Bounding Data-driven Model Errors in Power Grid Analysis

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Abstract—Data-driven models analyze power grids under incomplete physical information, and their accuracy has been mostly validated empirically using certain training and testing datasets. This paper explores error bounds for data-driven models under all possible training and testing scenarios, and proposes an evaluation implementation based on Rademacher complexity theory. We answer key questions for data-driven models: how much training data is required to guarantee a certain error bound, and how partial physical knowledge can be utilized to reduce the required amount of data. Our results are crucial for the evaluation and application of data-driven models in power grid analysis. We demonstrate the proposed method by finding generalization error bounds for two applications, i.e., branch flow linearization and external network equivalent under different degrees of physical knowledge. Results identify how the bounds decrease with additional power grid physical knowledge or more training data.

Index Terms—Learning theory, Rademacher complexity, power flow, linear regression, support vector machine

I. INTRODUCTION

Data-driven models are widely applied in power systems to model the system stability, the power grid control and optimization strategies, and electrical consumer behaviors. In this paper, we focus on one type of data-driven models that extract mappings among the power grid from operational data such as voltage and power injection measurements, e.g., data-driven power flow modeling [1], power network equivalence [2], line failures detection [3], and operational security rules learning [4], etc. Data-driven models are preferred when physical knowledge are too complex [5] or unavailable [2], or when the power grid analysis involves non-parametric factors such as renewable uncertainties [6] or human behaviors [7]. Nonetheless, the accuracy of data-driven models is usually evaluated empirically on certain testing data and is often unreliable over unfamiliar input data. Some recent works address this problem by integrating partial physical knowledge into data-driven models [2], [3], [8] that intuitively improve the model accuracy. However, these approaches are unable to provide any theoretical conclusions about the generalization error, i.e., the model error over all possible model outcomes.

The inability of bounding the generalization error is a major obstacle that prevents wide spread adoption of data-driven models in the power industry. Power system operators must estimate the worst-case model outcome (i.e. the upper bound of errors) for robust operation, and must be able to explain and reinforce the data-driven model with their physical knowledge of the system. In addition, how much data is required to bound a data-driven model to a desired accuracy is yet an open question [9], as it closely relates to the data quality and model complexity. Simply using more training data may not be ideal due to the trade-off between stable performance and real-time adaptivity [10], i.e., do we want to find a model that best fits all known data, or do we only use recent datasets so the model better adapts to changes in the system states or ambient conditions.

We address the aforementioned challenges by quantifying a theoretical bound on generalization errors based on the Rademacher complexity theory [11]. Rademacher complexity is a notation of complexity that measures the richness of a class of real-valued functions. The formulation is interpretable and has been applied to derive generalization bounds in classification problems [12]. However, existing Rademacher complexity bounds for regression problems are theoretically loose [13], and cannot consider the integration of any physical knowledge. We propose a modified Rademacher complexity (MRC) generalization bound that is tighter for regression problems and incorporates physical knowledge. We derive the bound using the modified logarithmic Sobolev inequality [14] that satisfies the conditions of regression problems (where the output of the regression is continues without explicit bound).

The contribution of our work is summarized as follows:

1) We provide a tighter bound than conventional Rademacher complexity bound for the generalization error in regression problems, which are common for conducting data-driven power grid analysis.

2) We show how much data is required to theoretically bound a data-driven model under all possible training and testing datasets, which is critical to guarantee the reliability of data-driven models in power grid applications.

3) We quantify how physical knowledge can reduce generalization error by incorporating physical knowledge as problem constraints in the MRC model.

4) Our method applies in power flow analysis and in external network equivalence, which involve the use of linear regression and support vector regression (SVR).

The remainder of this paper is organized as follows. Section II introduces the preliminaries and the problem statements. In section III, we propose the MRC generalization error bound, which includes the theoretical results and the computation methods. Section IV and section V provide the case studies. Finally, section VI draws the conclusions.

II. PRELIMINARIES AND PROBLEM STATEMENT

A. Generalization Error

We start by introducing the formal definition of generalization error and the probably approximately correct (PAC)
Learning framework, firstly proposed by Valiant [15]. Subsequently, further work on generalization error theory includes Vapnik Chervonenkis (VC) dimension [16], PAC-Bayes [17], and Rademacher complexity [11] have been established over the PAC learning framework.

Definition 1 (Generalization error). Given a sample $x \in \mathcal{X}$ from an underlying distribution $D$, a hidden ground truth mapping $f(\cdot)$, and a hypothesis class (a.k.a. a data-driven model class such as linear regression) $h \in \mathcal{H}$, the generalization error, $L(h)$, is:

$$L(h) = E_{x \sim D} [ l(h, x) ],$$

where $l(h, x)$ is the loss function mapping from $\mathcal{H} \times \mathcal{X} \rightarrow \mathbb{R}$.

The loss function calculates the loss from an input hypothesis $h$ and sample point $x$. In this paper, we use the absolute error as the loss function:

$$l(h, x) = |f(x) - h(x)|.$$

Definition 2 (Empirical error). The empirical error $\hat{L}_m(h)$ over the $m$ training samples $\{x_i\}_{i=1}^m$ given a hypothesis $h$ is:

$$\hat{L}_m(h) = \frac{1}{m} \sum_{i=1}^m l(h, x_i).$$

Definition 3 (PAC learning). A hypothesis class $\mathcal{H}$ is said to have generalization error $\epsilon$ with probability $1 - \delta$, if under the unknown distributions $D$, the generalization error $L(h)$ of any hypothesis $h \in \mathcal{H}$ satisfies the following inequality:

$$Pr_{x \sim \mathcal{D}} [ L(h) \leq \epsilon ] \geq 1 - \delta.$$

The VC dimension is a pioneering theory to measure the complexity of a hypothesis class [16] but does not consider sample distributions, which makes VC bounds loose with conservative estimation of the generalization error [18]. PAC-Bayes bound is a generic theory to evaluate generalization errors in a Bayesian learning framework, which has been extensively explored recently [19], [20]. Different from other theories that bound the generalization error $L(h)$, PAC-Bayes bounds the error according to a posterior distribution $\pi$ over $\mathcal{H}$: $E_{h \sim \pi} L(h)$, where parameters in $h$ are not definite, but is according to the posterior distribution $\pi$. This approach for measuring the bound, though can help to develop better learning algorithms, may lose their physical meaning in practical engineering applications.

The Rademacher complexity bound uses the information of the sample distribution and derives a tighter bound compared to VC dimension [13]. It also directly bounds the $L(h)$ compared with the PAC-Bayes bound, and shows great potential in analyzing data-driven models of engineering problems. The definition of the Rademacher complexity is as follows:

Definition 4 (Rademacher complexity [11]). Given samples $x = \{x_i\}_{i=1}^m \sim D$, the Rademacher complexity of a hypothesis class $\mathcal{H}$ is:

$$\mathcal{R}(\mathcal{H}) = E_{x \sim D} \left[ \mathcal{R}(\mathcal{H}) \right].$$

where $\mathcal{R}(\mathcal{H})$ is the empirical Rademacher complexity based on the loss function of the samples, i.e.:

$$\hat{\mathcal{R}}(\mathcal{H}) = E_{x \sim D} \left[ \sup_{h \in \mathcal{H}} \frac{1}{m} \sum_{i=1}^m \sigma_i l(h, x_i) \right].$$

where $\sigma = (\sigma_1, \ldots, \sigma_m)^T$ are i.i.d. random variables with $Pr[\sigma_i = 1] = Pr[\sigma_i = -1] = 0.5$, and $\sup$ denotes the supremum of the formulation.

The Rademacher complexity measures the expected $(E_{\sigma})$ richness of a function family $\mathcal{H}$: how well functions in $\mathcal{H}$ can best correlate $(\sup_{h \in \mathcal{H}})$ with random noise $(\sigma_i)$. However, Rademacher theory primarily handles classification problems and is less often applied to regression problems [12], [21], [22], while numerical calculation strategies of Rademacher complexity is seldom developed. We therefore propose a MRC generalization bounds based on the modified logarithmic Sobolev inequality [14], to provide a tighter bound for regression problems. We show that although Rademacher complexity is mostly developed for classification problems, the MRC is also suitable for regression problem.

B. Physical Knowledge in Data-driven Models

The physical knowledge space $\mathcal{P}$ describes what we know about the target system in addition to measurements. For instance, in power grid analysis, this includes topology, line impedance, or physical principles such as power flow models. Incorporation of physical knowledge stabilizes data-driven model performance as it reduces model complexity by intersecting the hypothesis class space with the physical knowledge space $\mathcal{H} \cap \mathcal{P}$ according to Definition 1.

Definition 5 (Data-driven models with physical knowledge). Given samples $x = \{x_i\}_{i=1}^m \sim D$ and the physical knowledge based space $\mathcal{P}$ derived from some physical rules, the model aims at finding the hypothesis $h \in \mathcal{H} \cap \mathcal{P}$ while minimizing the empirical error $\hat{L}_m(h)$.

In practice, physical knowledge $\mathcal{P}$ can be described as data-driven model parameter constraints (i.e. $p(x, h) \leq 0$) during the training stage. For example, Yu et al. [2] added external network parameter constraints (derived from system maximum and minimum operating modes) to least squares regression models; Karagiannopoulos et al. [8] added box constraints (derived from imbalanced control penalties) to SVR models.

C. Problem Statement

We seek a generalization error bound $\epsilon$ that reflects the underlying hypothesis space $\mathcal{H}$, the physical knowledge space $\mathcal{P}$, and the training samples $\mathcal{x}$, formally stated as follows:

$$\epsilon = MRC(\mathcal{H} \cap \mathcal{P}, \mathcal{x})$$

Our proposed approach provides a way to benchmark the choice of model, training data size, and physical constraints in data-driven grid analysis. For example, a linear regression model with more regressors achieves better training results but its generalization error may increase due to over-fitting, as illustrated in Fig [1]a); while incorporating physical knowledge improves the generalization error, this improvement diminishes with larger training datasets, as illustrated in Fig [1]b).
III. THE MODIFIED RADEMACHER COMPLEXITY BOUND

In this Section, we introduce the proposed MRC bound. We first present the theoretical derivation of the bound. Then, we adopt an iteration strategy to further tighten the bound. At last, we provide the approach to numerically evaluate the bound.

A. Theoretical Result

We start by introducing the main Theorem, which states that the empirical error of a hypothesis \( h \) can be bounded based on the sample-based empirical Rademacher complexity:

**Theorem 6** (Empirical modified Rademacher complexity bound). We can bound the generalization error, for \( \forall \delta \in (0, 1) \) and \( \forall h \in \mathcal{H}(e) \), with at least \( 1 - \delta \) probability:

\[
L(h) \leq \tilde{L}_\infty(h) + 2\mathfrak{R}(\mathcal{H}(e)) + 3e \sqrt{(2\log \frac{2}{\delta})/m},
\]

where \( \tilde{L}_\infty(h) \) is the empirical error as in **Definition 2** \( \delta \) is the PAC learning probability as in **Definition 3** \( m \) is the sample size, and \( e \) is an upper bound of the mean square error (MSE) over arbitrary \( m \) testing samples \( x = \{x_i\}^m \sim \mathcal{D} \) after arbitrary \( m \) training samples \( \forall x' = \{x'_i\}^m \sim \mathcal{D} \), defined below as:

\[
\frac{1}{m} \sum_{i=1}^{m} l(h, x_i)^2 \leq e^2, h \in \mathcal{H}(e)
\]

where \( \text{Tr}(\cdot) \) is the training of the data-driven model, and \( \mathcal{H}(e) \) denotes the narrowed hypothesis class bounded by the MSE of \( e^2 \) after training any \( m \) samples. The Rademacher complexity generalization can be intuitively interpreted as follows: The generalization error of a trained hypothesis class \( \mathcal{H}(e) \) has a high probability to be large when: 1) the empirical error (training error) is large (the first part of (8)); 2) the hypothesis class \( \mathcal{H}(e) \) is “complex” (the second part of (8)); 3) the training sample size is small (the third part of (8)). The first part of (8) can be obtained after training. The third part of (8) can be directly calculated by the value of \( e, \delta, \) and \( m \). We will introduce how to evaluate the second part in Section III-C.

Assumption (9) denotes that the MSE is bounded after training arbitrary \( m \) samples. It is more flexible than assuming maximum value of the loss function \( l(h, x_i) \) is bounded in the traditional Rademacher complexity bound [11]. This is reasonable in classification problems yet difficult to be applied in regression problems, because \( l(h, x_i) \) may be extremely large. In our MRC bound, however, one only need to set an upper bound of MSE, which is more applicable in regression problems. We use an iterative strategy to configure the upper bound for MSE, as shown in Section III-B.

The proof of **Theorem 6** is based on two key results. First we show that the empirical error can be bounded by the Rademacher complexity (which is the expectation of the empirical Rademacher complexity) under \( 1 - \delta \) probability as

\[
L(h) \leq \tilde{L}_\infty(h) + 2\mathfrak{R}(\mathcal{H}(e)) + e \sqrt{(2\log \frac{2}{\delta})/m}.
\]

whose proof is primarily based on the use of the modified logarithmic Sobolev inequality from Section 6.4 of [14]. Starting with this inequality, we can derive the bound of the generalization error \( L(h) \) from assumption (9). We then show that the Rademacher complexity can be bounded by the empirical Rademacher complexity under \( 1 - \delta/2 \) probability:

\[
\mathfrak{R}(\mathcal{H}) \leq \tilde{\mathfrak{R}}(\mathcal{H}) + e \sqrt{(2\log \frac{2}{\delta})/m},
\]

which is derived by combining (11) and (10). The full proof is listed in the Appendix.

**Remark 7** (Physical knowledge). The physical knowledge \( P \) narrows the hypothesis space and reduces the Rademacher complexity: \( \tilde{\mathfrak{R}(\mathcal{H} \cap P)} \leq \tilde{\mathfrak{R}}(\mathcal{H}) \). The bound in (8) is also valid for \( \tilde{\mathfrak{R}(\mathcal{H} \cap P)} \).

B. Iteration Strategy

In this section, we implement an iteration strategy for the configuration of the upper bound of the MSE \( e^2 \). The basic idea is to assume an initial \( e \) and narrow the \( e \) and \( L(h) \) through iterations.

1) **Step 1**: Assume a large enough initial \( e \). Set the maximum iteration step \( I \) and the current iteration step \( i = 1 \).

2) **Step 2**: Evaluate the generalization bound \( L(h) \) using **Theorem 6** (equation (8)).

3) **Step 3**: Update \( e \) by \( e^{new} \leftarrow kL(h) \), where \( k \) is a constant factor that represents how tight we can bound the MSE \( e^{new} \) of the next iteration from the mean absolute error (MAE) bound \( L(h) \) of this iteration. See Appendix for the configuration of factor \( k \). If \( e^{new} < e \) and \( i < p \), set \( i \leftarrow i + 1 \) and do **Step 2**. Else, do **Step 4**.

4) **Step 4**: Output the final generalization bound as \( L(h) \).

Finally, we divide the evaluation of \( L(h) \) in equation (8) (in **Step 2**) into three parts: the empirical error, the empirical Rademacher complexity, and the randomness of sample distribution. The iterative framework is shown in Fig 2.

C. Computation of Empirical Rademacher Complexity

To calculate the empirical Rademacher complexity as in **Definition 4**, we generate \( n \) samples of the Rademacher variable vector \( \sigma_j \in \{-1, 1\}^m \) each with \( m \) elements. The empirical Rademacher complexity can thus be calculated using the generated samples as

\[
\hat{\mathfrak{R}}(\mathcal{H}(e) \cap P) \approx \frac{1}{n} \sum_{j=1}^{n} \sup (\sigma_j, x, l)
\]

(12a)
This is a necessary condition of the transformation in (14).

\[(13c)\] ensure that at least one of \(d\) decision variable. The big M related constraints \((15c)\) and the problem.

is non-convex. We adopt the following theorem to convexify

where \(\sigma\) demonstrates in Section IV and Section V.

Fig. 2. Flowchart of modified Rademacher complexity bound evaluation.

\[\sup(\sigma_j, x, h) = \sup_{h \in \mathcal{H}(e) \cap \mathcal{P}} \frac{1}{m} \sum_{i=1}^{m} \sigma_{ij}l(h, x_i),\]

where \(\sigma_{ij}\) denotes the \(i\)th element of the \(j\)th vector of Rademacher variables \(\sigma_j\). Afterwards, we cast the sup in \((12b)\) as a maximization problem:

\[
\begin{align*}
\max_h \sum_{i=1}^{m} \sigma_{ij}l(h, x_i) \\
\sum_{i=1}^{m} |f(x_i) - h(x_i)|^2 \leq me^2 \\
p(x, h) \leq 0,
\end{align*}
\]

\[(13a)\]

\[(13b)\]

\[(13c)\]

where the maximum value of \((13a)\) is \((1/m)\sup(\sigma_j, x, h).

\[(13b)\] denotes the upper bound of MSE as assumed in \((9)\), and \((13c)\) represents the physical constraints. The physical constraints may relate to the samples \(x\) or the parameters of the hypothesis \(h\). Specified formulations of \((13c)\) will be demonstrated in Section IV and Section V.

Then, we cast the absolute value formulations in \((13)\) as a differentiable problem, by introducing complementary auxiliary variables:

\[|f(x_i) - h(x_i)| = d_i^+ + d_i^- \quad f(x_i) - h(x_i) = d_i^+ - d_i^- .\]

Applying the big M method, problem \((13)\) becomes:

\[
\begin{align*}
\max_{h, d_i^+, d_i^-} & \quad \sum_{i=1}^{m} \sigma_{ij} \left( d_i^+ + d_i^- \right) \\
h(x_i) - f(x_i) = d_i^+ - d_i^- , & \forall i \\
0 \leq d_i^+ \leq M u_i , & \forall i \text{ s.t. } \sigma_{ij} = +1 \\
0 \leq d_i^- \leq M (1 - u_i) , & \forall i \text{ s.t. } \sigma_{ij} = +1 \\
\sum_{i=1}^{m} \left( d_i^+ + d_i^- \right)^2 \leq me^2 \\
p(x, h) \leq 0,
\end{align*}
\]

\[(15a)\]

\[(15b)\]

\[(15c)\]

\[(15d)\]

\[(15e)\]

\[(15f)\]

where \(M\) denote the big M value, \(u_i\) denotes the \(i\)th 0-1 decision variable. The big M related constraints \((15c)\) and \((13c)\) ensure that at least one of \(d_i^+\) and \(d_i^-\) should be zero. This is a necessary condition of the transformation in \((14)\). We only need to add the above constraints when \(\sigma_{ij} = +1\). Because when \(\sigma_{ij} = -1\), minimizing \(d_i^+ + d_i^-\) will guarantee no violation of \((15c)\) and \((13c)\) \([23]\). Note that constraint \((15c)\) is non-convex. We adopt the following theorem to convexify the problem.

Proposition 8. Assume after training of \(m\) samples, the MAE

\[\frac{1}{m} \sum_{i=1}^{m} |f(x_i) - h(x_i)| \leq e .\]

Then, the empirical Rademacher complexity under assumption \((16)\) \(\mathcal{R}(\mathcal{H}(e) \cap \mathcal{P})\) is the upper bound of the empirical Rademacher complexity under assumption \((9)\) \(\mathcal{R}(\mathcal{H}(e) \cap \mathcal{P})\):

\[\mathcal{R}(\mathcal{H}(e) \cap \mathcal{P}) \leq \mathcal{R}(\mathcal{H}(e) \cap \mathcal{P}).\]

Proof. Denote \(|f(x_i) - h(x_i)| = d_i\) \(\forall h\) satisfies \((9)\), we have:

\[\frac{1}{m} \sum_{i=1}^{m} d_i \leq \left( \frac{1}{m} \sum_{i=1}^{m} d_i^2 \right)^{1/2} \leq e ,\]

where the first inequality holds by the general means inequality \([24]\), the second inequality is from \((9)\). Thus, any hypothesis \(h\) that satisfies \((9)\) also satisfies \((16)\), which proves \((17)\).

From Proposition 8, we evaluate \(\mathcal{R}(\mathcal{H}(e) \cap \mathcal{P})\) by substituting constraint \((15e)\) to:

\[\sum_{i=1}^{m} (d_i^+ + d_i^-) \leq me .\]

In many applications, \(h(x_i)\) and \(p(x, h)\) in \((15)\) are linear or quadratic corresponding to the parameters of \(h\), thus the numerical evaluation of \(\mathcal{R}(\mathcal{H}(e) \cap \mathcal{P})\) turns into a mixed-integer linear programming (MILP) problem or a mixed-integer quadratically-constrained program (MIQCP) problem, which can be solved by many commercial solvers such as Gurobi and Cplex.

IV. BRANCH FLOW LINEARIZATION

A. Problem Formulation

The branch flow linearization problem searches for an optimal mapping function between the branch flow and the voltage of the connected buses from historical operational data \([1], [25]\). The linearized branch flow function has better performance in terms of computational speed and convergence in power flow applications, such as probabilistic load flow analysis and the network pricing problems \([26]\). For simplicity, we only consider branch flow linearization in this paper, which is the basis process of linearized power flow. The well-known branch flow equations are as follows:

\[
\begin{align*}
P_{ij} &= g_{ij} (v_i^2 - v_i v_j \cos \theta_{ij}) - b_{ij} v_i v_j \sin \theta_{ij} \\
Q_{ij} &= -b_{ij} (v_i^2 - v_i v_j \cos \theta_{ij}) - g_{ij} v_i v_j \sin \theta_{ij},
\end{align*}
\]

where subscript \(i/j\) denote the bus number, \(v_i/v_j\) denote the voltage magnitudes of bus \(i/j\), and \(g_{ij}/b_{ij}, P_{ij}/Q_{ij}\), and \(\theta_{ij}\) denote conductance/susceptance, active/reactive power flow, and voltage angle of branch \((i,j)\), respectively. In this paper, we use the following linearized branch flow formulations:

\[h_{ij}^{bf}(v, \theta) = \alpha_{bf} v_i^2 + \alpha_{bf} v_j^2 + \alpha_{bf} \theta_{ij} + \alpha_{bf} \theta_j + \alpha_{bf},\]

where \(h_{ij}^{bf}(v, \theta)\) denotes the linearized formulation of active or reactive branch flow \(P_{ij}\) or \(Q_{ij}\), and \(\alpha_{bf} \sim \alpha_{bf}\) denote the
parameters of $h_{ij}^{bf}(v, \theta)$. In (21), branch flow is a linearized form with respect to $v^2$ and $\theta$, which is a recommended representation in [25]. The parameters of $\alpha_1^{bf} \sim \alpha_5^{bf}$ are computed from historical operational data by the ordinary least squares (OLS) regression algorithm. Parameters of different systems and different branches are different, to best fit the system and its operational characteristics.

B. Physical Knowledge

From (20) and (21), we can observe that the voltage angle only appears in the form of $\theta_{ij}$. In other words, the coefficient of $\theta_i$ is the negative of the coefficient of $\theta_j$. Thus, we adopt the following constraints as the physical constraints of the problem:

$$-\Delta^{bf} \leq \alpha_1^{bf} + \alpha_4^{bf} \leq \Delta^{bf}, \quad (22)$$

where $\Delta^{bf}$ is a non-negative small value. Furthermore, we can obtain the expressions of $\alpha_1^{bf} \sim \alpha_5^{bf}$ by first order expansion, and thus set the maximum and minimum bounds $B_1^{bf}$ and $B_4^{bf}$ considering the boundary operational conditions [2]:

$$B_1^{bf} \leq \alpha_1^{bf} \leq B_4^{bf}, \quad i = 1 \sim 5. \quad (23)$$

Finally, set (21) as the hypothesis $h$ in (15), and set (22) or (23) as the physical constraints in (15). The evaluation of $\mathcal{R}(\mathcal{H}(e) \cap P)$ then becomes an MILP problem.

C. Experimental Results

We generate the data using Monte Carlo simulation, with the aid of MATPOWER 6.0 [27]. Then, all the data are normalized to the interval $[0, 1]$. The data generation strategy of power system operational data is the same as in [1]. The optimization problem is solved by Gurobi 8.1 with Python interface. We use IEEE 118-bus system in this case study. Set the non-negative small value $\Delta^{bf} = 10^{-2}$ and the number of Rademacher variables in [25] to $n = 10$.

We analyze the generalization error of the reactive flow in Branch #96 which has the largest training error in all branches. The generalization error bounds of three cases under different amount of training data are compared: 1) NonPhys: Without any physical knowledge; 2) Angle: Consider the voltage angle constraint (22); 3) Box: Consider the maximum and minimum parameter bound constraints (23). Fig. 3 shows that the generalization error bound of all the three cases decrease as the training data amount increases.

The addition of physical knowledge significantly decreases the generalization error bounds, especially when the training size is below 700. Furthermore, Box has a more significant effect of reducing the generalization bounds than Angle. As shown in Fig. 3, to obtain the generalization bound of 0.1 p.u., the effect of physical knowledge Angle is equivalent to nearly 50 snapshots of training data, while the effect of Box is equivalent to nearly 100 snapshots. In practice, the above results can be used to design the implementation of physical knowledge. Fig. 3 suggests that Box is far more effective than Angle, and that the physical knowledge has more influence for small training datasets.

We then demonstrate different parts of the generalization error bounds in each iteration step in Fig. 4. The complexity of the data-driven model, the randomness of the sample distribution, and the total generalization error bound decrease through iterations. The total generalization bound difference of NonPhys and Box increases through iterations. At iteration step 1, the difference of the total generalization bounds is small because the initial $e$ is the same so that the randomness of the sample distribution is the same. Then, the difference of the total generalization bounds results in the difference of $e$ in the next iteration step. Therefore, the small difference accumulates through iterations and results in a significant difference in Fig. 4.

V. EXTERNAL NETWORK EQUIVALENT

A. Problem Formulation

In interconnected power systems, the power flow model of external networks can be simplified through an equivalent network representation. Such equivalence is essential for interconnected systems where the information is not shared, and can also reduce the computational complexity of system optimization problems. The equivalence model can be used in a wide range of applications such as contingency analysis, optimal power flow dispatch, and static voltage stability analysis, etc. In this section, we use the model in [2] as shown in Fig. 5, where the border PMU data is used to estimate the parameters of the model.
The model can be formulated as follows:

\[ P_i = -P_{Li} - \sum_{j \neq i} P_{ij} - P_{ie} \]  
\[ Q_i = -Q_{Li} - \sum_{j \neq i} Q_{ij} + b_i \]  
where \( P_i/Q_i, P_{Li}/Q_{Li}, P_{ij}/Q_{ij} \), and \( P_{ie}/Q_{ie} \) denote the active/reactive branch flow of the border bus \( i \) to the internal network, the equivalent active/reactive load of border bus \( i \), the active/reactive branch flow from bus \( i \) to \( j \), and the active/reactive branch flow from bus \( e_i \) to \( i \), respectively. By substituting the branch flow equations (20) into (24), the active/reactive branch flow \( P_i/Q_i \) can be formulated as:

\[ h_{\text{ex}}^e(v, \theta) = \sum_{j \neq i} \left[ \alpha_{ij}^+ (v_i^2 - v_i v_j \cos \theta_{ij}) + \alpha_{ij}^- v_i v_j \sin \theta_{ij} \right] + \alpha_{ex}^+ v_i^2 + \alpha_{ex}^- v_i + \alpha_{ex}^0. \]  
(25)

Similar to the case of branch flow linearization, the parameters \( \alpha_{\text{ex}}^e = [\alpha_{j1}^+, \alpha_{j2}^+, \alpha_{j3}^-, \alpha_{j4}^-, \alpha_{j5}^0] \) can be obtained from historical operational data by OLS algorithm.

The values of \( \alpha_{\text{ex}}^e \) are related to the power system and its operational characteristics. Thus, one can implement physical knowledge to constrain the value of \( \alpha_{\text{ex}}^e \), see [2] for details.

\[ B_{\text{ex}}^\leq \leq \alpha_{\text{ex}}^e \leq B_{\text{ex}}^\geq. \]  
(26)

The above data-driven models are linear regression models. To compare cases under different data-driven models, we also implement the support vector regression (SVR) method to learn the external network model. SVR has shown high accuracy in learning power flow models with appropriate setting of inputs [28]. Note that the aforementioned physical knowledge [26] can only be applied in linear regression method rather than SVR method. For border bus \( i \), we set the input vector as \( x_i = [v_i, v_j, \sin \theta_{ij}, \cos \theta_{ij}] \), where \( j \) represents all other border buses. Given \( m \) snapshots \( x_1^m \ldots x_m^m \), the SVR model can learn the active/reactive branch flow from the following formulation:

\[ h_{\text{ex}}^\text{svr}(x_i) = \sum_{i=k}^m (\alpha_i^+ - \alpha_i^-) K(x_i^k, x_i) + b, \]  
(27)

where \( \alpha_i^+ / \alpha_i^- \), \( b \), and \( K(\cdot) \) are the dual variables in the SVR optimization process, the constant term, and the kernel function, respectively. Note that for simplicity, we only introduce the dual form of the SVR problem. The non-linearity of the SVR comes from the kernel function \( K(\cdot) \). Considering the formulation of power flow equations, the second order polynomial kernel has sufficient richness to learn the power flow model:

\[ K(x_i^k, x_i) = (x_i^k x_i^T + c)^2, \]  
(28)

where \( c \) is a constant term. The parameters \( \alpha_i^+ / \alpha_i^- \) have two characteristics: 1) The values are constrained considering the optimization problem of SVR:

\[ 0 \leq \alpha_i^+ \leq C, 0 \leq \alpha_i^- \leq C, \]  
(29)

where the constant term \( C \) denotes the weight of loss in the primal optimization problem. 2) \( \alpha_i^+ / \alpha_i^- \) are sparse. \( \alpha_i^+ \) is non-zero only when the difference of the real value and the prediction value are larger than a threshold \( \epsilon_{\text{svr}} \): \( y_i - h_{\text{svr}}(x_i) > \epsilon_{\text{svr}} \). Similarly, \( \alpha_i^- \) is non-zero only when \( h_{\text{svr}}(x_i) - y_i > \epsilon_{\text{svr}} \). We adopt the big M method to satisfy the aforementioned two characteristics:

\[ M(u_i^+ - 1) \leq d_i^- - \epsilon_{\text{svr}} \leq M u_i^+ 0 \leq \alpha_i^+ \leq Cu_i^+ \]  
(30a)
\[ M(u_i^- - 1) \leq d_i^+ - \epsilon_{\text{svr}} \leq M u_i^- 0 \leq \alpha_i^- \leq Cu_i^- \]  
(30b)

B. Experimental Results

The experimental setup is the same as in Section IV. Hyper parameters only in this Section are set as: \( C = 0.2, \epsilon_{\text{svr}} = 0.01, \) and \( l = 2 \). We use the IEEE 39-bus system in this case study, with external buses: \#1-\#2, \#25-\#30, and \#37-\#39; border buses: \#3, \#9, and \#17; and internal buses: \#4-\#8, \#10-\#16, \#18-\#24, and \#31-\#36. We generate 500 snapshots of training data, and test the accuracy on 500 newly generated snapshots using the least squares method. The errors of different methods on different border buses are listed in Table I.

| \( P_i, \#3 \) | \( P_i, \#9 \) | \( P_i, \#17 \) | \( Q_i, \#3 \) | \( Q_i, \#9 \) | \( Q_i, \#17 \) |
|---|---|---|---|---|---|
| Errors | 0.0408 | 0.0283 | 0.0534 | 0.0047 | 0.0352 | 0.0070 |

As shown in Table I, the active branch flow of border bus \#17 has the largest testing error. Hence, we evaluate the generalization bound of the active branch flow of border bus \#17.

Three different methods are compared: 1) LR: The linear regression model without any physical knowledge. Set (25) as the hypothesis in (15). 2) LRBox: The linear regression model with physical knowledge. Set (25) as the hypothesis in (15), with the maximum and minimum parameter bound constraints (26) as the physical constraints in (15); 3) SVR: The SVR model. Set (27) as the hypothesis in (15), with constraints (30) added to the problem.

We bound generalization errors of methods LR, LRBox, and SVR under different amount of training data, as shown in Fig 6. An interesting result is that the generalization bound of the linear regression model LR is larger than that of the nonlinear SVR model. This is because without the physical knowledge, the parameters of LR are not constrained. In contrast, the parameters of SVR are constrained by (30). From Definition 4, model LR has more richness to fit random noise.
If \( \phi \) is the active branch flow of Branch #17. The total generalization bounds of LR, LRBox, and SVR under different amount of training data are compared. The bound of LRBox is the lowest among all the methods. The results in Fig. 6 suggest that when physical knowledge of linear regression method is not available (e.g. due to information barriers), SVR has more accurate generalization error bounds; and when physical knowledge of linear regression method is available, LRBox has more accurate generalization error bounds.

VI. CONCLUSION

Our work provides theoretical insights into the error bounds of data-driven models in power grid analysis, accounting for the influence of different data-driven models, physical knowledge, and the amount of training data. We extend the existing theory and propose a new MRC bound, by adopting a new concentration inequality. Our proposed method is theoretically tighter on regression problems. Furthermore, the evaluation of the bound is formulated as a mathematical programming problem, which can consider the effects of physical knowledge in power grid analysis. We conduct two case studies: branch flow linearization and external network equivalent, to demonstrate how our MRC bound can be used to evaluate the performance of different data-driven models. Our work rethinks the design and validation of data-driven models towards more widespread power industry applications. Further research will focus on expanding the applications of the proposed MRC bound method and improving the tightness of the bound.

APPENDIX A

PROOF OF THEOREM 6

A. Proof of inequality (10)

For simplicity, we denote \( \mathcal{H}(m) \) as \( \mathcal{H} \) in the Appendix. We firstly restate a theorem from Section 6.4 of [14].

Theorem 9 (Bounded variance inequality). Given function \( \phi : \mathcal{X}^m \rightarrow \mathbb{R} \), let:

\[
\sigma_i = |\phi(x_1, \ldots, x_i, \ldots, x_m) - \phi(x_1, \ldots, x_i', \ldots, x_m)|.
\]

If \( \phi \) satisfies: \( \sum_{i=1}^{m} \sigma_i^2 \leq v \), then for all \( t \leq 0 \):

\[
\Pr[|\phi(x_1, \ldots, x_m) - \mathbb{E}[\phi(x_1, \ldots, x_m)]| \geq t] \leq e^{-t^2/2v}. \tag{32}
\]

Then we introduce the following Lemma to discover the relationship between \( L(h) \) and \( \hat{L}_x(h) \):

Lemma 10. Set \( \phi \) as the supreme delta value of the generalization error and the empirical error:

\[
\phi(x_1, \ldots, x_m) = \sup_{h \in \mathcal{H}} \left( L(h) - \hat{L}_x(h) \right) \tag{33a}
\]

\[
= \sup_{h \in \mathcal{H}} \left( L(h) - \frac{1}{m} \sum_{i=1}^{m} |f(x_i) - h(x_i)| \right) \tag{33b}
\]

Then, under the assumption in (9), for all \( \delta \in (0, 1) \), with probability at least \( 1 - \delta \), the following holds:

\[
\phi(x_1, \ldots, x_m) \leq \mathbb{E}_{x \sim \mathcal{D}}[\phi(x_1, \ldots, x_m)] + \epsilon \sqrt{\frac{2 \log 2 \delta}{m}}. \tag{34}
\]

Proof. From the definition of (31) and (33b), we have:

\[
c_i = (1/m) |f(x_i) - h(x_i)|. \tag{35}
\]

From assumption (9), we have:

\[
\sum_{i=1}^{m} c_i^2 = \frac{1}{m^2} \sum_{i=1}^{m} |f(x_i) - h(x_i)|^2 \leq \frac{e^2}{m} = v. \tag{36}
\]

Apply Theorem 9 with \( v = e^2/m \) and \( t = \epsilon \sqrt{2 \log(2/\delta)/m} \) and finish the proof. \( \square \)

Then, from the definition of (33), we have:

\[
\mathbb{E}_{x \sim \mathcal{D}}[\phi(x_1, \ldots, x_m)] = \mathbb{E}_{x \sim \mathcal{D}} \left[ \sup_{h \in \mathcal{H}} \left( L(h) - \hat{L}_x(h) \right) \right] \tag{37a}
\]

\[
= \mathbb{E}_{x \sim \mathcal{D}} \left[ \sup_{h \in \mathcal{H}, x' \sim \mathcal{D}} \left( \hat{L}_{x'}(h) - \hat{L}_x(h) \right) \right] \tag{37b}
\]

\[
= \mathbb{E}_{x \sim \mathcal{D}} \left[ \sup_{h \in \mathcal{H}, x' \sim \mathcal{D}} \left( \hat{L}_{x'}(h) - \hat{L}_x(h) \right) \right] \tag{37c}
\]

\[
\leq \mathbb{E}_{x, x' \sim \mathcal{D}, \sigma} \left[ \sup_{h \in \mathcal{H}} \left( \hat{L}_{x'}(h) - \hat{L}_x(h) \right) \right], \tag{37d}
\]

where (37b) denotes the fact that generalization error is the expectation of empirical error over \( x' \sim \mathcal{D} \); (37c) uses the fact that sample \( x \) and \( x' \) are independent; and (37d) holds by the famous Jensen’s inequality, using the convexity of supremum function.

We build sample set \( \hat{x} \) and \( \hat{x}' \) from \( x \) and \( x' \), by randomly swapping samples between \( x \) and \( x' \) with the probability of 0.5. Denote \( x_i \in x \) and \( x'_i \in x' \). Recall the definition of Rademacher variables \( \sigma \) in Definition 4, we have:

\[
\hat{L}_{x'}(h) - \hat{L}_x(h) = \frac{1}{m} \sum_{i=1}^{m} \sigma_i (l(h, x'_i) - l(h, x_i)). \tag{38}
\]

Since \( x, x', \hat{x}, \) and \( \hat{x}' \) are from same distribution, we have:

\[
\mathbb{E}_{x, x' \sim \mathcal{D}, \sigma} \left[ \frac{1}{m} \sup_{h \in \mathcal{H}} \left( \sum_{i=1}^{m} \sigma_i (l(h, x'_i) - l(h, x_i)) \right) \right] \tag{39a}
\]

\[
= \mathbb{E}_{x, x' \sim \mathcal{D}, \sigma} \left[ \frac{1}{m} \sup_{h \in \mathcal{H}} \left( \sum_{i=1}^{m} \sigma_i (l(h, x'_i) - l(h, x_i)) \right) \right] \tag{39b}
\]
\[ \sum_{i=1}^{m} \sigma_i l(h, x_i) \leq E_{x \sim D, \sigma} \left[ \frac{1}{m} \sum_{h \in H} \sigma_i l(h, x_i) \right] + E_{x \sim D, \sigma} \left[ \frac{1}{m} \sum_{h \in H} \sigma_i l(h, x_i) \right] \]

\[ = 2 E_{x \sim D, \sigma} \left[ \frac{1}{m} \sum_{h \in H} \sigma_i l(h, x_i) \right] = 2\delta(H), \quad (39c) \]

where (39c) comes from (38); (39d) holds by the sub-additivity of the supremum function \( \max(x+y) \leq \max(x) + \max(y) \);

(39d) holds by Definition 4. Finally, the proof is finished by combining Lemma 10 and (37)–(39):

\[ L(h) - L^* (h) \leq \sup_{h \in H} \left( L(h) - L^*(h) \right) \leq 2\delta(H) + \epsilon \sqrt{2 \log \frac{2}{\delta}/m}. \quad (40a) \]

\[ \sum_{i=1}^{m} \sigma_i l(h, x_i)^2 \leq k \left( \frac{1}{m} \sum_{i=1}^{m} l(h, x_i) \right)^{1/2} \quad (41) \]

In practice, \( k \) can be obtained by assuming a certain distribution of the error and then sampling on this distribution. For example, we assume the error \( f(x_i) - h(x_i) \) follows a Gaussian distribution in the case study. Then we sample the ratio of the square root mean to the arithmetic mean of \( l(h, x_i) \) and find that the value of \( k = 1.4 \) can bound the ratio under Gaussian assumption. One can also apply different assumptions on the error distribution to get the value of \( k \).

### Appendix B

#### Configuration of \( k \) in Step 3

The factor \( k \) is used to update the bound of MSE by \( e^{\text{new}} \leftarrow k L(h) \), where \( e^{\text{new}} \) is the bound of MSE and \( L(h) \) is the bound of MAE. The \( e^{\text{new}} \) is used to calculate the empirical Rademacher complexity \( \delta(H) \) and the sample uncertainty \( \epsilon^2 \sqrt{2 \log(2/\delta)/m} \). For the update of \( e^{\text{new}} \), \( k \) is determined by the following inequality, indicating that the square root mean is smaller than the arithmetic mean times \( k \).

\[ \left( \frac{1}{m} \sum_{i=1}^{m} l(h, x_i)^2 \right)^{1/2} \leq k \left( \frac{1}{m} \sum_{i=1}^{m} l(h, x_i) \right) \quad (41) \]

In practice, \( k \) can be obtained by assuming a certain distribution of the error and then sampling on this distribution. For example, we assume the error \( f(x_i) - h(x_i) \) follows a Gaussian distribution in the case study. Then we sample the ratio of the square root mean to the arithmetic mean of \( l(h, x_i) \) and find that the value of \( k = 1.4 \) can bound the ratio under Gaussian assumption. One can also apply different assumptions on the error distribution to get the value of \( k \).

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