Abstract—This work revisits the joint beamforming (BF) and antenna selection (AS) problem, as well as its robust beamforming (RBF) version under imperfect channel state information (CSI). Such problems arise in scenarios where the number of the radio frequency (RF) chains is smaller than that of the antenna elements at the transmitter, which has become a critical consideration in the era of large-scale arrays. The joint (R)BF&AS problem is a mixed integer and nonlinear program, and thus finding optimal solutions is often costly, if not outright impossible. The vast majority of the prior works tackled these problems using continuous optimization-based approximations—yet these approximations do not ensure optimality or even feasibility of the solutions. The main contribution of this work is threefold. First, an effective branch and bound (B&B) framework for solving the problems of interest is proposed. Leveraging existing BF and RBF solvers, it is shown that the B&B framework guarantees global optimality of the considered problems. Second, to expedite the potentially costly B&B algorithm, a machine learning (ML)-based scheme is proposed to help skip intermediate states of the B&B search tree. The learning model features a graph neural network (GNN)-based design that is resilient to a commonly encountered challenge in wireless communications, namely, the change of problem size (e.g., the number of users) across the training and test stages. Third, comprehensive performance characterizations are presented, showing that the GNN-based method retains the global optimality of B&B with provably reduced complexity, under reasonable conditions. Numerical simulations also show that the ML-based acceleration can often achieve an order-of-magnitude speedup relative to B&B.

Index Terms—Beamforming, Antenna Selection, Global Optimum, Machine Learning, Graph Neural Networks

Beamforming lies at the heart of transmit signal design of multiple antenna systems. In the past decade, a plethora of beamforming algorithms have been proposed under various scenarios; see, e.g., [1]–[7]. Among the most challenging scenarios is the joint beamforming and antenna selection (BF&AS) problem (see, e.g., [5]–[7]), which often arises for practical considerations. For example, in downlink transmission, a base station (BS) may have a limited number of radio frequency (RF) chains—due to the RF chain’s costly nature [8]. The number of the RF chains may be (much) smaller than that of the antennas. Since the RF chains are responsible for encoding/modulating the transmit information, this limits the number of antennas that can be operated simultaneously in practice. To avail the advantages of multi-antenna systems, a proper antenna selection strategy is needed to be part of the transmit waveform design. In addition, when using a subset of the antennas can serve the users well, it may be more energy-economical to not activate all the antenna elements—which may be important for the sustainability and battery life of moving base stations and relays, e.g., unmanned aerial vehicle (UAV)-carried antenna arrays.

Jointly designing the beamformers and selecting antennas is a mixed integer nonlinear program, which is known to be NP-hard [9]. The vast majority of the literature tackles this problem using continuous programming-based approximations. For example, [5]–[7], [10] used convex and nonconvex group sparsity-promoting regularization to encourage turning off antenna elements. However, the continuous approximations are often NP-hard problems as well (especially when the sparsity promotion is done via nonconvex quasi-norms as in [5]), and thus it is unclear if they can solve the problem of interest optimally. In addition, works using greedy methods to assist antenna selection also exist (see, e.g., [9], [11]–[13]), which often offer better efficiency relative to continuous optimization. But the optimality of joint (R)BF&AS is still not addressed in these works.

In recent years, machine learning (ML) approaches are employed to handle the joint BF and AS problem. In [14], a supervised learning approach was proposed. The basic idea is to use a continuous optimization algorithm to produce training pairs (i.e., channel matrices and sparse beamformers), and then learn a neural network-based regression function using such pairs. Similar ideas were used in [15], [16] with various settings. This type of approach in essence mimics the training pair-generating algorithms at best, and thus the optimality of their solutions is again not guaranteed.

Contributions. In this work, we revisit the joint BF and AS and its extension under imperfect CSI, namely, the joint robust beamforming (RBF) and AS problem. We are interested in the unicast BF and RBF formulations in [2] and [17], respectively. The goal is to satisfy the users’ quality-of-service (QoS) constraints while minimizing the power consumption, with only a subset of the antenna elements activated. Our detailed contributions are as follows:

- Optimal Joint (R)BF&AS via Branch and Bound. Our first contribution lies in an optimal computational framework to attain the global optimal solutions to the joint (R)BF&AS problems. To this end, we propose a Branch and Bound (B&B)
[18], [19] framework that is tailored for the problems of interest. Our design leverages problem structures of unicast BF and RBF, which allows for branching only on a subset of the optimization variables—thereby having reduced complexity and being effective. Unlike continuous optimization-based approximations in [5]–[7], [10] whose solutions are often sub-optimal or infeasible, the proposed B&B is guaranteed to return an optimal solution.

- **An ML-based Acceleration Scheme.** B&B is known for its relatively weak scalability. To improve efficiency, an idea from the ML community (see, e.g., [20], [21]) is to learn a binary classifier offline using multiple problem instances. The classifier determines whether or not any encountered intermediate state of the B&B algorithm could be “skipped”, as skipping these states saves computational resources and expedites the B&B process. Generic ML learning functions (e.g., support vector machines (SVM)) used in existing works like [20], [22] do not reflect the problem structure in wireless communications. In this work, we propose a graph neural network (GNN) [23] based learning function designed to exploit the physics of the (R)BF problem—which offers an enhanced classification accuracy. More importantly, the GNN is agnostic to the change of scenarios (e.g., problem size) during training and testing. This feature is designed to meet the need of wireless communication systems, as the number of users served by a base station could change quickly in practice.

- **Theoretical Understanding.** We present comprehensive performance characterizations for the proposed approaches. In particular, we show that the ML-based acceleration retains the global optimality of the B&B procedure with high probability, under reasonable conditions. ML-based B&B acceleration has limited theoretical studies, and the results were developed under often overly ideal settings (e.g., convex classifier) [20], [24]. There is a lack of understanding of the impacts of key factors such as nonconvexity, limited training samples, and the employed ML model’s structure. Our analysis takes into consideration of key aspects such as the nonconvexity of the GNN learning process, the GNN’s structure and complexity, the GNN’s function approximation error, and the amount of available samples. As a consequence, the analysis offers insights to reveal key trade-offs in practice.

**Related Works.** B&B was proposed for beamforming problems in [25], [26], and antenna selection problems in [27]–[29]. Particularly, the work in [25] considered single group multicast beamforming problem, the work in [28] considered a joint power allocation and antenna selection problem, the work in [27] considered antenna selection-assisted rate maximization in wiretap channels, and [29] considered receive antenna selection for sum rate maximization. However these are different from the QoS-constrained downlink transmit beamforming formulation considered in our work, which requires new B&B designs. ML-based B&B acceleration so far has been mostly used for mixed integer and linear programs (MILPs) in the ML community, e.g., [20], [30], where the B&B design is standard. Such methods have also been adopted in wireless communications in [22], [31] where resource allocation tasks are framed as mixed integer and nonlinear programs (MINPs).

However, the joint (R)BF&AS problem has not been considered. In addition, comprehensive theoretical understanding to such ML-acceleration procedures has been elusive.

**Notation:** \( x, x \) and \( X \) denote a scalar, a vector, and a matrix, respectively. \( x_n \) denotes the \( n \)th column of \( X \). We use the matlab notation \( X(n,:) \) to denote the \( n \)th row of \( X \). \( |N| \) denotes the set \{1, 2, ..., \( N \)\}. \( \|x\|_2, \|x\|_\infty, \|X\|_2, \|X\|_F, \|X\|_{row=0} \) denote the vector \( \ell_2 \) norm, vector \( \ell_\infty \) norm, matrix spectral norm, matrix Frobenius norm, and the number of non-zero rows in the matrix, respectively. \( Tr(X) \), \( X^H \), and \( X^T \) denote the trace, hermitian, and transpose of \( X \). \( |X| \) denotes the cardinality of the set \( X \). \( E[\cdot] \) denotes the expectation operator. \( X \succeq 0 \) denotes that \( X \) is positive semi-definite matrix. \( X(S,:) \) with \( S \subseteq \{1, 2, \ldots, \|N|\} \) denotes the submatrix of \( X \in \mathbb{C}^{N\times M} \) containing only the rows of \( X \) contained in the set \( S \). \( X_{-n} \) denotes the submatrix of \( X \) with the \( n \)th column removed. \( f(\cdot) \) is \( C \)-Lipschitz continuous iff \( \|f(x) - f(y)\|_2 \leq C\|x - y\|_2 \).

**I. Background**

Consider a classic single-cell downlink communication scenario where the base station (BS) has \( N \) antennas [2], [17]. The BS serves \( M \) single antenna users. Suppose that the BS has \( L \) RF chains where \( L < N \). This limits the maximal number of active antenna elements to \( L \). Denote \( w_m \in \mathbb{C}^N \) as the beamforming vector for serving user \( m \). The message signal for user \( m \) is represented by \( s_m(t) \). Given the channel \( h_m \in \mathbb{C}^N \) between the BS and user \( m \), the signal received by user \( m \) can be expressed as follows:

\[
y_m(t) = h_m^H w_m s_m(t) + \sum_{\ell \neq m} h_m^H w_\ell s_\ell(t) + n_m,
\]

where \( n_m \) is zero-mean circular symmetric white Gaussian noise with variance \( \sigma_n^2 \). Assume w.l.o.g. that \( \{s_m(t)\}_{M=1} \) are mutually uncorrelated and temporally white with zero-mean and unit-variance. Then, the total transmission power is given by \( \sum_{m=1}^M \|w_m\|^2 := \|W\|_F^2 \), where \( W = [w_1, \ldots, w_M] \). The signal to interference and noise ratio (SINR) at the \( m \)th receiver is expressed as:

\[
\text{SINR}_m = \frac{\|w_m^H h_m\|^2}{\sum_{\ell \neq m} |w_\ell^H h_m|^2 + \sigma_n^2}.
\]

**A. Beamforming and SOCP**

One of the most popular formulations for beamforming is the so-called QoS formulation [32]–[34] that tries to maintain a pre-specified SINR level for all users. When \( h_m \) is known, the BF problem can be formulated as follows:

\[
\text{minimize } \|W\|_F^2 \tag{2a} \\
\text{subject to } \sum_{\ell \neq m} |w_\ell^H h_m|^2 + \sigma_n^2 \geq \gamma_m, \quad m \in [M]. \tag{2b}
\]

Problem (2) appears to be nonconvex, but it can be recast as a second-order cone program (SOCP):
Lemma 1 ([35]). Eq. (2b) can be equivalently written as a second-order cone constraint:

\[
\frac{1}{\sqrt{\gamma_m}} \Re(w_m^H h_m) \geq \sqrt{\sum_{\ell \neq m} |w_{\ell}^H h_m|^2 + 1},
\]

for all \( m \in [M] \). Therefore, any algorithm for solving SOCP can be used to solve (2) optimally.

B. Robust Beamforming and SDR

When the BS only has imperfect CSI, the following worst-case RBF formulation is often considered [17]:

\[
\begin{align*}
\text{minimize} & \quad \|W\|_F^2, \\
\text{subject to} & \quad \min_{\mathcal{U}_m} \frac{|w_m^H h_m|^2}{\sum_{\ell \neq m} |w_{\ell}^H h_m|^2 + \sigma_m^2} \geq \gamma_m, \\
& \quad \forall m \in [M],
\end{align*}
\]

(4b)

where \( \mathcal{U}_m := \{ h_m + e_m \mid \|e_m\|_2 \leq \varepsilon_m \} \), \( h_m \) is the approximate channel vector available at the BS, and \( \varepsilon_m \) is the bound on the approximation error. Problem 4 cannot be directly converted to a convex program as in the perfect CSI case (cf. Lemma 1). However, Problem (4) can be tackled by a convex relaxation technique, namely, semidefinite relaxation (SDR) [36]. Let \( W_m := w_m w_m^H \). Then the SDR of (4) is given by

\[
\begin{align*}
\text{minimize} & \quad \sum_{i=1}^M \text{Tr}(W_m) \\
\text{subject to} & \quad \min_{\mathcal{U}_m} \frac{\tilde{h}_m^H W_m \tilde{h}_m}{\sum_{j \neq m} \tilde{h}_m^H W_j \tilde{h}_m + \sigma_m^2} \geq \gamma_m, \\
&W_m \succeq 0, \quad \forall m \in [M].
\end{align*}
\]

(5b)

Note that (5) and (4) are equivalent if the constraint \( W_m = w_m w_m^H \) (or, \( \text{rank}(W_m) = 1 \)) has not been relaxed. Problem (5) can be further re-expressed as a standard semidefinite program (SDP) using the S-Lemma; see details in [17]. Interestingly, this relaxation procedure turns out to be tight under reasonable conditions:

Lemma 2 ([17, Theorem 1]). Suppose that Problem (4) is feasible. Let \( \Pi_m := I - H_m (H_m^H H_m)^{-1} H_m^H \) be the orthogonal complement projector of \( H_m \). If

\[
\frac{\|\Pi_m h_m\|_2^2}{\varepsilon_m^2} > 1 + M + (M - \frac{1}{M}) \gamma_m, \forall m,
\]

then the optimal solution of (4) can be obtained using SDR.

The condition in (6) means that if the downlink channels associated with different users are sufficiently different, then the SDR is tight.

C. Joint (R)BF&AS: Existing Approaches

In this work, we consider the joint (R)BF&AS problem:

\[
\begin{align*}
\text{minimize} & \quad \|W\|_F^2, \\
\text{subject to} & \quad C(w_m, h_m, \varepsilon_m, \sigma_m) \geq \gamma_m, \\
& \quad \|W\|_{\text{row}-0} \leq L.
\end{align*}
\]

(7c)

where the row-0 function \( \| \cdot \|_{\text{row}-0} \) counts the number of nonzero rows in \( W \) and

\[
C(w_m, h_m, \varepsilon_m, \sigma_m) := \left\{ \begin{array}{ll}
\sum_{\ell \neq m} |w_{\ell}^H h_m|^2 + \sigma_m^2, & \text{if BF is considered}, \\
\min_{\mathcal{U}_m} \sum_{\ell \neq m} |w_{\ell}^H h_m|^2 + \sigma_m^2, & \text{if RBF is considered}.
\end{array} \right.
\]

Problem (7) is a non-convex combinatorial problem, and it is NP-hard [37]. In the literature, Problem (7) and its variants are often handled by continuous approximation. For example, a representative continuous approximation technique was used in [5] for handling the multicast BF&AS problem. Using the same idea for (7), one can recast the problem as a regularized formulation as follows:

\[
\begin{align*}
\text{minimize} & \quad \|W\|_F^2 + \lambda \|W\|_{\text{row}-0} \\
\text{subject to} & \quad C(w_m, h_m, \varepsilon_m, \sigma_m) \geq \gamma_m, \quad m \in [M].
\end{align*}
\]

(8)

Following the idea in [5], the row-0 function can be approximated by an \( l_{\infty,1} \) norm, i.e., \( \|W\|_{\text{row}-0} \approx \sum_{n=1}^N \|W(n,:)\|_{\infty} \) and its nonconvex counterpart \( \|W\|_{\text{row}-0} \approx \sum_{n=1}^N \log ((\|W(n,:)\|_{\infty} + \varepsilon)\|) \) [38]. Similar ideas were used in [10]. Such continuous approximations allow the use of standard nonlinear program techniques to tackle (8). However, as mentioned, these methods do not provide any optimality guarantees. In addition, the feasibility of \( \|W\|_{\text{row}-0} \leq L \) is often not met by the approximate solutions.

More recently, a number of learning-based approaches are proposed to tackle the joint (R)BF&AS problem; see, e.g., [14], [39], [40]. In [14], a multicast version of (7) was considered. There, an existing joint multicast BF&AS algorithm (e.g., the continuous approximation algorithm in [5]) was used to generate “training pairs” by simulating a large number of problem instances:

\[
\{ H_t, \bar{W}_t \}_{t=1}^T
\]

where \( t \) is the instance index, \( \bar{W}_t \) is a (row-sparse) solution produced by the training-pair generating algorithm. Then, a deep neural network (DNN) \( f_\theta(H) \) is trained via

\[
\hat{\theta} \leftarrow \arg \min_\theta \frac{1}{T} \sum_{t=1}^T \ell(\hat{W}_t, f_\theta(H_t)),
\]

(9)

where \( \theta \) represents the parameters of the DNN and \( \ell(x, y) \) measures the divergence between \( x \) and \( y \). When a new \( H \) is seen in the test stage, one can use the learned DNN to predict the solution, i.e., \( \hat{W} = f_{\hat{\theta}}(H) \). Finally, antennas corresponding to the \( L \) largest \( \|\hat{W}(n,:)\|_2 \)'s are selected. This “supervised learning” idea is similar to a line of work in deep learning based wireless system design; see, e.g., [41], [42]. Notably, it cannot exceed the performance of the algorithm that produces the training pairs or ensure producing a row sparse
solution in the test stage. Other deep learning-based ideas were seen in [16], [39], [40], [43] using either supervised learning or unsupervised learning variants, but similar challenges remain.

II. OPTIMAL JOINT (R)BF&AS VIA B&B

A natural idea for solving hard optimization problems is to employ a global optimization technique, e.g., the B&B procedure [18], [19], [44]. Designing a practically working B&B algorithm is often an art—it normally involves judicious exploitation of problem structures. That is, not every hard problem enjoys an efficient B&B algorithm. Nonetheless, as we will see, the special properties of BF and RBF allows for an effective B&B design.

A. Preliminaries of B&B

We follow the notations from the tutorial in [44] to give a brief overview of B&B’s design principles. Consider a nonconvex problem

\[
\begin{align*}
\text{minimize } & f(x) \\
\text{subject to } & x \in X.
\end{align*}
\]

(10a)

(10b)

where both the objective function and the constraint can be nonconvex. Suppose that there is a partition of the space \(X = \mathcal{X}_1 \cup \ldots \cup \mathcal{X}_S\), and that lower and upper bounds of \(f(x)\) over each \(\mathcal{X}_i\) is easier to find (relative to directly solving (10)). Let \(\Phi_{lb}(\mathcal{X}_i)\) and \(\Phi_{ub}(\mathcal{X}_i)\) be the algorithms that return lower and upper bounds of the optimal solution of (10) over the set \(\mathcal{X}_i\), respectively. Then, the following holds:

\[
\min_{1 \leq i \leq S} \Phi_{lb}(\mathcal{X}_i) \leq \Phi(\mathcal{X}) \leq \min_{1 \leq i \leq S} \Phi_{ub}(\mathcal{X}_i). \tag{11}
\]

where \(\Phi(\mathcal{X})\) represents the optimal solution of (10) over the feasible region \(\mathcal{X}\). A premise of the success of B&B is that one could find a partition \(\mathcal{X}_i\) for \(i = 1, \ldots, S\) and a pair of functions \(\Phi_{lb}\) and \(\Phi_{ub}\) which can make the following hold:

\[
\min_{1 \leq i \leq S} \Phi_{ub}(\mathcal{X}_i) - \Phi_{lb}(\mathcal{X}_i) \leq \epsilon \tag{12}
\]

where \(\epsilon > 0\) is a pre-specified error tolerance parameter.

The effectiveness of B&B relies on two key factors. First, the design of the lower and upper bounding algorithms represented by \(\Phi_{lb}(\mathcal{X}_i)\) and \(\Phi_{ub}(\mathcal{X}_i)\), respectively, plays a central role. Second, the way of partitioning the space \(X\) also matters. It often requires a problem-specific way to progressively and judiciously partition the constraint set \(X\) (usually from rough to fine-grid), so that the difference in (12) could shrink quicker than exhaustive search. Meeting either of the design requirements is not necessarily easy. Moreover, the key designs in B&B algorithms (e.g., the \(X\) partition strategies) are highly problem-dependent; that is, there is hardly a “standard recipe” for B&B algorithm design.

B. Proposed B&B for Joint (R)BF&AS

Problem (7) involves optimization in discrete and continuous spaces simultaneously. Designing a B&B algorithm for such problems can be difficult due to the large search space. However, the special structure of (R)BF in (7) allows us to bypass the continuous (beamforming) part when branching the feasible space.

Fig. 1. Illustration of B&B tree for problem (7). Here, \(n_i \in \mathbb{N}\) are the branching variables selected at each node.

1) B&B Tree Construction: We illustrate the idea of systematically partitioning the feasible region of Problem (7) in Fig. 1. Here, \(N_i^{(l)}\) denotes the feasible region corresponding to the \(i\)th node at the \(l\)th level. In the sequel, we will use the term “node” and the associated feasible region interchangeably. The root is denoted as \(N^{(0)}\), and we have

\[
N^{(0)} = \{W \mid W \text{satisfies (7b), (7c)}\}.
\]

In the first level, the region represented by the root node is split into two regions represented by two child nodes, namely,

\[
N_1^{(1)} = \{W \mid W(n_1,:) = 0, W \text{satisfies (7b), (7c)}\},
\]

\[
N_2^{(1)} = \{W \mid W(n_1,:) \in C^M, W \text{satisfies (7b), (7c)}\}.
\]

where \(n_1 \in \mathbb{N}\) is an antenna index selected by a certain criterion (e.g., via random sampling). Up to the first level of the tree, the status (“include (activate)” or “exclude (shut down)”) of all antennas other than antenna \(n_1\) have not been decided.

Note that the nodes in the B&B tree could constitute a partition in various forms. For example, for nodes in the same level, we have

\[
N_1^{(l)} \cup \ldots \cup N_S^{(l)} = N^{(0)};
\]

where \(S = 2^l\) is the number of nodes in the \(l\)th level of the tree. In addition, we have

\[
N_1^{(l)} = N_{s_1}^{(l+1)} \cup N_{s_2}^{(l+1)}, \quad \text{where } s_1 := 2(s - 1) + 1 \quad \text{and } s_2 := 2(s - 1) + 2
\]

represents the left and right children developed from \(N_s^{(l)}\) in the full tree. In fact, the children of \(N_s^{(l)}\) in any level and \(N_{s_1}^{(l)}\) also present a partition of the root node, where \(N_{s_2}^{(l)}\) is the union of \(N_1^{(l)}, \ldots, N_{s_2}^{(l)}\) with \(N_s^{(l)}\) excluded.

The B&B algorithm starts from the first level to compute lower and upper bounds of (7) over the node-defined regions. Then, the B&B algorithm picks a node to “branch”, i.e., to further partition, according to a certain heuristic-based metric; see [18]. Going deeper in the tree towards the final leaves will allow us to progressively decide which antennas to activate or shut off. Let \(t\) denote the iteration index of the B&B algorithm, where an iteration corresponds to a branching (partitioning a node) operation. Use \(P(t)\) to denote the collection of \((s, l)\)
Lemma 3. procedure for solved for all nodes in the B&B tree. It also helps derive a \[ \ell \] solving the following relaxation of (14):

\[ N \]

\[ N \]

\[ s \] have been activated and shut down at node \( B \) reaching the stopping criterion in (12). The hope is that one would not need to visit all nodes of tree before reaching the stopping criterion in (12).

2) Lower and Upper Bounds: In order to compute \( \Phi_{lb}(N_s^{(t)}) \) and \( \Phi_{ub}(N_s^{(t)}) \), let us define \( A_s^{(t)} \subseteq [N] \) and \( B_s^{(t)} \subseteq [N]\backslash A_s^{(t)} \) to be the index sets of the antennas that have been activated and shut down at node \( s \) in level \( t \), respectively. Note that \( A_s^{(t)} \cup B_s^{(t)} \subseteq [N] \) constitute the set of decided antennas at the node. Then, finding the upper and lower bounds of \( \| W \|_F^2 \) at this node amounts to finding those of the following optimization problem:

\[
\begin{align*}
\text{minimize} & \quad \| W \|_F^2 \\
\text{subject to} & \quad C(w_m, h_m, e_m, \sigma_m) \geq \gamma_m, \forall m, \\
& \quad W(n, :) = 0, \quad \forall n \in B_s^{(t)}, \\
& \quad \| W \|_F \leq L, \quad n \in [N].
\end{align*}
\]

(14)

For any given node \( N_s^{(t)} \), the lower bound can be obtained by solving the following relaxation of (14):

\[
\begin{align*}
\Phi_{lb}(N_s^{(t)}) &= \text{minimize} \quad \| W \|_F^2 \\
\text{subject to} & \quad C(w_m, h_m, e_m, \sigma_m) \geq \gamma_m, \forall m, \\
& \quad W(n, :) = 0, \quad \forall n \in B_s^{(t)},
\end{align*}
\]

(15a)

where we have dropped \( \| W \|_{row-0} \leq L \).

In the following lemma, we show that (15) can be optimally solved for all nodes in the B&B tree. It also helps derive a procedure for \( \Phi_{lb}(\cdot) \).

Lemma 3. Regarding (15), the following hold:

(a) Consider the BF case where perfect CSI is given. Then, (15) can be optimally solved by using SOCP.

(b) Consider the RBF case where imperfect CSI is given. Assume that

\[
\frac{\| \Pi_m \tilde{h}_m \|_2^2}{\varepsilon_m^2} > 1 + \frac{M-1}{M} \gamma_m, \forall m,
\]

(16)

where \( \Pi_m := I - \tilde{H}_m (\tilde{H}_m^H \tilde{H}_m)^{-1} \tilde{H}_m^H \), holds for \( \tilde{H} \in \{ H(S, :)|\forall S \subseteq [N], |S| \geq L \} \). Then, Problem (15) can be optimally solved using SDR.

(c) Under the same conditions of (a) and (b), solving the following gives a valid upper bound of (14) under the BF and RBF cases, respectively:

\[
\begin{align*}
\Phi_{ub}(N_s^{(t)}) &= \text{minimize} \quad \| W \|_F^2 \\
\text{subject to} & \quad C(w_m, h_m, e_m, \sigma_m) \geq \gamma_m, \forall m, \\
& \quad W(n, :) = 0, \quad \forall n \in \tilde{B}_s^{(t)},
\end{align*}
\]

(17a)

where \( \tilde{B}_s^{(t)} \subseteq C_s^{(t)} \cup B_s^{(t)} \) represents the set of \( N - L \) antennas to be excluded, and \( C_s^{(t)} \subseteq [N]\backslash (A_s^{(t)} \cup \tilde{B}_s^{(t)}) \) is the index set of undecided antennas that have been assigned the minimum power in the solution of (15).

The proof of Lemma 3 is relegated to Appendix B.

3) Node Selection and Branching: After (15) and (17) are computed in iteration \( t \), \( \ell_G^{(t+1)} \) and \( \epsilon_G^{(t+1)} \) are updated. If the stopping criterion \( \epsilon_G^{(t)} - \ell_G^{(t)} \leq \varepsilon \) is not met, one needs to pick a node in \( \mathcal{P}^{(t)} \) to further partition. To this end, we employ the “lowest lower bound first” principle that is often used in the literature [18]. To be specific, we pick a non-leaf node \( N_s^{(t+1)} \) such that

\[ (\ell, s) \in \arg \min_{(\ell, s) \in \mathcal{P}^{(t)}} \Phi_{lb}(N_s^{(t)}) \]

(18)

where \( S_{leaf} := \{ (\ell, s) : |A_s^{(\ell)}| = L, |B_s^{(\ell)}| = N - L \} \) is the set of leaf nodes. To partition the region \( N_s^{(t+1)} \), we need to pick an undecided antenna and decide whether to include or exclude it in our solution. We select the antenna that has been assigned the largest power among the undecided antennas in iteration \( t \), i.e.,

\[ n^* = \arg \max_{i \in [N]\backslash (A_s^{(t)} \cup B_s^{(t)})} \| W_{s^{(t)}(i, :)\}} \|_2^2 \]

(19)

where \( W_{s^{(t)}(i, :)\}} \) is the minimum power in the solution of (15) at \( N_s^{(t)} \). Then, \( n^* \) is used to partition \( N_s^{(t)} \) into two child nodes (i.e., excluding and including antenna \( n^* \) on top of the decided antennas in \( N_s^{(t)} \)). The associated include/exclude sets in the child nodes, \( N_s^{(t+1)} \), \( i \in \{1, 2\} \), are updated as follows:

\[ B_s^{(t+1)} = B_s^{(t)} \cup \{ n^* \}, \quad A_s^{(t+1)} = A_s^{(t)}, \]

(15) \[ A_s^{(t+1)} = A_s^{(t)} \cup \{ n^* \}, \quad B_s^{(t+1)} = B_s^{(t)}. \]

Note that if any of the child nodes, have \( L \) included or \( N - L \) excluded antennas, we apply the following update:

\[ B_s^{(t+1)} = [N] \backslash A_s^{(t+1)} \quad \text{if} \quad |A_s^{(t+1)}| = L \]

(20) \[ A_s^{(t+1)} = [N] \backslash B_s^{(t+1)} \quad \text{if} \quad |B_s^{(t+1)}| = N - L. \]

This ensures that we do not generate any new nodes that do not satisfy (7c). Finally, the two children replace \( N_s^{(t)} \) in \( \mathcal{P}^{(t)} \) to form \( \mathcal{P}^{(t+1)} \). Note during the process, some nodes in the B&B tree can be simply discarded, or, “fathomed”—as in the standard terminologies of B&B [18]. After iteration \( t \), one can potentially find a set of \( (s', t') \) such that

\[ \Phi_{lb}(N_s^{(t')}) > u_G^{(t)}. \]
The above means that $\mathcal{N}_{s}^{(t)}$ needs not to be further partitioned in the next iteration. Hence, we can form a set $\mathcal{F}^{(t)}$ in each iteration, which only contains the nodes that need to be further considered, i.e.,

$$
\mathcal{F}^{(t)} = \left\{(s', \ell') \in \mathcal{P}^{(t)} \mid \Phi_{\text{BB}} \left(\mathcal{N}_{s'}^{(t)}\right) \leq u_{G}^{(t)}\right\}
$$

This is arguably the most important for attaining efficiency against exhaustive search. The B&B procedure can be found in Appendix A.

4) An Alternative B&B Method: It is interesting to note that there is often more than one way to come up with a B&B procedure for a given problem. For example, a commonly used approach for deriving B&B of mixed integer and linear programs (MILPs), and more generally, subset selection problems (see, e.g., [22], [45]) can also be used for our problem (7). The method is by introducing auxiliary Boolean variables. Specifically, problem (7) can be expressed as follows:

$$
\begin{align}
\text{minimize} & \quad \|W\|^2_F, \\
\text{subject to} & \quad C(w_m, h_m, \varepsilon_m, \sigma_m) \geq \gamma_m, \\
& \quad z \in \{0,1\}^N, \\
& \quad z^T 1 \leq L, \\
& \quad \|W(n,:)\|_2 \leq C(z(n), \forall n \in [N]).
\end{align}
$$

(21)

where $C < \infty$ is a large positive constant and $z(n) = 0$ means that the $n$th antenna is excluded whereas $z(n) = 1$ indicates the opposite. The constraint in (21b) can be relaxed to be $z \in [0,1]^N$ for finding the lower bound (see Appendix C-B2 for details). In this procedure, the branching operations are imposed on the new variable $z$ [22], [45]. The reason that we do not choose formulation (21) to design B&B for our joint (R)BF&AS problem is that this approach could be computationally (much) less efficient compared to the proposed approach (see a proof in Theorem 1). The computational efficiency of our method comes from the fact that the computation of upper and lower bounds in (15) and (17) can be reused for many nodes; see the proof of Theorem 1. However, it is not obvious if such kind of computation reduction is still possible for the formulation in (21).

C. Optimality

We show that the proposed algorithm will produce optimal solutions for the problem of interest:

Theorem 1. Regarding the proposed B&B procedure (see Appendix A), the following statements hold:

(a) When BF is considered, the proposed B&B solves (7) optimally.

(b) When RBF is considered, if the conditions in Lemma 3(b) are satisfied, the proposed B&B solves (7) optimally.

(c) The total number of SOCPs/SDRs solved by the proposed B&B is upper bounded by

$$
Q_{\text{Compute}} = \binom{N}{L} + \sum_{i=2}^{N-L+1} \binom{N-i}{L-1}.
$$

The number of SOCPs/SDRs needed by the B&B associated with the alternative formulation in Sec. II-B4 is upper bounded by $Q'_{\text{Compute}} = 2\binom{N}{L} - 1$.

The proof of Theorem 1 is in Appendix C. At the first glance, it feels a bit surprising that the B&B algorithms could use more than $\binom{N}{L}$ SOCP/SDRs to find the optimal solution, since this seems to be worse than exhaustive search. This is because, in the worst case, B&B visits many more intermediate states in the search tree—but exhaustive search only visits the leaves. Nonetheless, in practice, B&B is often much more efficient than exhaustive search since B&B does not really exhaust all the nodes. Theorem 1 (c) spells out the advantage of our B&B design relative to the more classic B&B idea as in (21) from the MILP literature. Note that the reduction of complexity shown in (c) could be substantial. For example, when $(N, L) = (12, 8)$, $Q_{\text{Compute}} = 660$, whereas $Q'_{\text{Compute}} = 989$. Hence, there is a potential saving of 339 SOCPs/SDRs (reduction by 34%) in the worst case.

III. ACCELERATED JOINT (R)BF&AS VIA ML

The challenge of any B&B algorithm lies in the large number of nodes in the tree. This means that in the worst case, many SOCPs and SDRs need to be solved. An idea from the ML community is to “train” a classifier to recognize the relevant nodes, i.e., nodes that lead to leaves containing the optimal solution [20]. If a node is deemed to be “irrelevant”, the B&B algorithm would simply skip branching on this node, and thus could save a substantial amount of time. In this section, we will show that a similar idea can be used for accelerating our B&B based joint (R)BF&AS algorithm—with carefully designed neural models to meet the requirements arising in wireless communications. More importantly, we will present comprehensive performance characterizations, including sample complexity and global optimality retention, which are currently lacking in the existing literature.

A. Preliminaries: Node Classification and Imitation Learning

1) Node Classification: Let us denote

$$
\pi_{\theta} : \mathbb{R}^P \rightarrow [0,1]
$$

as the node classifier parameterized by $\theta$, which returns the probability of a node being relevant. Let $\phi(\mathcal{N}_s^{(t)}) \in \mathbb{R}^P$ be the mapping from a node to its feature representation. When $\pi_{\theta}(\phi(\mathcal{N}_s^{(t)})) < 0.5$, then the node is deemed irrelevant. Otherwise, the node is branched.

To train such a classifier, denote $\{(\mathcal{N}_s, y_s)\}_{s=1}^T$ as the (node, label) training data, where we have removed the level indices of the nodes for notation simplicity. To create the training pairs, one could run random problem instances of (7) using the B&B procedure. Note that the label $y_s$ is annotated according to the following rule:

$$
y_s = \begin{cases} 
1, & A_s \subseteq A^* \text{ and } B_s \subseteq \{N\} \setminus A^*, \\
0, & \text{otherwise},
\end{cases}
$$

(22)
where $\mathcal{A}_s$ and $\mathcal{B}_s$ are the index sets of included and excluded antennas at node $s$, respectively, and $\mathcal{A}^*$ is the index set of the active antennas of the optimal solution found by B&B of the associated problem instance.

2) *Imitation Learning*: The simplest supervised learning paradigm would learn $\pi_\theta$ using the following risk minimization criterion:

$$
\min_{\theta} \frac{1}{T} \sum_{t=1}^{T} \mathcal{L}(\pi_\theta(\phi_s), y_s) + r(\theta),
$$

where $\phi_s := \phi(N_s)$, $\mathcal{L}(x, y)$ is a certain loss function, e.g., the logistic loss, and $r(\theta)$ is a regularization term, e.g., $r(\theta) = \lambda \|\theta\|^2$. Unfortunately, such a supervised learning approach often does not work well, since it ignores the fact that the node processing is sequential and interactive with the node classifier in the test stage. In ML-based MILP, the remedy is to adopt the *imitation learning* (IL) [24] approach, where $\pi_\theta$ is integrated in the training data generation process [20]. To be more specific, the training data generation process is done in a batch-by-batch manner with online optimization. The IL training criterion is as follows (see Section III-C for data generation and training process):

$$
\theta^{(i+1)} = \arg\min_{\theta} \frac{1}{I} \sum_{t=1}^{I} \frac{1}{|D_t|} \sum_{(\phi_s, y_s) \in D_t} \mathcal{L}(\pi_\theta(\phi_s), y_s) + r(\theta),
$$

where $D_t$ is the $t$th batch of training pairs. The learned model parameter $\hat{\theta}$ is selected from $\theta^{(i)}$’s via the following:

$$
\hat{\theta} = \arg\min_{\theta} \frac{1}{I} \sum_{t=1}^{I} \mathbb{E}_{(\phi_s, y_s) \in D_t} [\mathcal{L}(\pi_\theta(\phi_s), y_s)],
$$

where $I$ is the total number of batches generated during the training process. In practice, one can use a validation set to approximate the above expectation. In the test stage, the proposed B&B algorithm is run with the assistance of $\pi_{\hat{\theta}}$.

The key of using IL to accelerate the proposed B&B for joint (R)BF&AS is twofold, namely, a practical node classifier tailored for wireless communications and a convergent online training algorithm. We will detail our designs to address the two requirements in the next subsections.

B. GNN-based Node Classifier for Joint (R)BF&AS

To design the node classifier, a critical consideration in wireless communications is that the number of users to serve could drastically change from time to time. This requires us to design an ML model that is agnostic to such changes, as re-training a model when change happens is not affordable. Towards this end, we design a GNN-based node classifier [23]. Note that GNNs learn aggregation operators over a graph, and thus is naturally robust to the change of entities on the graph. We will leverage this property to design our node classifier.

To describe the GNN-based node classifier, we first define a graph to represent $\mathcal{N}_s^{(i)}$. Fig. 2 illustrates the idea, where the antennas and users represent the vertices, and the channel represent the edge between the vertices. It is important to design the features of the vertices and the edges, so that they represent the essential information of the node $\mathcal{N}_s^{(i)}$. To be specific, We let

$$
\begin{align*}
\mathbf{x}_n &\in \mathbb{R}^{V_n}, \ n \in [N], \\
\mathbf{x}_{N+m} &\in \mathbb{R}^{V_m}, \ m \in [M], \text{ and} \\
\mathbf{e}_{n,N+m} &\in \mathbb{R}^{V_m}, \ n \in [N], \ m \in [M]
\end{align*}
$$

represent the feature vectors of antenna $n$ (a vertex), user $m$ (a vertex), and the channel between the antenna $n$ and the user $m$ (an edge), respectively. Layer $d$ of the GNN “aggregates” the embedding of graph neighbors to update the $d$th vertex for all $u \in [M+N]$. The definition of such aggregation can be flexible. For example, in the *message passing neural network* [46], the aggregation is done by the following:

$$
\mathbf{q}_u^{(d)} = \xi(\mathbf{Z}_d \mathbf{q}_u^{(d-1)} + \sum_{v \in \mathcal{E}_u} \xi(\mathbf{Z}_e \mathbf{q}_v^{(d-1)} + \mathbf{Z}_e \mathbf{e}_{u,v})),
$$

where $\mathbf{q}_u^{(0)} = \mathbf{x}_u$; $\mathbf{Z}_d$ for $i = 1, 2, 3$ are the aggregation operators of the GNN; $\xi(\cdot)$ represents the activation functions of layer $d$; and $\mathcal{E}_u$ is the index set of all the one-hop neighbors of vertex $u$ on the graph. The output of the GNN is

$$
\pi_\theta(\phi_s) = \frac{1}{U} \sum_{u \in [U]} \zeta(\beta^T \mathbf{q}_u^{(D)}), \ \phi_s = \phi(N_s) \in \mathbb{R}^P
$$

where $U = M + N$ is the total number of vertices; $\phi_s = [\mathbf{x}_1, \ldots, \mathbf{x}_{N+m}, \mathbf{e}_{1,N+1}, \ldots, \mathbf{e}_{N,N+m}]^T$; and $\zeta(\cdot)$ is a sigmoid function. Here, the parameter to be optimized is given by $\theta := [\vec{(\mathbf{Z}_1)}, \vec{(\mathbf{Z}_2)}, \vec{(\mathbf{Z}_3)}]^T$. Since $\theta$ does not depend on $(N, M, L)$, the learned model can naturally work when the number of users changes, as long as $V_a$, $V_u$, and $V_e$ remain the same.

Table I shows the detailed feature descriptions. We design two types of features, namely, problem size-dependent (containing information of $(N, M, L)$) and problem size-independent features; see Appendix G for detailed conversion from these features to $\mathbf{x}_u$ and $\mathbf{e}_{u,v}$. Note that the special structure of GNN allows us to employ problem-size dependent features, as the sizes of aggregation matrices $\mathbf{Z}_d$ are determined by the feature vector size, instead of the numbers of vertices $(N + M)$ and edges. However, if one uses SVM as in [20] or other types of neural networks (e.g., fully connected network (FCN) and convolutional neural network (CNN)), these features cannot be used. We should remark that our feature design is not “optimal” in any sense, but using problem size-dependant features arguably provides more comprehensive information about the node and could often enhance the node classification accuracy.

Table II shows numerical evidence to support our postulate. There, different classifiers are trained by IL using problem instances as described in Sec. IV. The FCN has two hidden
layers with 32 hidden units in each layer, a sigmoid activation function on the output layer, and ReLU activations on the remaining layers. The architecture of the GNN is described in Appendix F. The SVM and FCN could only use the problem size-independent features. The GNN with both types of features clearly offers a lower node classification error.

### C. Data Generation and Online Training

We use an IL framework to train the GNN, which is summarized in Algorithm 1. The framework is based on the online learning method in [24]. The work in [24] was proposed for convex learning criteria. Necessary modifications are made in Algorithm 1 to accommodate our nonconvex learning problem.

Algorithm 1 consists of two steps in each iteration: data collection and classifier improvement. In the ith iteration, the accumulated dataset \( D_i \) is obtained by solving B&B on \( R \) problem instances using the current classifier learned from the previous data batches, \( \pi_{\theta(i)} \). Then, the classifier is retrained using \( \cup_{i=1}^{j} D_i \) and

\[
\hat{\theta}^{(i+1)} = \arg \min_{\theta \in \Theta} g_i(\theta) + r(\theta)
\]

where \( \Theta \) specifies the constraints of the GNN parameters [cf. Eq (28)]; the loss function \( g_i(\cdot) \) is defined as follows:

\[
g_i(\theta) := \frac{1}{|D_i|} \sum_{(\phi_s, y_s) \in D_i} L(\pi_{\theta}(\phi_s), y_s);
\]

(27)

Additionally, we select \( r(\theta) = -\psi^T \theta \) in which \( \psi \) is sampled from exponential distribution in each iteration. This specific choice of \( r(\theta) \) plays an important role in our nonconvex learning problem (where the nonconvexity arises due to the use of GNN). To be more specific, such a random perturbation-based \( r(\theta) \) is advocated by recent developments from nonconvex online learning [47]. It was shown in [47] that using \( r(\theta) = -\psi^T \theta \) ensures no-regret type convergence of nonconvex online learning. This property is a critical stepping stone towards establishing learning guarantees of our GNN-based framework. This will become clearer in the proofs of Theorem 2.

The training data generation subroutine is given in Algorithm 2. To generate \( D_i \), the algorithm first runs B&B on a given problem instance to find the optimal solution. Next, B&B is run again but with \( \pi_{\theta(i)} \) to generate nodes. The training pairs \((\phi_s, y_s)\) are annotated by utilizing the optimal solution obtained in the first run.

The overall GNN-accelerated B&B procedure is summarized in Algorithm 3. The algorithm is termed as Machine Learning-based fast Branch and Bound for Joint Beamforming and antenna Selection (MLBB-JOBS). The node classifier is used in Line 11.

### D. Performance Characterizations

Our goal is to characterize the performance of MLBB-JOBS, e.g., under what conditions (e.g., the amount of training...
Algorithm 3: Main Algorithm: MLBB-JOBS

1. Input: Problem instance \((A_m, \sigma_m, \gamma_m, \epsilon_m), \forall m\), trained pruning policy \(\pi_{\theta}\), relative error \(\epsilon\).
   // Add the root node first
2. \(A_1(0) \leftarrow \emptyset, B_1(0) \leftarrow \emptyset\).
3. Select node using (18) for \(N_x(0)\).
4. \(W_{incumbent} \leftarrow \text{solution to (17)}\).
5. \(F(0) \leftarrow \{(0,1)\};
6. \(\ell(0) \leftarrow \|W(0)\|_2; u_G(0) \leftarrow \|W_{incumbent}\|_2\);\n7. \(t \leftarrow 0;\)
8. \(\text{while } |F(t)| > 0 \text{ and } \|u_G(t) - u_G(t-1)\| > \epsilon\) do
9. \(\text{Select a non-leaf node } (t', s') \text{ using (18);}\n10. \(\text{Remove the selected node } F(t) \leftarrow F(t) \setminus N_x(t');\n11. \text{if } \pi_{\theta}(\Phi_{t'}(s')) > 0.5 \text{ then}\n12. \quad \text{Select variable } n^* \text{ using (19);}\n13. \quad \text{Generate child nodes } N_x(t'+1) \text{ and } N_x(t'+1) \text{ using (13) and}\n14. \quad \text{and append to } F(t')\n15. \quad k \leftarrow \arg\min_{i \in \{1,2\}} \Phi_{ab}(\Lambda_{i}^x(t'+1));\n16. \quad \text{if } \Phi_{ab}(\Lambda_{i}^x(t'+1)) \leq u_G(0) \text{ then}\n17. \quad \quad u_G(t'+1) \leftarrow \Phi_{ab}(\Lambda_{i}^x(t'+1));\n18. \quad W_{incumbent} \leftarrow \text{solution to (17) for } N_x(t'+1);\n19. \end{end}\n20. \(F(t'+1) \leftarrow \{(s', t') \in F(t) \mid \Phi_{ab}(\Lambda_{i}^x(t')) \leq u_G(t'+1)\};\n21. \(t \leftarrow t + 1;\)
22. \(\text{end}\)
23. \(\text{end}\)
24. \(\text{Return } W_{incumbent};\)

MLBB-JOBS can accelerate the proposed B&B without losing its optimality. To our best knowledge, such performance characterization have not been provided for ML-based B&B acceleration, even when the learning problem is convex.

To proceed, we will use the following assumptions:

**Assumption 1.** Assume that the following statements about the data features and the GNN in Sec. III-B hold:

(a) The input features are bounded, i.e., \(\|x_u\|_2, \|e_u\|_2 \leq B_x, \forall u, v,\)
(b) The activation functions \(\xi(\cdot)\) and \(\zeta(\cdot)\) are \(C_\xi\)-Lipschitz and \(C_\zeta\)-Lipschitz continuous, respectively. In addition, \(\xi(0) = 0\).
(c) Let \(L : \mathbb{R} \times \mathbb{R} \rightarrow [-BC, BC]\) be \(C_\xi\)-Lipschitz in its first argument, i.e., \(|L(x, y) - L(x', y)| \leq C_\xi |x - x'|\).
(d) The parameters of the GNN are bounded; i.e., \(\|Z_i\|_2 \leq B_Z, \forall i \in \{1, 2, 3\}\) and \(\|\beta\|_2 \leq B_\beta\).

Let us define the set of parameters \(\mathcal{X}\) as follows:

\[\mathcal{X} := \{\theta = [\text{vec}(Z_1)^\top, \text{vec}(Z_2)^\top, \text{vec}(Z_3)^\top, \beta]^\top \mid \|Z_i\|_2 \leq B_Z, \beta \leq B_\beta, i \in \{1, 2, 3\}\}.\]

Using the above, we first characterize the generalization error of the GNN with the following Lemma:

**Lemma 4** (Generalization Error of GNN). Consider a GNN \(\pi_{\theta}\) in Sec. III-B and \(G = \{\phi_k, y_k\}_{k=1}^K\) of i.i.d. samples. Then, for \(\theta \in \Theta\), the following holds with probability at least \(1 - \delta\):

\[\text{Gap}(\delta, K) = E\left[\mathcal{L}(\pi_{\theta}(\phi), y) - 1/K \sum_{(\phi, y) \in G} \mathcal{L}(\pi_{\theta}(\phi), y)\right] \leq \frac{24C_\xi B \epsilon}{K} + \frac{24 \epsilon C_\xi}{K} \frac{C_\xi}{\epsilon} \frac{C_\xi}{\epsilon} \sqrt\left(3E^2 + E \log \Lambda + 3B \sqrt{3} + \frac{C_\xi}{\epsilon} \frac{C_\xi}{\epsilon} \right),\]

where \(\Lambda = 1 + 12\sqrt{E K/3} + 12\sqrt{E K/3} + 12\sqrt{E K/3}\)

Note that our GNN generalization error bound is rather different from some existing results, e.g., [48], as edge features (i.e., \(e_u,v\)) were not considered in their work. Lemma 4 can be used to understand the GNN’s performance with a single batch. To characterize the node classification accuracy of the GNN learned through the described imitation learning algorithm, we need the following assumptions:

**Assumption 2.** Let \(\sup_{\theta_1, \theta_2} \|\theta_1 - \theta_2\|_\infty \leq H, \text{ for some } H < \infty\). Let all the loss functions \(g_i(\cdot)\) [cf. Eq. (27)] for \(i = 1, \ldots, I\) are \(G\)-Lipschitz continuous with respect to the \(\ell_1\)-norm, i.e.

\[|g_i(\theta_1) - g_i(\theta_2)| \leq G \|\theta_1 - \theta_2\|_1, \forall i.\]

**Assumption 3.** The minimal empirical loss over the aggregated dataset is bounded by \(\nu\).

\[\min_{\theta \in \Theta} \frac{1}{I} \sum_{i=1}^I \sum_{(\phi, y) \in D_i} E_{\psi}[\mathcal{L}(\pi_{\theta}(\phi), y)] \leq \nu.\]

Assumption 2 is not hard to meet if the data features and the network parameters are bounded. Assumption 3 characterizes the expressiveness of the GNN.

To present our main theory, we compute the expected number of nodes that will be visited (with the associated SOCPs/SDRs solved) by Algorithm 3 when run with \(\pi_{\theta}\) in the testing stage. Let us denote \(\rho_\phi\) as the probability with which the classifier accurately classifies a node. Also denote \(S\) as the set of all possible B&B trees that can be realized by Algorithm 3 under a given instance. Let \(\text{Pr}(s; \theta), s \in S\) be the probability with which a particular tree \(s\) is realized. Let \(Q_\theta\) denote the number of visited nodes in tree \(s\). Let \(Q_\theta = E[Q_\theta]\) where the expectation is taken over the probability mass function \(\text{Pr}(s; \theta), s \in S\). In the following theorem, we characterize the classification accuracy, \(\rho_\phi\), and present a bound on \(Q_\theta\).

**Theorem 2.** Suppose that Assumptions 2, 3 hold, and that the GNN in MLBB-JOBS is parameterized by \(\theta\) in (25). In addition,
assume that every single batch $\mathcal{D}_i$ consists of i.i.d. samples, and that Algorithm 1 is used for GNN learning. Then, we have

$$Q_\hat{\theta} \leq \frac{2N (2\tilde{\rho}_\theta - \rho_\theta^N)}{2\rho_\theta - 1} + 1.$$  

Further, when $\hat{\theta}$ is selected using (25), with a probability at least 1 $-$ $\delta$,

$$\mathbb{E}_{\rho, s} \left[ \mathcal{L} \left( \pi_{\hat{\theta}}(\phi_s), y_s \right) \right]$$  

$$\leq \nu + O \left( \frac{1}{I^{1/3}} \right) + \text{Gap} \left( \frac{\delta}{2}, \mathcal{I} \right) \sqrt{\frac{2 \log(2/\delta)}{I}}.$$  

Assume the logistic loss function $\mathcal{L}$ is employed. Then, the node classification accuracy

$$\rho_{\hat{\theta}} \geq \exp \left( -\mathbb{E}_{\rho, s} \left[ \mathcal{L} \left( \pi_{\hat{\theta}}(\phi_s), y_s \right) \right] \right).$$  

In addition, MLBB–JOBS returns an optimal solution with probability at least $\rho_{\hat{\theta}}^N$.

The proof of Theorem 2 is relegated to Appendix E. This result bounds the number of nodes visited by the proposed algorithm under a given classification accuracy. It also characterizes the classification accuracy that can be achieved by the proposed training procedure. One can see that when the batch size is large enough, Gap is close to zero. Additionally, when the GNN is expressive (and thus $\nu$ is small) and the algorithm is run for large enough iterations $I$, the accuracy of the classifier, i.e., $\rho_{\hat{\theta}}$, approaches 1 [cf. Eq. (30)]. Consequently, the total number of nodes visited will be close to $2N + 1$ at most. This shows linear dependence of the computational complexity of the proposed method on $N$, which is a significant saving compared to $\binom{N}{2}$ for the exhaustive search.

Remark 1. We should remark that the results in Theorem 2 has a couple of caveats. First, we assumed that the samples in each $\mathcal{D}_i$ are i.i.d. If every node created by $\pi_{\theta}^{(i)}$ in Algorithm 2 is used, then the samples in $\mathcal{D}_i$ are likely not i.i.d., as the nodes in the same B&B tree are generated in a sequential manner. Nonetheless, simple remedies can assist creating an i.i.d. batch $\mathcal{D}_i$, e.g., by taking only one random node from a B&B tree. This is inevitably more costly, and seems not to be necessary in practice—as using nodes from Algorithm 2 for training works fairly well in our simulations. Second, the expectation based criterion (25) is only approximated in practice, e.g., via using empirical averaging. Characterizing the empirical version of (25) can be done via concentration theorems in a straightforward manner. However, this would substantially complicate the expressions yet reveals little to no additional insight. Hence, we leave it out of this work.

IV. Numerical Results

In this section, we showcase the effectiveness of the proposed B&B algorithm and its machine learning based acceleration using numerical simulations. We use CVXPY [49] to solve the SOCPs/SDRs in (15) and (17). The elements of Rayleigh fading channel vectors $\{h_m\}_{m=1}^M$ are sampled independently from circularly symmetric zero mean Gaussian distribution with unit variance. Throughout the experiments, we set the noise variance for all users to $\sigma_n^2 = 1, \forall m \in [M]$. Similarly, we set $\varepsilon_m = 0.1, \forall m \in [M]$ unless otherwise specified. Implementation of the proposed methods can be found on the authors’ website.

A. Evaluation of B&B for Joint (R)BF&AS

In Fig. 3, we verify the convergence of the proposed B&B algorithm under both the perfect and the approximate CSI cases. The figure shows the convergence of the global upper and lower bounds (i.e., $u_c^{\ell}$ and $u_c^{U}$) computed by the proposed B&B procedure for $(N, M, L) = (8, 4, 4)$. One can see that the global bounds converge to the optimal objective value in both the perfect and approximate CSI case. This verifies our optimality claim in Theorem 1. Note that the B&B algorithm for both cases converges in less than 24 iterations (i.e., visiting 48 nodes). This is much less than the worst-case complexity of B&B, i.e., visiting 139 nodes. The empirical complexity is also better than the worst-case complexity of exhaustive search, which is 70 node visits in this case.

Table III gives a closer look at the effectiveness of the proposed B&B framework. Specifically, Table III shows the performance of the proposed B&B procedure for various problem sizes, compared to the exhaustive search strategy for the perfect CSI case. The result is averaged over 30 Monte Carlo trials. One can see that the B&B algorithm can constantly attain reduced complexity, in terms of the number of nodes visited (i.e., the number of SOCPs solved). In particular, when the number of users is relatively small, the B&B can attain an around 8-fold acceleration (cf. the case where $(N, M, L) = (12, 2, 8)$). Similar results can be seen in Table IV, where the imperfect CSI case is considered.

Table V compares our B&B and the alternative B&B using the formulation (21) in the perfect CSI case. One can see that the proposed procedure consistently solves fewer SOCPs. This supports Theorem 1 (c).

1https://github.com/XiaoFuLab/BeamSelection-and-Beamforming-with-BandB-and-ML.git
We term this method iteratively reweighted convex relaxation-based optimization (IrCvxOpt). We use a GNN tailored for our beamforming setting (see details in Appendix F). We set λ-tuning method for 30 iterations as well. The test set consists of 5000 test instances, and the algorithm under test is run for 30 iterations. The run-time of method under test is recorded and averaged over 30 different random test instances. Note that the run-time could not find a feasible solution.

In this section, we demonstrate the efficacy of ML-accelerated B&B for Joint (R)BF&AS

We use a GNN tailored for our beamforming setting (see details in Appendix F). We set λ-tuning method for 30 iterations as well. The test set consists of 5000 test instances, and the algorithm under test is run for 30 iterations. The run-time of method under test is recorded and averaged over 30 different random test instances. Note that the run-time could not find a feasible solution.

In this section, we demonstrate the efficacy of ML-accelerated B&B for Joint (R)BF&AS.

As a baseline, we use the continuous optimization-based idea in [5] and modify it to solve the unitcast cases as in this work. Although [5] did not explore their method for the approximate CSI case, we note that the same idea can be used after proper modifications to the subproblems (i.e., using the S-lemma to come up with an S-DR formulation of the subproblem). We term this method iteratively reweighted convex relaxation-based optimization (IrCvxOpt).

1) Baseline Setting: Following the implementation instruction of [5], we run IrCvxOpt for at most 30 iterations with its bisection-based λ-tuning method for 30 iterations as well. The algorithm is stopped if the relative change of the reweighting matrix is smaller than 10−4 or a solution comprising of ≤ L antennas is found. If the algorithm returns > L antennas, we conclude that IrCvxOpt could not find a feasible solution.

2) Training Details: We use a GNN tailored for our beamforming setting (see details in Appendix F). We set λ-tuning method for 30 iterations as well. The test set consists of 5000 test instances, and the algorithm under test is run for 30 iterations. The run-time of method under test is recorded and averaged over 30 different random test instances. Note that the run-time could not find a feasible solution.

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speedup compared to the B&B algorithm increases along with the growth of $N$. In terms of speedup, one can see that MLBB-JOBS even achieves better speedup relative to IrCvxOpt, compared to the perfect CSI cases. The proposed method also always finds a feasible solution with exact $L$ active antennas, yet IrCvxOpt fails to do so.

**C. Performance under Training-Test Mismatch**

In a wireless communication environment, the number of users being served by a BS varies frequently. Hence, it is highly likely that the node classifier is trained using $M$ users but $M'$ users (where $M' \neq M$) appear in the test stage. Therefore, we evaluate the performance of MLBB-JOBS in cases where there are such mismatches between in training and test.

Table VIII shows the performance of the model trained on problem instances of size $(N, M, L) = (8, 4, 4)$. The test stage uses various $M$’s. One can see that the optimality gap attained by MLBB-JOBS is consistently below 1% in all cases. Similarly, there is no significant degradation in the speedup. Finally, the feasibility rate is consistently 100% in all cases. This shows that the proposed GNN based classifier generalizes well across unseen problem sizes, which is an important consideration in any wireless communication systems.

**V. Conclusion**

In this work, we revisited the joint beamforming and antenna selection problem under perfect and imperfect CSI and proposed a machine learning-assisted B&B algorithm to attain its optimal solution. Unlike the vast majority of existing algorithms that rely on continuous optimization to approximate the hard mixed integer and nonconvex optimization problem without optimality guarantees, our B&B algorithm leverages the special properties of joint (R)BF&AS to come up with optimal solutions. More importantly, we proposed a GNN-based machine learning method to help accelerate the B&B algorithm. Our analysis showed that the design ensures provable acceleration and retains optimality with high probability, under proper GNN design and given a sufficiently enough sample size. To our best knowledge, this is the first comprehensive characterization for ML-based B&B. Our GNN design also easily handles a commonly seen challenge in communications, namely, the problem size change across training and test sets, without visible performance losses. Simulations corroborated our design goals and theoretical analyses.

**REFERENCES**

APPENDIX A
PROPOSED B&B PROCEDURE

The proposed B&B procedure is essentially Algorithm 3 without any pruning of the nodes based on node classifier. The B&B procedure is outlined in Algorithm 4.

Algorithm 4: BB

1. Input: Problem instance \((h_m, \sigma_m, \gamma_m, \varepsilon_m), \forall m\), trained pruning policy \(\pi_\theta\), relative error \(\epsilon\);
2. // Add the root node first
3. \(A_1^{(0)} \leftarrow \emptyset, B_1^{(0)} \leftarrow \emptyset\);
4. Select node using (18) for \(N_1^{(0)}\);
5. \(W_{\text{incumbent}} \leftarrow \text{solution to (17)}\);
6. \(l_G^{(0)} \leftarrow \|W_1^{(0)}\|_F^2, u_G^{(0)} \leftarrow \|W_{\text{incumbent}}\|_F^2\);
7. \(F^{(0)} \leftarrow \{(0, 1)\}\);
8. \(t \leftarrow 0;\)
9. while \(|F^{(t)}| > 0\) and \(|u_G^{(t)} - l_G^{(t)}|/|l_G^{(t)}| > \epsilon\) do
10. Select a non-leaf node \((\ell, s')\) using (18);
11. Remove the selected node \(F^{(t)} \leftarrow F^{(t)} \setminus N_{s'}^{(t)}\);
12. Select variable \(n^*\) using (19);
13. Generate child nodes \(N_{s'}^{(t+1)}\) and \(N_{s''}^{(t+1)}\) using (13) and append to \(F^{(t)}\);
14. \(k \leftarrow \arg\min_{m \in \{1, 2\}} \Phi_{\text{ub}}(N_{s'}^{(t+1)})\);
15. if \(\Phi_{\text{ub}}(N_{s'}^{(t+1)}) \leq u_G^{(t)}\) then
16. \(u_G^{(t+1)} \leftarrow \Phi_{\text{ub}}(N_{s'}^{(t+1)})\);
17. \(W_{\text{incumbent}} \leftarrow \text{solution to (17) for } N_{s'}^{(t+1)}\);
18. end
19. \(l_G^{(t+1)} \leftarrow \min_{(s, \ell) \in F^{(t)}} \Phi_{\text{lb}}(N_{s'}^{(t+1)})\);
20. \(F^{(t+1)} \leftarrow \{(s', \ell) \in F^{(t)} | \Phi_{\text{lb}}(N_{s'}^{(t+1)}) \leq u_G^{(t+1)}\}\);
21. \(t \leftarrow t + 1;\)
22. Return \(W_{\text{incumbent}}\);
B. Proof of (c)

1) Amount of SOCPs/SDRs Solved by Proposed B&B: In the given B&B procedure, (15) and (17) are equivalent for any node and its right child node, i.e.,

\[
\Phi_{lb} \left( N_s^{(l+1)} \right) = \Phi_{lb} \left( N_{s2}^{(l+1)} \right),
\]

\[
\Phi_{ub} \left( N_s^{(l)} \right) = \Phi_{ub} \left( N_{s2}^{(l+1)} \right).
\]

The first equation is because \( B_s^{(l)} = B_s^{(l+1)} \) and the second equation is because \( B_s^{(l)}, \forall (l, s) \) in (17) is determined using the solution to (15). Hence, one can avoid redundant computations in the nodes by storing and reusing the results of (15) and (17). Using this observation, in the following, we derive an upper bound of the number of SOCPs/SDRs that need to be solved by the proposed B&B procedure.

Consider a B&B tree where none of the nodes are fathomed (see illustration in Fig. 4). Note that there are \( Q_{\text{Leaf}} = \binom{N}{L} \) leaf nodes (squares in Fig. 4). Therefore, there are \( Q_{\text{Total}} = 2^{\binom{N}{L}} - 1 \) nodes in total (all circles and squares). Each non-leaf node (circles) is branched into a right child node and a left child node. Hence, there are \( Q_{\text{Right}} = \binom{N}{L} - 1 \) right child nodes (shaded solid circles and squares) and \( Q_{\text{Left}} = \binom{N}{L} - 1 \) left child nodes (unshaded solid circles and squares).

The constraints of the SOCPs/SDRs corresponding to the leaf nodes can be different from that of its parent even if they correspond to a right child node, i.e., shaded squares. This is because of the update step in (20) for the leaf nodes. To explain, a right child node, \( N_s^{(l+1)} \), is converted into a leaf node if \( L \) of the decided antennas are included, i.e., \( |A_s^{(l)}| = L \). For this node,

\[
B_s^{(l)} = [N] \setminus A_s^{(l)},
\]

i.e., all remaining undecided antennas are excluded. Since \( B_s^{(l)} \) will be different from that of its parent node, the solutions of (15) and (17) can be different from that of its parent node.

Therefore, only the non-leaf right child nodes (shaded solid circles) can reuse previously stored upper bound and lower bound solutions from their parents. Let \( Q_{\text{RightLeaf}} \) denote the number of right child leaf nodes (shaded squares). Then, the total number of nodes whose associated SOCPs/SDRs that need to be solved in the worst case is as follows:

\[
Q_{\text{Compute}} = Q_{\text{Total}} - Q_{\text{Right}} + Q_{\text{RightLeaf}}.
\]

To count \( Q_{\text{RightLeaf}} \), notice that the right and left child nodes of a parent node correspond to ‘including’ and ‘excluding’ an antenna, respectively. A parent node is branched into a right child leaf node if it contains exactly \( L - 1 \) included antennas and fewer than or equal to \( N - L - 1 \) excluded antennas. This implies that there can be fewer than or equal to \((L-1) + (N-L-1) = N-2\) decided antennas. Hence, a right child leaf node is created whenever a node has \( \leq N-2\) decided antennas, where \( L-1 \) of them are included, is branched. Therefore, we have the following holds:

\[
Q_{\text{RightLeaf}} = \binom{N-2}{L-1} + \binom{N-3}{L-1} + \cdots + \binom{L-1}{L-1} = \sum_{i=2}^{N-L+1} \binom{N-i}{L-1}.
\]

Consequently,

\[
Q_{\text{Compute}} = \binom{N}{L} + \sum_{i=2}^{N-L+1} \binom{N-i}{L-1}.
\]

Note that \( Q_{\text{Compute}} \) nodes may correspond to \( 2Q_{\text{Compute}} \) SOCPs/SDRs (cf. (15) and (17) for each node). However, for the leaf nodes (15) and (17) are identical. Hence there are only \( Q_{\text{Compute}} - \binom{N}{L} \) instances of (15). Moreover, there can be at most \( \binom{N}{L} \) instances of (17), since \( \binom{N}{L} \) correspond to selecting \( L \) out of \( N \) antennas. Therefore, there are at most \( Q_{\text{Compute}} \) SDRs/SOCPs solved by the B&B procedure.

2) The SOCPs/SDRs Needed in B&B for Problem (21):

To complete the proof, let us examine the number of SOCPs/SDRs that are needed to exhaust the B&B tree of the formulation in (21).

A node problem of (21), for the node \( N_s^{(l)} \) is as follows:

\[
\begin{align*}
\text{minimize} & \quad \|W\|_F^2 \\
\text{subject to} & \quad C(w_m, h_m, \varepsilon_m, \sigma_m) \geq \gamma_m, \\
& \quad z \in \{0,1\}^N, \\
& \quad z^T1 \leq L, \\
& \quad z(n) = 0, n \in B_s^{(l)}, \\
& \quad z(n) = 1, n \in A_s^{(l)}, \\
& \quad \|W(n,:)\|_2 \leq Cz(n), \forall n \in [N].
\end{align*}
\]

The lower bound is obtained by solving the convex relaxation of the above, i.e., \( z \in \{0,1\} \) is relaxed to \( z \in [0,1]^N \). One can see that the lower bounds obtained at the parent node and both child nodes may be different. It is because (35) depends upon both \( A_s^{(l)} \) and \( B_s^{(l)} \) and each child node will differ from its parent in one of the two sets, i.e, \( B_s^{(l+1)} \neq B_s^{(l)} \) and \( A_{s2}^{(l+1)} \neq A_s^{(l)} \). The above implies that the number of SOCPs/SDRs with B&B using (35) has an upper bound of \( Q_{\text{Compute}} = 2 \binom{N}{L} - 1 \) (specially, with \( \binom{N}{L} \) instances of (17) and \( \binom{N}{L} - 1 \) instances of (15)).

### APPENDIX D

#### PROOF OF LEMMA 4

We use the empirical Rademacher complexity of the GNN class to assist finding the expected risk’s error, which is a
First, consider the following lemma:

**Lemma 5** ([1, Theorem 3.1]). Let \( T \) be a family of functions mapping from \( X_\phi \times \{0, 1\} \) to \([-b, b]\). Assume \( G \) consists of \( K \) i.i.d. samples \( \{\phi_k, y_k\}_{k=1}^K \). With probability at least \( 1 - \delta \) over the samples \( G \), for any \( \tau \in T \),

\[
\mathbb{E}[\tau(\phi, y)] - \frac{1}{K} \sum_{(\phi_k, y_k) \in G} \tau(\phi_k, y_k) \leq 2\tilde{\mathcal{R}}_G(T) + 3b\sqrt{\frac{\log(2/\delta)}{2K}},
\]

where \( \tilde{\mathcal{R}}_G(T) \) is the empirical Rademacher complexity [1] of the set \( T \) with respect to the samples \( G \).

Let us define the set \( T := \{(\phi, y) \mapsto \mathcal{L}(\pi_\theta(\phi), y) \mid \theta \in \Theta\} \), a class of functions that maps from \( X_\phi \times \{0, 1\} \) to \([-B, B] \). Then, applying Lemma 5 to \( T \) over the set \( G \) ensures that with probability at least \( 1 - \delta \) over \( \Theta \), \( \forall \theta \in \Theta \),

\[
\mathbb{E}[\mathcal{L}(\pi_\theta(\phi), y)] - \frac{1}{K} \sum_{i \in [K]} \mathcal{L}(\pi_\theta(\phi_i), y_i) \leq 2\tilde{\mathcal{R}}_G(T) + 3b\sqrt{\frac{\log(2/\delta)}{2K}},
\]

In the following, we derive an upper bound on \( \tilde{\mathcal{R}}_G(T) \). To this end, we instead define a set \( \Pi := \{\phi \mapsto \pi_\theta(\phi) \mid \theta \in \Theta\} \), and derive \( \tilde{\mathcal{R}}_G(\Pi) \). With this, we can use Talagrand’s Lemma [1, Lemma 4.2] to obtain \( \tilde{\mathcal{R}}_G(T) = \tilde{\mathcal{C}}_G \tilde{\mathcal{R}}_G(\Pi) \).

In order to derive \( \tilde{\mathcal{R}}_G(\Pi) \), we use Dudley’s entropy integral [2, Lemma A.5], which provides an upper bound on the empirical Rademacher complexity by using the covering number of \( \Pi \). To clarify, a \( \mu \)-cover of \( \Pi \) is any set \( C \subseteq \Pi \) such that \( \forall \pi_\theta \in \Pi, \exists \pi_\theta \in C \) such that

\[
\max_{\phi \in X_\phi} |\pi_\theta(\phi) - \pi_\theta(\phi)| \leq \mu.
\]

Similarly, the covering number of the set \( \Pi \) at scale \( \mu \) is denoted by \( N(\Pi, \mu) \) and defined as the minimum cardinality of a \( \mu \)-cover set of \( \Pi \). The following lemma summarizes the Dudley’s entropy integral that uses the covering number of a set to bound its empirical Rademacher complexity.

**Lemma 6** ([2, Lemma A.5]). Given samples \( G \) of size \( K \), the empirical Rademacher complexity of the set \( \Pi \) with respect to the samples \( G \) is upperbounded as follows:

\[
\tilde{\mathcal{R}}_G(\Pi) \leq \inf_{\alpha > 0} \left[ \frac{4a}{\sqrt{K}} + \frac{12}{\sqrt{a}} \int_a^{\sqrt{N(\Pi, \mu)}} \sqrt{\log(N(\Pi, \mu))} d\mu \right].
\]
Solving the recursion in the last inequality, and using $\Gamma_u^{(0)} = 0, \forall u$, we get

$$\Gamma_u^{(D)} \leq \Sigma Z_i \left\| Z_i - \bar{Z}_i \right\|_2 + \Sigma Z_i \left\| Z_i - \bar{Z}_i \right\|_2,$$

where

$$\Sigma Z_i = U C x^2 B x Z_x \alpha^{(D+1)} - 2 \alpha + 1 - (\alpha - 1)^2,$$

$$\Sigma Z_i = U^2 C x^4 B x Z_x \alpha^{(D+1)} - 2 \alpha + 1 - (\alpha - 1)^2,$$

$$\Sigma Z_i = U C x^2 B x Z_x \alpha^{(D+1)} - 2 \alpha + 1 - (\alpha - 1)^2.$$

Using the above bound on $\Gamma_u^{(D)}$ in (38), we get

$$|\pi_\theta(\phi) - \pi_\theta(\phi)| \leq \Sigma Z_i \left\| \beta - \bar{Z}_i \right\|_2 + \Sigma Z_i \left\| Z_i - \bar{Z}_i \right\|_2,$$

where $\Sigma Z_i = C z^2 \beta \alpha^{(D)} + C \eta U C x^2 B x Z_x \alpha^{(D+1)}$, $\Sigma Z_i = C z^2 \beta \Sigma Z_i$, $\Sigma Z_i = C \eta U C x^2 B x Z_x \Sigma Z_i$, and $\Sigma Z_i = C z^2 \beta \Sigma Z_i$.

Eq. (40) implies that for any $\theta \in \Theta$, the existence of the cover set such that $|\pi_\theta(\phi) - \pi(\phi)| \leq \mu$ can be satisfied by ensuring the existence of $(\beta, Z_i, Z_i, Z_i)$ such that the right hand side of (40) $\leq \mu$. Hence, if we construct $\eta / 4 \Sigma Z_i$-cover of $X_\beta$, and $|\Sigma Z_i|$-cover of $X_\beta$, $\forall i \in \{1, 2, 3\}$, the Cartesian product of the four sets correspond to a $\mu$-cover of $\Pi$. Hence, the covering number of $\Pi$ at scale $\mu$ can be upper bounded by the product of the covering numbers of the four sets as follows:

$$N(\Pi, \mu) \leq N\left(X_\beta, \frac{\mu}{4 \Sigma Z_i}\right) \times \prod_{i=1}^3 N\left(X_\beta, \frac{\mu}{4 \Sigma Z_i}\right).$$

In addition, the covering number for $X_\beta$ can be upper bounded using [3, Lemma 8] as follows:

$$N(X_\beta, \mu) \leq \left(1 + \frac{2 \sqrt{E} B \Sigma Z_i}{\mu}\right)^E.$$

Similarly, the covering number for $X_\beta$ can be upper bounded as follows [4]:

$$N(X_\beta, \mu) \leq \left(3 B \beta \mu\right)^E.$$

Using the above bounds in (41), we get

$$N(\Pi, \mu) \leq \left(\frac{12 B \beta \Sigma Z_i}{\mu}\right)^E \times \prod_{i=1}^3 \left(1 + \frac{8 \sqrt{E} B \Sigma Z_i}{\mu}\right)^E \leq \left(1 + \frac{12 \sqrt{E} B \max \left\{ B \beta \Sigma Z_i, \Sigma Z_i, \Sigma Z_i, \Sigma Z_i\right\}}{\mu}\right)^3 E^2 + E.$$

Finally, we can use Lemma 6 to obtain a bound on $\hat{R}_\theta(\Pi)$. To this end, we upper bound the integral on the right hand side of (37) as follows:

$$\int_{\mu} \sqrt{\log N(\Pi, \mu)} d\mu \leq \sqrt{K \log N(\Pi, \alpha)}.$$

The above inequality holds because $\sqrt{\log N(\Pi, \mu)}$ increases monotonically with the decrease of $\mu$. Taking $\alpha = 1/\sqrt{\pi}$, we get the following:

$$\hat{R}_\theta(\Pi) \leq \frac{4}{K} + \frac{12 \sqrt{E} B \max \left\{ B \beta \Sigma Z_i, \Sigma Z_i, \Sigma Z_i, \Sigma Z_i\right\}}{\sqrt{K}}.$$

Combining the above with $\hat{R}_\theta(\Pi) \leq C L \hat{R}_\theta(\Pi)$ and substituting in (36), we get the final result.

**APPENDIX E**

**PROOF OF THEOREM 2**

Proof of Theorem 2 can be divided into two parts. In the first part we bound the expected loss under of the learned GNN. For this we will use the proof idea from [5]. However, the proof technique in [5] hinges on the convexity of their online learning problem. Hence, we make appropriate modifications to accommodate our non-convex GNN-based learning problem. In the second part, using the expected loss, we characterize the number of nodes needed to be visited by Algorithm 3 for solving a given problem instance optimally.

**A. Expected Loss of Algorithm 1**

Note that the online learning algorithm in Algorithm 1 is a no-regret algorithm. The definition of regret is as follows:

**Definition 1** (Regret). *Regret of an online algorithm that produces a sequence of policies $\theta(t) = \{\theta(1), \theta(2), \ldots, \theta(I)\}$ is denoted by $R_\theta$. It is the average loss of all policies with respect to the best policy in hindsight, i.e.,

$$R_\theta := \frac{1}{I} \sum_{i=1}^I \sum_{(\Phi, y) \in D_i} [L(\pi_\theta(\Phi, y), y)] - \min_{\Phi \in \Theta} \frac{1}{I} \sum_{i=1}^I \sum_{(\Phi, y) \in D_i} [L(\pi_\theta(\Phi, y), y)].$$

**Definition 2** (No-regret Algorithm). *A no-regret algorithm is an algorithm that produces a sequence of policies $\theta(t)$ such that the average regret goes to 0 as $N$ goes to $\infty$:

$$R_\theta \leq \gamma I \text{ and } \lim_{I \to \infty} \gamma I \to 0.$$

For strongly convex $L$, the work in [5] shows that Algorithm 1 is a no-regret algorithm with $\eta = \infty$, i.e., $\psi = 0$ (recall that $\eta$ is the parameter of the exponential distribution, i.e., $\psi \sim \text{Exp}(\eta)$, where $\text{Exp}(\eta) := \eta(\text{Exp}(-\eta))$). However, for non-convex $L$ we cannot guarantee that Algorithm 1 is a no-regret algorithm [6]. But with $0 < \eta < \infty$, under Assumption 2, Algorithm 1 was shown to be a no-regret algorithm [6].

**Lemma 7.** *[6, Theorem 1] When Assumption 2 holds, the regret after $N$ iterations can be bounded by:

$$\text{E}_{\eta \sim \text{Exp}(\eta)}[R_\theta] \leq \gamma I \leq O(1/I^{1/3}).$$

Finally, the following lemma establishes the expected loss of the policy returned by Algorithm 1.
Lemma 8. For Algorithm 1, with probability at least $1 - \delta$,
\[
\min_{\theta \in \Theta_{1,1}} E_{(\phi_s, y_s) \sim p_{\theta, \psi}} \left[ L(\pi_{\theta}(\phi_s), y_s) \right] 
\leq \min_{\theta \in \Theta_{1,1}} \frac{1}{I} \sum_{i=1}^{I} \frac{1}{J} \sum_{(\phi_s, y_s) \in D_i} E_{\psi} \left[ L(\pi_{\theta}(\phi_s), y_s) \right] 
+ \gamma_I + \text{Gap} \left( \frac{\delta}{2}, J \right) \sqrt{\frac{2 \log(\frac{1}{\delta})}{I}}.
\] (42)
Proof: Define $\omega_i, \forall i \in [I]$ as:
\[
\omega_i := E_{p_{\theta}(\phi_s), \psi} \left[ L(\pi_{\theta}(\phi_s), y_s) \right] 
- \frac{1}{J} \sum_{(\phi_s, y_s) \in D_i} E_{\psi} \left[ L(\pi_{\theta}(\phi_s), y_s) \right].
\]
Next, we use Lemma 4 to obtain a bound on $\omega_i, \forall i$; i.e., with probability at least $1 - \delta/2$, the following holds simultaneously for $\omega_i, \forall i \in [I]$:
\[
\omega_i \leq \text{Gap} \left( \frac{\delta}{2}, J \right).
\]
Consequently, $\Omega_i := \sum_{i=1}^{I} \omega_i, i = \{1, \ldots, I\}$ forms a martingale sequence, i.e.,
\[
E[\Omega_{i+1}|\Omega_1, \ldots, \Omega_{i-1}] = \Omega_{i-1}.
\]
Also, we have $|\Omega_{i+1} - \Omega_i| \leq \text{Gap}(\delta/2, J), \forall i \in [I-1]$ with probability $1 - \delta/2$. Next, consider the following lemma:

Lemma 9 (Azuma-Hoeffding’s Inequality). Let $X_0, \ldots, X_I$ be a martingale sequence and $|X_i - X_{i-1}| \leq c_i$. Then with probability $1 - \delta$,
\[
\Pr(X_I - X_0 \geq c) \leq \exp \left( \frac{-c^2}{2 \sum_{i=1}^{I} c_i^2} \right).
\]
Using Lemma 9, we have the following holds with probability at least $(1 - \delta/2)^2 \geq 1 - \delta$,
\[
\Omega_i \leq \text{Gap} \left( \frac{\delta}{2}, J \right) \sqrt{2I \log(2/\delta)}.
\] (43)
Now, consider the following inequality:
\[
\min_{\theta \in \Theta_{1,1}} E_{p_{\theta}, \psi} \left[ L(\pi_{\theta}(\phi_s), y_s) \right] 
\leq \frac{1}{I} \sum_{i=1}^{I} E_{p_{\theta}, \psi} \left[ L(\pi_{\theta}(\phi_s), y_s) \right] 
= \frac{1}{I} \sum_{i=1}^{I} \frac{1}{J} \sum_{(\phi_s, y_s) \in D_i} E_{\psi} \left[ L(\pi_{\theta}(\phi_s), y_s) \right] + \frac{1}{I} \sum_{i=1}^{I} \omega_i.
\]

Hence, with probability of at least $1 - \delta$, we have
\[
\min_{\theta \in \Theta_{1,1}} E_{p_{\theta}, \psi} \left[ L(\pi_{\theta}(\phi_s), y_s) \right] 
\leq \min_{\theta \in \Theta} \frac{1}{I} \sum_{i=1}^{I} \frac{1}{J} \sum_{(\phi_s, y_s) \in D_i} E_{\psi} \left[ L(\pi_{\theta}(\phi_s), y_s) \right] + O(1/I^{1/3})
+ \text{Gap} \left( \frac{\delta}{2}, J \right) \sqrt{\frac{2 \log(2/\delta)}{I}}
\]
\[
\leq \nu + O(1/I^{1/3}) + \text{Gap} \left( \frac{\delta}{2}, J \right) \sqrt{\frac{2 \log(2/\delta)}{I}},
\]
where (a) is by Lemma 7 and (43), and (b) is obtained via using Assumption 3.

When the loss function $L$ is selected to be binary cross-entropy loss, i.e.,
\[
L(x, y) = -y \log(x) - (1 - y) \log(1 - x),
\]
$1 - e^{-L(x, y)}$ corresponds to the classification error. Therefore, classification accuracy for any $\theta$, i.e., $\rho_{\theta}$ is given by
\[
\rho_{\theta} = E_{p_{\theta}, \psi} [\exp(-L(\pi_{\theta}(\phi_s), y_s))].
\]
Note that $\hat{\theta} = \arg \min_{\theta \in \Theta_{1,1}} E_{p_{\theta}, \psi} [\exp(-L(\pi_{\theta}(\phi_s), y_s))]$. Next, we characterize $\rho_{\hat{\theta}}$. To that end, the following follows from Lemma 8.
\[
\exp(E_{p_{\theta}, \psi} [\exp(-L(\pi_{\theta}(\phi_s), y_s))]) 
\geq \exp \left( -\nu - O(1/I^{1/3}) - \text{Gap} \left( \frac{\delta}{2}, J \right) \sqrt{\frac{2 \log(2/\delta)}{I}} \right)
\]
\[
\Rightarrow \rho_{\hat{\theta}} = E_{p_{\theta}, \psi} [\exp(-L(\pi_{\theta}(\phi_s), y_s))] 
\geq \exp \left( -\nu - O(1/I^{1/3}) - \text{Gap} \left( \frac{\delta}{2}, J \right) \sqrt{\frac{2 \log(2/\delta)}{I}} \right),
\]
where (b) follows from Jensen’s inequality.

B. B&B expected number of nodes and optimality

Let $\epsilon_{FP}$ denote the false positive error rate, i.e., the probability of classifying an irrelevant node as relevant. Also define $\epsilon_{FN}$ denote the false negative error rate, i.e., the probability of classifying a relevant node as irrelevant. Then the expected number of branches generated by using pruning policy on B&B was derived in [7]:

Lemma 10 (Theorem 1). Assume that the node selection method in (18) ranks an irrelevant node higher than a relevant node with probability $\epsilon_r$. Then the expected number of branches (number of non-leaf nodes) is
\[
\frac{Q_0 - 1}{2} \leq \left( \left( \frac{1 - \epsilon_{FN}}{1 - 2\epsilon_r \epsilon_{FP}} + \frac{\epsilon_{FN}}{1 - 2\epsilon_{FP}} \right) \epsilon_r \epsilon_{FP} \sum_{n=0}^{N} (1 - \epsilon_{FN})^n \right. 
+ \left( (1 - \epsilon_{FN})^{N+1} (1 - \epsilon_r) \epsilon_{FP} + 1 \right) N.
\]
Our node selection strategy is the lowest lower bound first as detailed in Section II. In the worst case scenario, $\epsilon_r = 1$. Therefore, using Lemma 10, the expected number of branches is
\[
\leq N \left( \frac{1 - \rho_{\hat{\theta}}}{2\rho_{\hat{\theta}} - 1} \sum_{n=0}^{N} \rho_{\hat{\theta}}^n + 1 \right)
\]
\[
\leq N \left( \frac{1 - \rho_{\hat{\theta}}}{2\rho_{\hat{\theta}} - 1} \sum_{n=0}^{N+1} \rho_{\hat{\theta}}^n + 1 \right)
\]
\[
= \frac{N(2\rho_{\hat{\theta}} - \rho_{\hat{\theta}}^N)}{2\rho_{\hat{\theta}} - 1}.
\]
Since the expected number of branches corresponds to the expected number of non-leaf nodes, the total number of nodes in the tree is
\[\leq 2N(2\rho_\theta - \rho_\theta^N) \frac{2\rho_\theta - 1}{2\rho_\theta - 1} + 1.\]

Next, we characterize the probability that Algorithm 3 provides the optimal solution. To this end, observe that there is only one relevant node at any depth \(n\) of the B&B algorithm. The probability of not pruning a relevant node is \(\geq \rho_\theta\). Therefore, the probability of not pruning a relevant node at any depth of the branch and bound tree is \(\geq \rho_\theta^N\) (since \(N\) is the maximum depth of the tree). Hence, the probability of obtaining an optimal solution is at least \(\rho_\theta^N\).

**APPENDIX F**

**GNN DESIGN IN SIMULATIONS**

In this section, we detail the GNN architecture used in the experiments. The GNN is designed to accommodate the unequal input feature dimensions for antennas and users. We enhance the expressiveness of the GNN by letting different layers to have different aggregation matrices in our experiments. The initial embeddings of a common size \(E\) are obtained being a single layer fully connected neural network, i.e.,
\[
q^{(0)}_n = \text{ReLU}(Z_1 x_n)
\]
\[
q^{(0)}_{N+m} = \text{ReLU}(Z_2 x_m)
\]
\[
e_{u,v} = \text{ReLU}(Z_3 e_{u,v}).
\]

where \(Z_1 \in \mathbb{R}^{E \times V_a}, Z_2 \in \mathbb{R}^{E \times V_e}, Z_3 \in \mathbb{R}^{E \times V_e}\), and \(\text{ReLU} : \mathbb{R}^E \to \mathbb{R}^E\) denotes elementwise nonlinear function such that \(\text{ReLU}(x) = \max(x, 0)\).

The first layer of GNN only updates the antenna vertices, i.e., \(q_n, n \in [N]\), as follows
\[
q^{(1)}_n = Z_9 \left(\text{ReLU} \left( Z_8 q^{(0)}_n + \sum_{m=1}^M Z_7 \left(\text{ReLU} \left( Z_6 q^{(0)}_n + Z_5 q^{(0)}_{N+m} + Z_4 e_{n,N+m} \right) \right) \right) \right), \forall n \in [N]
\]
\[
q^{(1)}_{N+m} = q^{(0)}_{N+m}, \forall m \in [M].
\]

The second layer only updates the user vertices as follows
\[
q^{(2)}_{N+m} = Z_{15} \left(\text{ReLU} \left( Z_{14} q^{(1)}_{N+m} + \sum_{n=1}^N Z_{13} \left(\text{ReLU} \left( Z_{12} q^{(1)}_{N+m} + Z_{11} q^{(1)}_n + Z_{10} e_{n,N+m} \right) \right) \right) \right), \forall m \in [M]
\]
\[
q^{(2)}_n = q^{(1)}_n, \forall n \in [N].
\]

Such “split updating” of different nodes’ embeddings in two layers has been advocated in [8] for the type of graph structure used in this work (i.e., a bipartite graph). Moreover, there is a potential saving in the computational cost in both training and testing [9] compared to updating all nodes’ embeddings in each layer.

Finally, \(\pi_\theta(\phi)\) is computed using the \(q^{(2)}_{N+m}, \forall m \in [M]\) as follows:
\[
\pi_\theta(\phi) = \text{Sigmoid} \left( \frac{1}{M} \sum_{m=1}^M \beta^I \text{ReLU}(Z_{16} q^{(2)}_{N+m}) \right),
\]

where \(Z_{1}, \ldots, Z_{16} \in \mathbb{R}^{E \times E}, \beta \in \mathbb{R}^E\), and \(\text{Sigmoid} : \mathbb{R} \to \mathbb{R}\) is the sigmoid function, i.e., \(\text{Sigmoid}(x) = \frac{1}{1 + \exp(-x)}\).

**APPENDIX G**

**CONSTRUCTION OF INPUT FEATURES (\(\phi(A^{(t)}_s)\))**

We assign the features tabulated in Table I among the elements of the following sets: \(\{x_i \mid i \in [N]\}, \{x_{N+i} \mid i \in [M]\}\), and \(\{e_{i,N+j} \mid i \in [N], j \in [M]\}\). Specifically, the problem size-dependent features that can be represented with a vector of dimension \(N\) (i.e., \(A^{(t)}_s\), and \(B^{(t)}_s\), \(||W_{t,s}(1,:)||^2_2, \ldots, ||W_{t,s}(N,:)||^2_2\)) are assigned to the elements of \(\{x_i \mid i \in [N]\}\) as follows:
\[
x_i(1) = \begin{cases} 1, & \text{if } i \in A^{(t)}_s \\ 0, & \text{otherwise,} \end{cases}
\]
\[
x_i(2) = \begin{cases} 1, & \text{if } i \in B^{(t)}_s \\ 0, & \text{otherwise, and} \end{cases}
\]
\[
x_i(3) = ||W_{t,s}(i,:)||^2_2.
\]

Similarly, the problem size-dependent features that can be represented by a vector of dimension \(M\) (i.e., \(W_{t,s}(i,:)^H h_m\) and the aggregated interference under \(W_{t,s}\) are assigned to the elements of \(\{x_{N+i} \mid i \in [M]\}\) as follows:
\[
x_{N+i}(1) = ||W_{t,s}(i,:)^H h_i||^2_2 \\
x_{N+i}(2) = \sum_{j \neq i} ||W_{t,s}(i,:)^H h_j||^2_2.
\]

The remaining problem size-dependent features can be represented by a vector of dimension \(NM\), and are assigned to the elements of \(\{e_{i,N+j} \mid i \in [N], j \in [M]\}\) as follows:
\[
(e_{i,N+j}(1), e_{i,N+j}(2), e_{i,N+j}(3)) = (\text{Re}(H(i,j)), \text{Im}(H(i,j)), |H(i,j)|)
\]
\[
(e_{i,N+j}(4), e_{i,N+j}(5), e_{i,N+j}(6)) = (\text{Re}(W_{\text{incumbent}}(i,j)), \text{Im}(W_{\text{incumbent}}(i,j)), |W_{\text{incumbent}}(i,j)|)
\]
\[
(e_{i,N+j}(7), e_{i,N+j}(8), e_{i,N+j}(9)) = (\text{Re}(W_{t,s}(i,j)), \text{Im}(W_{t,s}(i,j)), |W_{t,s}(i,j)|),
\]

where \(\text{Re}(\cdot)\) and \(\text{Im}(\cdot)\) returns the real and imaginary part of the complex number.

Finally, the problem size-independent features are assigned to the set \(\{x_{N+i} \mid i \in [M]\}\) as follows:
\[
(x_{N+i}(3), x_{N+i}(4), \ldots, x_{N+i}(8))
\]
\[
= (i^{(t)}_G, u^{(t)}_G, \Phi_{ib}(A^{(t)}_s), \Phi_{ab}(A^{(t)}_s), \ell, ||(\Phi_{ab}(A^{(t)}_s) - u^{(t)}_G) < \epsilon||).
\]
APPENDIX H

SOLVING SDR IN (5)

The method for solving SDR in (5) is explained in [10]. We detail the procedure below for the sake of completeness. The constraint (5b) can be equivalently written as a linear matrix inequality using the $S$-lemma. The equivalent optimization problem is then expressed as follows:

$$\begin{array}{l}
\text{minimize} \sum_{m=1}^{M} \text{tr}(W_m) \\
\text{subject to } Y_m = \begin{bmatrix} Q_m + t_m I & r_m \\ r_m^H & s_m - t_m^2 \end{bmatrix}, \quad m \in [M] \\
Y_m \succeq 0, \quad W_m \succeq 0, \quad t_m \geq 0, \quad m \in [M],
\end{array}$$

where,

$$\begin{align*}
Q_m &= \frac{1}{\gamma_m} W_i - \sum_{j \neq i} W_j, \\
r_m &= Q_m h_m, \\
s_m &= h_m^H Q_m h_m - \sigma_m^2.
\end{align*}$$

When the conditions in Lemma 2 are satisfied, the optimal beamforming matrix $W^* = [w^*_1, w^*_2, \ldots, w^*_M]$ can be obtained from optimal solution, $W^*_m, \forall m$, to the above problem as follows:

$$w^*_m = \sqrt{\lambda_1^{(m)} v_1^{(m)}}, \forall m \in [M], \quad (44)$$

where $\lambda_1$ and $v_1$ are the principal eigenvalue and eigenvector of $W^*_m$, respectively.

REFERENCES