - 2\delta)^{-1} m \times m_\ell.
\]

**Proof.** Suppose that the measure \( Q_\ell \) is the counting measure, \( Q_\ell(J) = |J| \) for \( J \subset \{1, \ldots, m_\ell\} \), and \( q_\ell \) is a density given by \( q_\ell(j) = w_j^{\ell} \) (\( j \in \{1, \ldots, m_\ell\} \)) with respect to the base measure \( Q_\ell \). Suppose that \( v_1, \ldots, v_m \in \{1, \ldots, m_\ell\} \) is an i.i.d. sequence distributed from \( q_\ell \) with \( Q_\ell \), then Bach [3] showed that this sequence satisfies the assertion given in Proposition 2.

Notice that

\[
E_v \left[ \sum_{j=1}^m q_\ell(v_j)^{-1} \right] = E_v(\ell) = \int_{[m]} q_\ell(v)^{-1} q_\ell(v) dQ_\ell(v) = \int_{[m]} dQ_\ell(v) = m_\ell, \text{ thus an i.i.d. sequence } \{v_1, \ldots, v_m\} \text{ satisfies } \frac{1}{m} \sum_{j=1}^m q_\ell(v_j)^{-1} \leq m_\ell/(1 - 2\delta) \text{ with probability } 2\delta \text{ by the Markov's inequality. Combining this with Proposition 2 the i.i.d. sequence } \{v_1, \ldots, v_m\} \text{ and } w_j = q_\ell(v_j) \text{ satisfies the condition in the statement with probability } 1 - (\delta + 1 - 2\delta) = \delta > 0. \text{ This ensures the existence of sequences } \{v_j\}_{j=1}^m \text{ and } \{w_j\}_{j=1}^m \text{ that satisfy the assertion.} \]

**A.2 Proof of Theorem 1**

First, we show the first inequality (3). Since Lemma 1 with \( \delta = 1/5 \) states that if \( m_\ell^2 \geq 5\hat{N}_t(\lambda_t) \log(80\hat{N}_t(\lambda_t)) \), then there exists \( J \subset \{1, \ldots, m_\ell\} \) and \( u' \in \mathbb{R}^{m_\ell} \) (which is given by Eq. (9)) such that

\[
\inf_{\alpha \in \mathbb{R}^{|J|}} \|z^\top \phi - \alpha^\top \phi_J\|^2 + \lambda|J|\|\alpha\|^2_{u'} \leq 4\lambda z^\top \hat{\Sigma}_t(\hat{\Sigma}_t + \lambda I)^{-1}z \quad \forall z \in \mathbb{R}^{m_\ell},
\]
and \( \sum_{j=1}^{m_\ell} w_j^{-1} \leq \frac{5}{3} m_\ell \times m_\ell^2 \) is satisfied.

If we limit the candidate of \( z \in \mathbb{R}^{m_\ell} \) to a set \( \{z = Z_t^\top u \mid \|u\| \leq 1\} \), then we obtain that

\[
\sup_{u : \|u\| \leq 1} \inf_{\alpha \in \mathbb{R}^{|J|}} \|u^\top Z_t \phi - \alpha^\top \phi_J\|^2_n + \lambda|J|\|\alpha\|^2_{u'} \leq 4\lambda \|Z_t \hat{\Sigma}_t \hat{\Sigma}_t + \lambda I\|^{-1} Z_t^\top u \leq 4\lambda \|Z_t \hat{\Sigma}_t \hat{\Sigma}_t + \lambda I\|^{-1} Z_t^\top \|u\|_{op}.
\]

for the same \( J \) as above. Letting \( u = \lambda m_\ell^2 w' (= \lambda \ell_J|w'|) \), this indicates that \( L^{(A)}(J) \leq 4\lambda \|Z_t \hat{\Sigma}_t \hat{\Sigma}_t + \lambda I\|^{-1} Z_t^\top \|u\|_{op} \). It also indicates \( L^{(A)}(J) \leq 4\lambda \|Z_t \hat{\Sigma}_t \hat{\Sigma}_t + \lambda I\|^{-1} \|u\|_{op} \leq 4\lambda \).

Therefore, by minimizing \( \theta L^{(A)}(J) + (1 - \theta)L^{(B)}(J) \) with respect to \( J \), it holds that

\[
\theta L^{(A)}(J) + (1 - \theta)L^{(B)}(J) \leq 4\lambda \theta[\theta + (1 - \theta)]\|Z_t \hat{\Sigma}_t \hat{\Sigma}_t + \lambda I\|^{-1} Z_t^\top \|u\|_{op}.
\]

Hence, for all \( j \in J \), by noticing \( \hat{W}_{j,t}^{(f)} \in \{u^\top Z_t \mid u \in \mathbb{R}^{m_{\ell+1}}\} \) and \( \|Z_t \|_{op} \leq 1 \) for all \( 1 \leq j \leq m_{\ell+1} \), we obtain

\[
\inf_{\alpha \in \mathbb{R}^{|J|}} \|\hat{W}_{j,t}^{(f)} \phi - \alpha^\top \phi_J\|^2_n + \lambda|J|\|\alpha\|^2_{u'}.
\]
If we further impose the constraint then we obtain the first assertion (6). By substituting this solution to Eq. (12) and (13), we obtain

$$\leq \theta \|\hat{W}_{j,\ell}^{(f)}\|^2 L_w^A(J) + (1 - \theta) \max \{\|\hat{W}_{j,\ell}^{(f)}\|^2\} L_w^B(J)$$

$$\leq \max \{\|\hat{W}_{j,\ell}^{(f)}\|^2\} \theta L_w^A(J) + (1 - \theta) L_w^B(J)$$

$$\leq 4\lambda_{\ell} \max \{\|\hat{W}_{j,\ell}^{(f)}\|^2\} \left[\theta + (1 - \theta)\|Z_{\ell} \hat{\Sigma}_{\ell} (\hat{\Sigma}_{\ell} + \lambda_{\ell} I)^{-1} Z_{\ell}^T\|_{op}\right].$$

(12)

As for $j \notin \tilde{J}_{\ell}$, we have that

$$\inf_{\alpha \in \mathbb{R}^{\tilde{J}_{\ell}}} \|\hat{W}_{j,\ell}^{(f)} \phi - \alpha^T \phi_j\|_n + \lambda_{\ell} \|\alpha\|_{w'}$$

$$\leq \|\hat{W}_{j,\ell}^{(f)}\|^2 L_w^A(J)$$

$$\leq \max_{j' \notin \tilde{J}_{\ell}} \{\|\hat{W}_{j,\ell}^{(f)}\|^2\} \theta L_w^A(J) + (1 - \theta) L_w^B(J)$$

$$\leq 4\lambda_{\ell} \max_{j' \notin \tilde{J}_{\ell}} \{\|\hat{W}_{j,\ell}^{(f)}\|^2\} \left[\theta + (1 - \theta)\|Z_{\ell} \hat{\Sigma}_{\ell} (\hat{\Sigma}_{\ell} + \lambda_{\ell} I)^{-1} Z_{\ell}^T\|_{op}\right].$$

(13)

Combining (12) and (13), and noticing that the optimal $\alpha$ that attains the infimum is written as

$$\hat{\alpha} = (\hat{\Sigma}_{j,j} + \lambda_{\ell} I)_{\ell}^{-1} \hat{\Sigma}_{j,F} (\hat{W}_{j,\ell}^{(f)})^T = (\hat{W}_{j,\ell}^{(f)})^T,$$

then we obtain the first assertion (6). By substituting this solution to Eq. (12) and (13), we obtain a norm bound as

$$\|\hat{W}_{j,\ell}^{(f)} \hat{A}_j \text{diag}(w)^{1/2}\|^2 \leq 4\lambda_{\ell} \alpha_{j,\ell} \max_{j' \notin \tilde{J}_{\ell}} \{\|\hat{W}_{j,\ell}^{(f)}\|^2\} \left[\theta + (1 - \theta)\|Z_{\ell} \hat{\Sigma}_{\ell} (\hat{\Sigma}_{\ell} + \lambda_{\ell} I)^{-1} Z_{\ell}^T\|_{op}\right]$$

$$\leq \tilde{c}\lambda_{\ell} \alpha_{j,\ell} \max_{j' \notin \tilde{J}_{\ell}} \{\|\hat{W}_{j,\ell}^{(f)}\|^2\}.$$  

If we further impose the constraint $\sum_{j \in \ell} w_{j}^{-1} \leq \frac{3}{4} m_{\ell} m_{\ell}^2$ for all $1 \leq \ell \leq L$, then according to the construction of a network given in the proof of Lemma 2 of Suzuki [45], we have the approximation error bound (8) as

$$\|\hat{f} - \tilde{f}\|_n \leq \sum_{\ell=2}^L \left( \prod_{\ell' = \ell+1}^L \max_{j} \{\alpha_{j,\ell'}\} \right)^{\sqrt{e^{L-\ell+1} R^{L-\ell+1}}} \sqrt{\max_{j} \{\alpha_{j,\ell}\} \zeta_{\ell,\theta} \lambda_{\ell}}$$

where $\zeta_{\ell,\theta} = \theta + (1 - \theta)\|Z_{\ell} \hat{\Sigma}_{\ell} (\hat{\Sigma}_{\ell} + \lambda_{\ell} I)^{-1} Z_{\ell}^T\|_{op}$ and $\alpha_{j,\ell} = \theta^{-1} \max_{j' \notin \tilde{J}_{\ell}} \|\hat{W}_{j,\ell}^{(f)}\|^2$ (otherwise). The last assertion can be easily checked by noting $\alpha_{j,\ell} \leq \alpha_{\text{max}}$ for all $j, \ell$.

B Proof of Theorem 2 (Generalization error bound of the compressed network)

B.1 Notations

For a sequence of the width $m' = (m'_1, \ldots, m'_L)$ of a network, let

$$\hat{F}_{m'} := \{f(x) = (W^{(L)} \eta(\cdot) + b^{(L)}) \circ \cdots \circ (W^{(1)} x + b^{(1)}) | \|W^{(l)}\|_F \leq R, \|b^{(l)}\|_\infty \leq R_b, W^{(l)} \in \mathbb{R}^{m'_l \times m'_{l-1}}, b^{(l)} \in \mathbb{R}^{m'_l} (1 \leq l \leq L)\}.$$  

Lemma 3 of Suzuki [45] gives the following $\ell_\infty$-norm bound of the elements in $\hat{F}_{m'}$. 

Proposition 3. Under Assumption [2] the \( \ell_\infty \)-norm of \( f \in \hat{F}_{m'} \) is bounded as

\[
\|f\|_\infty \leq (\sqrt{\alpha_{\max}})^L R_L D_x + \sum_{\ell=1}^L (\sqrt{\alpha_{\max}} R)^{L-\ell} c_{R_b} \leq \tilde{R}^L D_x + \sum_{\ell=1}^L \tilde{R}^{L-\ell} \tilde{R}_b \leq \hat{R}_\infty,
\]

for any \( m' \in [m_2] \times \cdots \times [m_L] \).

Proof. The assertion is a direct consequence from Lemma 3 of Suzuki [45] (or Appendix A.2 of Suzuki [46]).\( \square \)

Note that, from Theorem [1] and Proposition [3] it holds that

\[
f^\sharp \in \hat{F}_{m'}
\]

for \( m^\sharp = (m_3^\sharp, m_3^\sharp, \ldots, m_L^\sharp) \). To bound the generalization error, we use the following proposition. Moreover, it is easy to check that

\[
\mathcal{F} \subset \hat{F}_m
\]

for \( m = (m_2, \ldots, m_L) \) by its definition.

Remind that the closest element in the model \( \mathcal{F} \) to the true function \( f^\circ \) is denoted by

\[
\hat{f}^* := \arg\min_{f \in \mathcal{F}} \|f - f^\circ\|_{L_2}.
\]

Accordingly, we define the distance between \( f^\circ \) and \( f^* \) as

\[
\gamma^* : = \|f^* - f^\circ\|_{L_2}^2.
\]

B.2 Proof of Theorem [2]

In this section, we give the proof of Theorem [2].

Step 1:

First we give the empirical \( L_2 \)-norm bound \( \|f^\sharp - f^\circ\|_n \). We will give the population \( L_2 \)-norm bound \( \|f^\sharp - f^\circ\|_{L_2} \) in Step 2 based on this bound. In this Step, we fix the input observations \( (x_i)^{n_1}_{i=1} \). Accordingly, all events considered in this Step is conditioned by \( (x_i)^{n_1}_{i=1} \).

Proposition 4 (Gaussian concentration inequality (Theorem 2.5.8 in [15])). Let \( (\xi_i)^{n_1}_{i=1} \) be i.i.d. Gaussian sequence with mean 0 and variance \( \sigma^2 \), and \( (x_i)^{n_1}_{i=1} \subset \mathcal{X} \) be a given set of input variables. Then, for a set \( \hat{F} \) of functions from \( \mathcal{X} \) to \( \mathbb{R} \) which is separable with respect to \( L_\infty \)-norm and \( \sup_{f \in \hat{F}} \left| \sum_{i=1}^n \xi_i f(x_i) \right| < \infty \) almost surely, it holds that for every \( r > 0 \),

\[
P \left( \sup_{f \in \hat{F}} \left| \sum_{i=1}^n \xi_i f(x_i) \right| \geq \mathbb{E} \left[ \sup_{f \in \hat{F}} \left| \frac{1}{n} \sum_{i=1}^n \xi_i f(x_i) \right| \right] + r \right) \leq \exp[-nr^2/2(\sigma^2||\hat{F}||_n)^2],
\]

where \( ||\hat{F}||_n^2 = \sup_{f \in \hat{F}} \frac{1}{n} \sum_{i=1}^n f(x_i)^2 \). Here the probability is taken with respect to \( (\xi_i)^{n_1}_{i=1} \).

For given input observations \( (x_i)^{n_1}_{i=1} \), let

\[
G_{\delta, m'} = \{ f - f^\circ \mid \|f - f^\circ\|_n \leq \delta, f \in \hat{F}_{m'} \} \cup \{ f - f' \mid \|f - f'\|_n \leq \delta, f, f' \in \hat{F}_{m'} \}.
\]

Here, it should be noted that, even though \( f^\sharp \) could be determined by both of input and output observations \( (x_i, y_i)^{n_1}_{i=1} \), the set \( G_{\delta, m'} \) is independent of the output observations \( (y_i)^{n_1}_{i=1} \) for a fixed \( m^\sharp \). However, \( m^\sharp \) could be dependent on the observations, we must construct a bound uniformly valid for all choices of \( m^\sharp \).

Proposition [3] tells that any \( f \in \hat{F}_{m'} \) satisfies \( \|f\|_n \leq \|f\|_\infty \leq \hat{R}_\infty \). Moreover, we have that \( \|f^\circ\|_n \leq \|f^\circ\|_\infty \leq \hat{R}_\infty \) by the definition of \( \hat{R}_\infty \). Therefore, we can see that every \( g \in G_{\delta, m'} \) satisfies \( \|g\|_\infty \leq 2\hat{R}_\infty \).
It is obvious that $G_{δ,m′}$ is separable with respect to $L_{∞}$-norm. Then, by the Gaussian concentration inequality, we have that

$$P \left( \sup_{g \in G_{δ,m′}} \left| \sum_{i=1}^{n} \frac{1}{n} \xi_i g(x_i) \right| \geq \mathbb{E} \left[ \sup_{g \in G_{δ,m′}} \left| \frac{1}{n} \sum_{i=1}^{n} \xi_i g(x_i) \right| \right] + r \right) \leq \exp[-nr^2/(2σδ)^2]$$

for every $r > 0$. By applying this inequality for $δ = 2^{−1} σ/√n$ for $j = 1, … , \lfloor \log_2(2R_∞√n/σ) \rfloor$ and for $m′ ∈ [m_2] × [m_3] × … × [m_L]$ (where $m := \{1, … , m\}$) uniformly, we can show that, for every $r > 0$ and $µ > 0$, with probability $1 - \exp(-r)$, it holds that

$$\frac{1}{n} \sum_{i=1}^{n} \left| f_i(x_i) - f′(x_i) \right|$$

$$\leq \mathbb{E} \left[ \sup_{g \in G_{δ,m′}} \left| \frac{1}{n} \sum_{i=1}^{n} \xi_i g(x_i) \right| \right] + 2δσ √ \left( \frac{r + \sum_{ℓ=1}^{L} \log(m_ℓ) + \log(\log(2R_∞√n/σ))}{2} \right)$$

$$\leq \mathbb{E} \left[ \sup_{g \in G_{δ,m′}} \left| \frac{1}{n} \sum_{i=1}^{n} \xi_i g(x_i) \right| \right] + \frac{µδ^2}{2} + \frac{σ^2}{2µ} \left( r + \sum_{ℓ=1}^{L} \log(m_ℓ) + \log(\log(2R_∞√n/σ)) \right),$$

(14)

uniformly for all $f ∈ \hat{F}_{m′}$ and $f′ ∈ \hat{F}_{m′} \cup \{f^o\}$ such that $||f - f^o||_n ≤ δ$ for any $δ ≥ σ/√n$ and any $m′ ∈ [m_2] × [m_3] × … × [m_L]$.

Lemma 2. There exists a universal constant $C$ such that, for any $δ > 0$ and $µ > 0$, it holds that

$$\mathbb{E} \left[ \sup_{f ∈ G_{δ,m′}} \left| \frac{1}{n} \sum_{i=1}^{n} \xi_i g(x_i) \right| \right] ≤ Cδ σ \sqrt{\frac{\sum_{ℓ=1}^{L} m_ℓ′ m_{ℓ+1}′}{n} \log \left( 1 + \frac{4\hat{G} \max\{\bar{R}, \bar{R}_b\}}{δ} \right)}$$

$$≤ \frac{µ}{2} δ^2 + \frac{σ^2}{2} C^2 \frac{\sum_{ℓ=1}^{L} m_ℓ′ m_{ℓ+1}′}{n} \log \left( 1 + \frac{4\hat{G} \max\{\bar{R}, \bar{R}_b\}}{δ} \right) \cdot φ(n, m′, δ).$$

Proof. Since $f \mapsto \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \xi_i f(x_i)$ is a sub-Gaussian process relative to the metric $||·||_n$. By the chaining argument (see, for example, Theorem 2.3.6 of [15]), it holds that

$$\mathbb{E} \left[ \sup_{g \in G_{δ,m′}} \left| \frac{1}{n} \sum_{i=1}^{n} \xi_i g(x_i) \right| \right] \leq 4\sqrt{2} σ \sqrt{\frac{\log(2N(ε, G_{δ,m′}, ||·||_n))}{ε}}.$$

Since $\log N(ε, G_{δ,m′}, ||·||_n) ≤ \log N(ε, \hat{F}_{m′}, ||·||_∞) ≤ 4\sum_{ℓ=1}^{L} m_ℓ′ m_{ℓ+1}′ \log \left( 1 + \frac{4\hat{G} \max\{\bar{R}, \bar{R}_b\}}{ε} \right)$, the right hand side is bounded by

$$\int_{0}^{2δ} \sqrt{\log(2N(ε, G_{δ,m′}, ||·||_n))} dε$$

$$\leq \int_{0}^{2δ} \sqrt{\log(2) + 4\sum_{ℓ=1}^{L} m_ℓ′ m_{ℓ+1}′ \log \left( 1 + \frac{4\hat{G} \max\{\bar{R}, \bar{R}_b\}}{ε} \right)} dε$$

$$≤ Cδ \sqrt{\frac{\sum_{ℓ=1}^{L} m_ℓ′ m_{ℓ+1}′}{n} \log \left( 1 + \frac{4\hat{G} \max\{\bar{R}, \bar{R}_b\}}{δ} \right)},$$

where $C$ is a universal constant. This gives the assertion. 

Combining Eq. (14) and Lemma 2 it holds that, with probability $1 - e^{-r}$, the following holds uniformly over all choices of $f ∈ \hat{F}_{m′} \cup \{f^o\}$ such that $||f - f′||_n ≤ δ$ for any $δ ≥ σ/√n$ and any
\( m' \in [m_2] \times [m_3] \times \cdots \times [m_L]: \)
\[
\left| \frac{1}{n} \sum_{i=1}^{n} \xi_i (f(x_i) - f'(x_i)) \right| \\
\leq \mu \delta^2 + \phi_n (m', \mu, \delta) + \frac{2 \sigma^2}{n \mu} \left( r + \sum_{\ell=1}^{L} \log(m_{\ell}) + \log(\ceil{\log_2(2\hat{R}_{\infty} \sqrt{n}/\sigma)}) \right),
\]
for any \( \mu > 0 \). By substituting \( \delta \leftarrow \left( \| f - f' \|_n \vee \sigma \frac{1}{\sqrt{n}} \right) \) and \( r \leftarrow \sigma r/\sqrt{n} \) to the right hand side, the right hand side yields
\[
\left| \frac{1}{n} \sum_{i=1}^{n} \xi_i (f(x_i) - f'(x_i)) \right| \\
\leq \mu \left( \| f - f' \|_n \vee \frac{\sigma}{\sqrt{n}} \right)^2 + \phi_n (m', \mu, \delta) + \frac{\sigma^2}{n \mu} \left( r + \sum_{\ell=1}^{L} \log(m_{\ell}) + \log(\ceil{\log_2(2\hat{R}_{\infty} \sqrt{n}/\sigma)}) \right) \\
\leq \mu \| f - f' \|_n^2 + \phi_n (m', \mu, \sigma/\sqrt{n}) + \frac{\sigma^2}{n \mu} \left( r + 2 \mu^2 + \sum_{\ell=1}^{L} \log(m_{\ell}) + \log(\ceil{\log_2(2\hat{R}_{\infty} \sqrt{n}/\sigma)}) \right) .
\]
For notational convenience, we write \( \| f - y \|_n^2 = \frac{1}{n} \sum_{i=1}^{n} (f(x_i) - y_i)^2 \) and similarly \( \langle f, y \rangle_n = \frac{1}{n} \sum_{i=1}^{n} f(x_i) y_i \) and \( \langle f, \xi \rangle_n = \frac{1}{n} \sum_{i=1}^{n} f(x_i) \xi_i \).
We give the generalization error bound for the situation \( \beta_n = \infty \) in Assumption\footnote{2}
First note that, since \( \| \hat{f} - y \|_n^2 \leq \| f^* - y \|_n^2 + \hat{\zeta} \), we have that
\[
\| \hat{f} - f^0 \|_n^2 \leq \| f^* - f^0 \|_n^2 - 2 \langle f^* - \hat{f}, \xi \rangle_n + \hat{\zeta} .
\]
Therefore, it holds that
\[
\| f^2 - y \|_n^2 = \| f^2 - \hat{f} + \hat{f} - y \|_n^2 \\
= \| f^2 - \hat{f} \|_n^2 + 2 \langle f^2 - \hat{f}, \hat{f} - y \rangle_n + \| \hat{f} - y \|_n^2 \\
= \| f^2 - \hat{f} \|_n^2 + 2 \langle f^2 - \hat{f}, \hat{f} - f^0 \rangle_n + 2 \| f^2 - \hat{f}, \xi \|_n + \| \hat{f} - y \|_n^2 \\
\leq \| f^2 - \hat{f} \|_n^2 + 2 \| f^2 - \hat{f} \|_n \| \hat{f} - f^0 \|_n + 2 \langle f^2 - \hat{f}, \xi \rangle_n + \| \hat{f} - y \|_n^2 \\
\leq \| f^2 - \hat{f} \|_n^2 + \| f^2 - \hat{f} \|_n^2 + (\| f^* - f^0 \|_n^2 - 2 \langle f^* - \hat{f}, \xi \rangle_n + \hat{\zeta}) - 2 \langle f^2 - \hat{f}, \xi \rangle_n + \| \hat{f} - y \|_n^2 .
\]
The right hand side is further bounded from above by
\[
2 \| f^2 - \hat{f} \|_n^2 + (\| f^* - f^0 \|_n^2 - 2 \langle f^* - f^0, \xi \rangle_n - 2 \langle f^* - f^0, \xi \rangle_n - 2 \langle f^2 - \hat{f}, \xi \rangle_n + \hat{\zeta}) \\
- 2 \langle f^2 - \hat{f}, \xi \rangle_n + \| \hat{f} - y \|_n^2 \\
= 2 \| f^2 - \hat{f} \|_n^2 + \| f^* - f^0 \|_n^2 - 2 \langle f^* - f^0, \xi \rangle_n - 2 \langle f^* - f^0, \xi \rangle_n - 4 \langle f^2 - \hat{f}, \xi \rangle_n + \| f^* - y \|_n^2 + 2 \hat{\zeta} .
\]
Therefore, we have that
\[
\| f^2 - f^0 \|_n^2 \leq 2 \| f^2 - \hat{f} \|_n^2 + 2 \| f^* - f^0 \|_n^2 \\
- 2 \langle f^* - f^0, \xi \rangle_n - 2 \langle f^* - f^0, \xi \rangle_n - 4 \langle f^2 - \hat{f}, \xi \rangle_n - 2 \langle f^* - f^0, \xi \rangle_n + 2 \hat{\zeta} .
\]
This yields that
\[
\| f^2 - f^0 \|_n^2 \leq 2 \| f^2 - \hat{f} \|_n^2 + 2 \| f^* - f^0 \|_n^2 - 4 \langle f^* - f^0, \xi \rangle_n - 4 \langle f^* - f^0, \xi \rangle_n - 2 \langle f^2 - \hat{f}, \xi \rangle_n + 4 \hat{\zeta} .
\]
This gives that
\[
\| f^2 - f^0 \|_n^2
\[ \leq 2\delta_1^2 + 2\|f^* - f^0\|^2_n + 4\|f^* - f^0\|^2_n + \frac{8\sigma^2 t}{n} \]
\[ + 4\mu\|f^* - f^0\|^2_n + 4\Phi_{n,e}(m^2, \mu) + 8\|f^* - \hat{f}\|_n \sqrt{\Phi_{n,e}(m, 1) + 2\zeta} \]
\[ \leq 2\delta_1^2 + 2\|f^* - f^0\|^2_n + 4\|f^* - f^0\|^2_n + \frac{8\sigma^2 t}{n} \]
\[ + 4\mu\|f^* - f^0\|^2_n + 4\Phi_{n,e}(m^2, \mu) + 8\delta_1\sqrt{\Phi_{n,e}(m, 1) + 2\zeta}. \]

Letting \( \mu = 1/8 \), it holds that
\[ \|f^* - f^0\|^2_n \leq 4\delta_1^2 + 12\|f^* - f^0\|^2_n + \frac{16\sigma^2 t}{n} + 8\Phi_{n,e}(m^2, 1/8) + 16\delta_1\sqrt{\Phi_{n,e}(m, 1) + 4\zeta}. \]

(15)

**Step 2:**

Based on the inequalities given in Step 1, we derive a bound for \( \|\hat{f} - f^*\|_L^2 \) instead of the empirical \( L^2 \)-norm \( \|\hat{f} - f^*\|_n \).

First note that, by Bernstein’s inequality
\[ P \left( \|f^0 - f^*\|^2_n \geq \gamma^2 + \sqrt{\frac{2R_{\infty}^2\gamma^2 t}{n}} + \frac{R_{\infty}^2}{n} \right) \leq e^{-t} \]
for any \( t > 0 \). Thus, with probability \( 1 - e^{-t} \), it holds that
\[ \|f^0 - f^*\|^2_n \leq \gamma^2 + \sqrt{\frac{2R_{\infty}^2\gamma^2 t}{n}} + \frac{R_{\infty}^2}{n} \leq \frac{3}{2\gamma^2} + \frac{2R_{\infty}^2}{n}, \]
where we used the arithmetic-geometric mean inequality.

To bound the difference between \( \|f^2 - f^0\|_L^2 \) and \( \|f^2 - f^0\|_n \), we need the following uniform bound known as Talagrand’s concentration inequality.

**Proposition 5** (Talagrand’s concentration inequality [47][8]). Let \( (x_i)_{i=1}^n \) be an i.i.d. sequence of input variables in \( X \). Then, for a set \( \mathcal{F} \) of functions from \( X \) to \( \mathbb{R} \) which is separable with respect to \( L_{\infty} \)-norm and \( \|f\|_\infty \leq R \) for all \( f \in \mathcal{F} \), it holds that for every \( r > 0 \),
\[ P \left( \sup_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^n f(x_i) - E[f^2] \right) \leq C \left\{ E \left[ \sup_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^n f(x_i)^2 - E[f^2] \right] + \sqrt{\frac{\mathcal{F}^2 r_{L^2}}{n} + \frac{rR^2}{n}} \right\} \]
\[ \leq \exp(-r), \]
where \( \|\mathcal{F}\|_{L^2} = \sup_{f \in \mathcal{F}} E[f(X)^4] \).

We are going to see how to apply this inequality to derive the population \( L^2 \)-norm bound. Let
\[ \mathcal{G}_{s,m'} \cdot \{ f - f' \mid \|f - f'\|_{L^2} \leq \delta, f \in \mathcal{F}_{m'}, f' \in \mathcal{F}_{m'} \cup \{ f^0 \} \}. \]

Since \( \|f\|_\infty \leq R_{\infty} \) for all \( f \in \mathcal{F}_{m'} \) (Proposition 3) and \( \|f^0\|_\infty \leq R_{\infty} \) by the definition of \( R_{\infty} \), \( \|g\|_\infty \leq 2R_{\infty} \) for all \( g \in \mathcal{G}_{s,m'} \). Therefore, we have \( \|\mathcal{G}_{s,m'}^2\|^2_{L^2} \leq 4R_{\infty}^2 \delta^2 \). Hence, Talagrand’s concentration inequality yields that
\[ \sup_{f \in \mathcal{G}_{s,m'}, \cdot} \left| \frac{1}{n} \sum_{i=1}^n f(x_i)^2 - E[f^2] \right| \leq C_1 \left\{ E \left[ \sup_{f \in \mathcal{G}_{s,m'}} \left| \frac{1}{n} \sum_{i=1}^n f(x_i)^2 - E[f^2] \right| \right] + \sqrt{\frac{\delta^2 \mathcal{F}_{L^2} r_{L^2}}{n} + \frac{rR_{\infty}^2}{n}} \right\} \]
\[ \leq \frac{1}{4} \delta^2 + C_1 E \left[ \sup_{f \in \mathcal{G}_{s,m'}} \left| \frac{1}{n} \sum_{i=1}^n f(x_i)^2 - E[f^2] \right| \right] + \frac{(C_1^2 + C_2)\delta R_{\infty}}{n} \]

(17)

with probability \( 1 - \exp(-r) \) where \( C_1 \) is a universal constant.
Lemma 3. There exists a universal constant $C > 0$ such that, for all $\delta > 0$,

$$
E \left[ \sup_{f \in \mathcal{G}_{\delta, m'}} \left| \frac{1}{n} \sum_{i=1}^{n} g(x_i)^2 - E[g^2] \right| \right] \leq C \left[ \delta \hat{R}_\infty \sqrt{\sum_{\ell=1}^{L} \frac{m'_\ell m'_{\ell+1}}{n} \log_+ \left( 1 + \frac{4\hat{G} \max \{ \hat{R}, \hat{R}_b \}}{\delta} \right)} \right] \\
+ \sqrt{\hat{R}_\infty^2 \sum_{\ell=1}^{L} \frac{m'_\ell m'_{\ell+1}}{n} \log_+ \left( 1 + \frac{4\hat{G} \max \{ \hat{R}, \hat{R}_b \}}{\delta} \right)} \\
\leq \frac{\delta^2}{4} + (C + C^2) \hat{R}_\infty^2 \sum_{\ell=1}^{L} \frac{m'_\ell m'_{\ell+1}}{n} \log_+ \left( 1 + \frac{4\hat{G} \max \{ \hat{R}, \hat{R}_b \}}{\delta} \right).
$$

Proof. Let $(\epsilon_i)_{i=1}^{n}$ be i.i.d. Rademacher sequence. Then, by the standard argument of Rademacher complexity, we have

$$
E \left[ \sup_{f \in \mathcal{G}_{\delta, m'}} \left| \frac{1}{n} \sum_{i=1}^{n} f(x_i)^2 - E[f^2] \right| \right] \leq 2E \left[ \sup_{f \in \mathcal{G}_{\delta, m'}} \left| \frac{1}{n} \sum_{i=1}^{n} \epsilon_i f(x_i)^2 \right| \right]
$$

(see, for example, Lemma 2.3.1 in van der Vaart & Wellner [48]). Since $\|f\|_\infty \leq 2\hat{R}_\infty$ for all $f \in \mathcal{G}_{\delta, m'}$, the contraction inequality Theorem 4.12 of Ledoux & Talagrand [31] gives an upper bound of the RHS as

$$
2E \left[ \sup_{f \in \mathcal{G}_{\delta, m'}} \left| \frac{1}{n} \sum_{i=1}^{n} \epsilon_i f(x_i)^2 \right| \right] \leq 4(2\hat{R}_\infty)E \left[ \sup_{f \in \mathcal{G}_{\delta, m'}} \left| \frac{1}{n} \sum_{i=1}^{n} \epsilon_i f(x_i) \right| \right].
$$

We further bound the RHS. By Theorem 3.1 in [16] or Lemma 2.3 of [37] with the covering number bound given by Suzuki [46] and Suzuki [45], there exists a universal constant $C'$ such that

$$
E \left[ \sup_{f \in \mathcal{G}_{\delta, m'}} \left| \frac{1}{n} \sum_{i=1}^{n} \epsilon_i f(x_i) \right| \right] \leq C' \left[ \delta \sqrt{\sum_{\ell=1}^{L} \frac{m'_\ell m'_{\ell+1}}{n} \log_+ \left( 1 + \frac{4\hat{G} \max \{ \hat{R}, \hat{R}_b \}}{\delta} \right)} \right] \\
+ \hat{R}_\infty \sum_{\ell=1}^{L} \frac{m'_\ell m'_{\ell+1}}{n} \log_+ \left( 1 + \frac{4\hat{G} \max \{ \hat{R}, \hat{R}_b \}}{\delta} \right).
$$

This concludes the proof. \qed

Let $\psi_{n, m'} := \sum_{\ell=1}^{L} \frac{m'_\ell m'_{\ell+1}}{n} \log_+ \left( 1 + \frac{4\sqrt{\hat{G} \max \{ \hat{R}, \hat{R}_b \}}}{\delta} \right)$. Then, applying the inequality [17] for $\delta = 2^{j-1} \hat{R}_\infty / \sqrt{n}$ for $j = 1, \ldots, \lfloor \log_2(\sqrt{n}) \rfloor$, it is shown that there exists an event with probability $1 - \lfloor \log_2(\sqrt{n}) \rfloor \exp(-r)$ such that, uniformly for all $g \in \mathcal{G}_{\delta, m'}$, it holds that

$$
\left| \frac{1}{n} \sum_{i=1}^{n} g(x_i)^2 - E[g^2] \right| \leq \frac{1}{2} \left( \delta^2 \sqrt{\frac{\hat{R}_\infty^2}{n}} + (C + C^2) \hat{R}_\infty^2 \psi_{n, m'} + (C_1 + C_1^2) \frac{\hat{R}_\infty^2 r}{n} \right) \\
\leq \frac{1}{2} \delta^2 + (C + C^2) \hat{R}_\infty^2 \psi_{n, m'} + \frac{\hat{R}_\infty^2 [(C_1 + C_1^2) r + 1]}{n},
$$

where $\delta$ is any positive real such that $\delta^2 \geq E[g^2]$. The right hand side can be further bounded by

$$
\frac{\delta^2}{2} + C_2 \hat{R}_\infty^2 \left( \psi_{n, m'} + \frac{r + 1}{n} \right)
$$

for an appropriately defined universal constant $C_2$. We apply this inequality uniformly for all $m' \in [m_2] \times \cdots \times [m_L]$, we have

$$
\left| \frac{1}{n} \sum_{i=1}^{n} g(x_i)^2 - E[g^2] \right| \leq \frac{E[g^2]}{2} + C_2 \hat{R}_\infty^2 \left( \psi_{n, m'} + \frac{r + 1 + \sum_{l=2}^{L} \log(m_l) + \log(\lfloor \log_2(\sqrt{n}) \rfloor)}{n} \right)
$$

(18)
for any $g \in G_{\delta,m'}$ with any $\delta > 0$ and $m' \in \{m_2\} \times \cdots \times \{m_L\}$. Applying this bound to those obtained in Step 1, we will obtain the assertion as follows.

Actually, Eq. (18) with Eq. (15) and Eq. (16) yields that

$$
\|f^\# - f^\circ\|_2^2 \leq 4\delta_1^2 + 12\|f^\ast - f^\circ\|_2^2 + \frac{16\delta_1^2 t}{n} + 8\Phi_{n,r}(m^\#, \mu) + 16\delta_1 \sqrt{\Phi_{n,r}(m, 1) + 4^i} \\
\Rightarrow \frac{1}{2}\|f^\# - f^\circ\|_2^2 \leq 4\delta_1^2 + 18\|f^\ast - f^\circ\|_2^2 + \frac{16\delta_1^2 t}{n} + 8\Phi_{n,r}(m^\#, \mu) \\
+ 16\delta_1 \sqrt{\Phi_{n,r}(m, 1) + 4^i} + \Psi_{n,r}(m^\#), \tag{19}
$$

with probability $1 - 3e^{-t} - 2e^{-r}$. Finally, we note that

$$
\delta_1 \sqrt{\Phi_{n,r}(m, 1)} \leq \delta_1 \sqrt{\phi_n(m, 1, \sigma/\sqrt{n})} + \delta_1 \sqrt{\frac{\sigma^2}{n} \left( r + 2\mu^2 + \sum_{\ell=1}^L \log(m_{\ell}) + \log(\lceil \log_2(2\hat{R}_\infty \sqrt{n}/\sigma) \rceil) \right)} \\
\leq \delta_1 \sqrt{\phi_n(m, 1, \sigma/\sqrt{n})} + \frac{1}{2}\delta_1^2 + \frac{\sigma^2}{2n} \left( r + 2\mu^2 + \sum_{\ell=1}^L \log(m_{\ell}) + \log(\lceil \log_2(2\hat{R}_\infty \sqrt{n}/\sigma) \rceil) \right).
$$

This yields the asserted generalization error bound.

\section{Proof of Proposition 1}

The proof is proven just by applying the Gaussian concentration inequality and the Bernstein inequality.

Let $\xi_i^l = y_i - f^\circ(x_i')$, then

$$
\frac{1}{n_{\text{val}}} \sum_{i=1}^{n_{\text{val}}} (y_i - \hat{f}(x_i'))^2 \leq \frac{1}{n_{\text{val}}} \sum_{i=1}^{n_{\text{val}}} (y_i - f^\#(x_i'))^2 + q_n \\
\Rightarrow \frac{1}{n_{\text{val}}} \sum_{i=1}^{n_{\text{val}}} (\hat{f}(x_i') - f^\circ(x_i'))^2 \leq \frac{1}{n_{\text{val}}} \sum_{i=1}^{n_{\text{val}}} (f^\#(x_i') - f^\circ(x_i'))^2 - \frac{2}{n_{\text{val}}} \sum_{i=1}^{n_{\text{val}}} \xi_i^l(f^\#(x_i') - \hat{f}(x_i')) + q_n.
$$

Let $P_{n_{\text{val}}} f = \frac{1}{n_{\text{val}}} \sum_{x_i', y_i'} f(x_i', y_i')$ and $P f = E[f(X, Y)]$. By applying the Gaussian concentration inequality, it holds that

$$
P \left( - \frac{1}{n_{\text{val}}} \sum_{i=1}^{n_{\text{val}}} \xi_i^l(f^\#(x_i') - \hat{f}(x_i')) \geq r\sigma \sqrt{\frac{2}{n_{\text{val}}} P_{n_{\text{val}}} (f^\# - \hat{f})^2 \mid \{x_i'\}_{i=1}^{n_{\text{val}}}} \right) \leq \exp(-r^2)
$$

for all $r > 0$. Therefore, with probability $1 - \exp(-r^2)$,

$$
- \frac{2}{n_{\text{val}}} \sum_{i=1}^{n_{\text{val}}} \xi_i^l(f^\#(x_i') - \hat{f}(x_i')) \leq 2r\sigma \sqrt{\frac{2}{n_{\text{val}}} P_{n_{\text{val}}} (f^\# - \hat{f})^2} \\
\leq 2r\sigma \sqrt{\frac{2}{n_{\text{val}}} \left( \sqrt{P_{n_{\text{val}}} (\hat{f} - f^\circ)^2} + \sqrt{P_{n_{\text{val}}} (f^\# - f^\circ)^2} \right)} \\
\leq \frac{1}{2} P_{n_{\text{val}}} (\hat{f} - f^\circ)^2 + \frac{1}{2} P_{n_{\text{val}}} (f^\# - f^\circ)^2 + \frac{4r^2\sigma^2}{n_{\text{val}}}
$$

and thus it holds that

$$
\frac{1}{2} P_{n_{\text{val}}} (\hat{f} - f^\circ)^2 \leq \frac{3}{2} P_{n_{\text{val}}} (f^\# - f^\circ)^2 + \frac{4r^2\sigma^2}{n_{\text{val}}} + q_n.
$$
Here, Bernstein’s inequality shows that for \( \|f\|_{\infty} \leq B \), it holds that
\[
P \left( |P_{n_{val}}f^2 - Pf^2| \geq \sqrt{\frac{2B^2 Pf^2 t}{n_{val}} + \frac{B^2 t}{n_{val}}} \right) \leq 2e^{-t}
\]
for any \( t > 0 \). Thus, with probability \( 1 - 2e^{-t} \), it holds that
\[
P_{n_{val}}f^2 \leq Pf^2 + \sqrt{\frac{2B^2 Pf^2 t}{n_{val}}} + \frac{B^2 t}{n_{val}} \leq \frac{3}{2} Pf^2 + \frac{2B^2 t}{n_{val}},
\]
and similarly it holds that
\[
P_{n_{val}}f^2 \geq Pf^2 - \sqrt{\frac{2B^2 Pf^2 t}{n_{val}}} - \frac{B^2 t}{n_{val}} \geq \frac{1}{2} Pf^2 - \frac{2B^2 t}{n_{val}}.
\]
Therefore, it holds that
\[
\frac{1}{4} P(\hat{f} - f^o)^2 \leq \frac{9}{4} P(f^2 - f^o)^2 + 4(\hat{R}_\infty)^2 t + \frac{4\sigma^2}{n_{val}} r + q_n,
\]
with probability \( 1 - 2 \exp(-t) - \exp(-r) \) for all \( t,r > 0 \). Therefore, we have that
\[
P(\hat{f} - f^o)^2 \leq 9P(f^2 - f^o)^2 + \frac{16(\hat{R}_\infty^2 + \sigma^2)}{n_{val}} t + q_n,
\]
with probability \( 1 - 3 \exp(-t) \) for all \( t > 0 \).

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