On the role of features in vertex nomination: Content and context together are better (sometimes)

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Abstract

Vertex nomination is a lightly-supervised network information retrieval (IR) task in which vertices of interest in one graph are used to query a second graph to discover vertices of interest in the second graph. Similar to other IR tasks, the output of a vertex nomination scheme is a ranked list of the vertices in the second graph, with the heretofore unknown vertices of interest ideally concentrating at the top of the list. Vertex nomination schemes provide a useful suite of tools for efficiently mining complex networks for pertinent information. In this paper, we explore, both theoretically and practically, the dual roles of content (i.e., edge and vertex attributes) and context (i.e., network topology) in vertex nomination. We provide necessary and sufficient conditions under which vertex nomination schemes that leverage both content and context outperform schemes that leverage only content or context separately. While the joint utility of both content and context has been demonstrated empirically in the literature, the framework presented in this paper provides a novel theoretical basis for understanding the potential complementary roles of network features and topology.

1 Introduction

Network data has become ubiquitous in the sciences, owing to the generality and flexibility of networks in modeling relations among entities. Networks appear in such
varied fields as neuroscience, genomics, the social sciences, economics and ecology, to name just a few (see, for example, [34]). As such, statistical analysis of network data has emerged as an important field within modern statistics [22, 23, 11]. Many classical statistical inference tasks, such as hypothesis testing [52, 53, 24, 16], regression [14, 31], and maximum likelihood estimation [4, 48, 2] have been adapted to network data. Inference tasks that are specific to network data, such as link-prediction [25], community detection [35, 44, 49], and vertex nomination [30, 8, 51, 12] have also seen increasing popularity in recent years. Among these network-specific tasks is the vertex nomination problem, in which the goal is to identify vertices similar to one or more vertices specified as being of interest to a practitioner. The vertex nomination (VN) task is similar in spirit to popular network-based information retrieval (IR) procedures such as PageRank [38] and personalized recommender systems on graphs [19]. In VN, the goal is as follows: Given vertices of interest in a graph $G_1$, produce a ranked list of the vertices in a second graph $G_2$ according to how likely they are judged to be interesting. Ideally, interesting vertices in $G_2$ should concentrate at the top of the ranked list. As an inference task, this formulation of VN is distinguished from other supervised network IR tasks by the generality of what may define vertices as interesting and the limited available training data in $G_1$. In contrast to typical IR problems, there is little or no training data available in the vertex nomination problem.

The vertex nomination problem was first introduced as a task involving only a single graph, and vertices of interest were modeled as belonging to a single community of vertices [8, 12, 28, 59]. The information provided by vertices with known community memberships, called seed vertices, was leveraged to rank vertices with unknown membership, with both network-topology and available vertex features being leveraged to produce ranking schemes [30, 9, 51]. This single-graph, community-based definition of the problem is somewhat limited in its ability to capture network models beyond the stochastic blockmodel [18]. Subsequent work lifted the problem to the two-network setting considered here [40], allowing a generalization of what defines interesting vertices and a generalization of the network models that could be considered [40, 29, 1].

In many settings, observed networks are endowed with features at the vertex and/or edge level. For example, in social networks, vertices typically correspond to users for whom we have demographic information, and edges correspond to different types of social relations. The theoretical advances in both the single- and multiple-graph VN problem recounted above were established in the context of networks where no such feature are available. It is natural, then, to seek to better understand the effect of network attributes on the theoretical VN framework developed in [29, 1]. Motivated by this, in the present work we develop VN on richly-featured networks, and we explore
how the incorporation of this information impacts the concepts of Bayes optimality and consistency for the VN problem. Furthermore, in Sections 4 and 5, adopting an information theoretic perspective, we give the first steps toward a theoretical understanding (which is born out in subsequent experiments) of the potential benefit of VN schemata that use both content and context versus one of content or context alone.

The remainder of the paper is laid out as follows. In Section 2, we outline the extension of the vertex nomination framework to the richly featured network setting, defining richly featured graphs in Section 2.1, VN schema in Section 2.2, and VN performance measures in Section 2.3. In Section 3, we derive the Bayes optimal VN scheme in the setting of richly featured networks, and in Sections 4 and 5 we compare VN performance in the richly featured setting to that in the featureless and graph-less settings, respectively. Experiments further illustrating the practical implications of the theory are presented in Section 6.

Notation: Please refer to Table 1 for a list of commonly used notation throughout the paper.

2 Vertex Nomination with Features

When the defining trait of interesting vertices was membership in a community of interest, graph models with latent community structure (e.g., the stochastic blockmodel [18, 20]) were sensible models for the underlying network structure. The need for more general notions of what renders a vertex interesting necessitated more nuanced models, culminating in the Nominatable Distribution network model introduced in [29]. We take this model as our starting point, and extend it by endowing it with both edge and vertex features.

2.1 Richly Featured Networks

We begin by defining the class of networks with vertex and edge features, which we call richly featured networks. We note here that there is a large literature on inference within attributed networks, with richly featured graphs arising in settings such as social network analysis [21, 58] and knowledge representation [36, 37], among others.

Definition 1. Let $\mathcal{V}$ and $\mathcal{E}$ be discrete sets of possible vertex and edge features, respectively. A richly featured network $g$ indexed by $(n, d_1, d_2, \mathcal{V}, \mathcal{E})$ is an ordered tuple $g = (g, x, w)$ where
| Symbol | Description | Definition |
|--------|-------------|------------|
| $\mathcal{V}$ | Denotes a discrete set of vertex features | - |
| $[n]$ | For $n \in \mathbb{Z}_{>0}$, this denotes $\{1, 2, 3, \ldots, n\}$ | - |
| $(S)$ | For a set $S$, this represents the set $\{u, v\}$ s.t. $u, v \in S$ | - |
| $\mathcal{E}$ | Denotes a discrete set of vertex features | - |
| $\tilde{\mathcal{E}}$ | The set $\mathcal{E} \cup \{\star\}$, where $\star$ is a special symbol representing unavailable data | Def. 1 |
| $\mathcal{G}_n$ | For $n \in \mathbb{Z}_{>0}$, the set of labeled, undirected graphs on $n$ vertices | - |
| $\mathcal{G}^{d_1, d_2}_{n, \mathcal{V}, \tilde{\mathcal{E}}}$ | For $n, d_1, d_2 \in \mathbb{Z}_{>0}$, the set of richly featured networks of order $(n, d_1, d_2)$ with vertex (resp., edge) features in $\mathcal{V}^{d_1}$ (resp., $\tilde{\mathcal{E}}^{d_2}$) | Def. 1 |
| $V_g$ | For graph $g \in \mathcal{G}_n$, $V_g$ denotes the set of vertices of $g$ | - |
| $E_g$ | For graph $g \in \mathcal{G}_n$, $E_g$ denotes the set of edges of $g$ | - |
| $N$ | The set $\begin{pmatrix} n \\ 2 \end{pmatrix}$ | - |
| $M$ | The set $\begin{pmatrix} m \\ 2 \end{pmatrix}$ | - |
| $\vec{0}$ | The vector of all 0’s | - |
| $X[i,:]$ | This denotes the $i$-th row of a matrix $X$ | - |
| $X[S,:]$ | For a set $S$, this denotes the submatrix of $X$ with rows indexed by $S$ | - |
| $\simeq$ | If $g_1, g_2 \in \mathcal{G}_n$ satisfy $g_1 \simeq g_2$, then $g_1$ is isomorphic to $g_2$ | - |
| $\simeq$ | If $g_1, g_2 \in \mathcal{G}^{d_1, d_2}_{n, \mathcal{V}, \tilde{\mathcal{E}}}$ satisfy $g_1 \simeq g_2$, then $g_1$ is feature-preserving isomorphic to $g_2$ | Def. 8 |

Table 1: Commonly used notation

i. $g = (V, E) \in \mathcal{G}_n$ is a labeled, undirected graph on $n$ vertices. The vertices of $g$ will be denoted via either $V = \{v_1, v_2, \ldots, v_n\}$ or $V = \{u_1, u_2, \ldots, u_n\}$.

ii. $x \in \mathcal{V}^{m \times d_1}$ denotes the matrix of $d_1$-dimensional vertex features, so that $x[v,:]$ is the vector of features associated with vertex $v$.

iii. Let $\tilde{\mathcal{E}} = \mathcal{E} \cup \{\star\}$, where we use $\star$ as a special symbol representing unavailable data. Letting $N = \begin{pmatrix} n \\ 2 \end{pmatrix}$, $w \in \tilde{\mathcal{E}}^{N \times d_2}$ denotes the matrix of $d_2$-dimensional edge features. Indexing $\begin{pmatrix} \mathcal{V} \\ 2 \end{pmatrix}$ lexicographically, for $e \in \begin{pmatrix} \mathcal{V} \\ 2 \end{pmatrix}$, we write $w[e,:]$ for the
vector of features associated with edge \( e \). The form of \( \mathbf{w} \) is then

\[
\mathbf{w} = \begin{pmatrix}
\mathbf{w} \{v_1, v_2\}, : \\
\mathbf{w} \{v_1, v_3\}, : \\
\mathbf{w} \{v_1, v_4\}, : \\
\vdots \\
\mathbf{w} \{v_{n-1}, v_n\}, : 
\end{pmatrix}.
\]

We further require that

\[
\mathbf{w}[e, :] = \begin{cases}
\left(\star, \star, \cdots, \star\right) \in \tilde{\mathcal{E}}^{d_2} & \text{if } e \notin E; \\
\in \mathcal{E}^{d_2} & \text{if } e \in E.
\end{cases}
\]

We will denote the set of richly featured networks indexed by \((n, d_1, d_2, \mathcal{V}, \mathcal{E})\) by \( \mathcal{G}^{d_1, d_2}_{n, \mathcal{V}, \mathcal{E}} \).

Let \( e \in \binom{\mathcal{V}}{2} \). In the definition of richly featured networks, for \( e \notin E \), we interpret the edge features \( \mathbf{w}[e, :] \) as unavailable data. This is a sensible assumption in practice, and is commonly made in richly featured network models (see, for example, [41, 61]). We note that the structure of \( \mathbf{w} \) encodes the edge structure of \( g \). We choose to keep the redundant \( g \) in Definition 1, as \( g \) encodes the purely topological structure of the graph, absent any edge- or vertex-level features, a fact that will prove useful in subsequent analyses.

Remark 2. We use discrete vertex and edge feature sets in Definition 1, as this is both rich enough to model many real world networks (where features encode types, characteristics or discrete weights, for example) and amenable to the theoretical derivations in vertex nomination. Considering continuous features is not a practical problem, but does raise subtle difficulties in the theoretical machinations to follow. See Remark 22 for further discussion.

Definition 3. Let \( N = \binom{n}{2} \). For \( \mathbf{w} \in \tilde{\mathcal{E}}^{N \times d_2} \), we define \( \gamma(\mathbf{w}) = (V_{\gamma(\mathbf{w})}, E_{\gamma(\mathbf{w})}) \in \mathcal{G}_n \) to be the graph compatible with the edge features in \( \mathbf{w} \); i.e., \( \gamma(\mathbf{w}) \in \mathcal{G}_n \), and

\[
\mathbf{w}[e, :] = \left(\star, \star, \cdots, \star\right) \text{ iff } e \notin E_{\gamma(\mathbf{w})} ;
\]

\[
\mathbf{w}[e, :] \in \mathcal{E}^{d_2} \text{ iff } e \in E_{\gamma(\mathbf{w})}.
\]

Example 4. Consider the graph \( g \in \mathcal{G}^{d_1, d_2}_{4, \mathcal{V}, \mathcal{E}} \) with \( g \) given by

\[
g = (V_g, E_g) = (\{1, 2, 3, 4\}, \{\{1, 2\}, \{1, 3\}, \{1, 4\}, \{3, 4\}\}).
\]
The edge features for this network would then be of the form

\[
\mathbf{w} = \begin{pmatrix}
    \mathbf{w}([v_1, v_2], :)
    \\
    \mathbf{w}([v_1, v_3], :)
    \\
    \mathbf{w}([v_1, v_4], :)
    \\
    \mathbf{w}([v_2, v_3], :)
    \\
    \mathbf{w}([v_2, v_4], :)
    \\
    \mathbf{w}([v_3, v_4], :)
\end{pmatrix} = \begin{pmatrix}
    \mathbf{w}([v_1, v_2], :) \in \mathcal{E}^d_2
    \\
    \mathbf{w}([v_1, v_3], :) \in \mathcal{E}^d_2
    \\
    \mathbf{w}([v_1, v_4], :) \in \mathcal{E}^d_2
    \\
    \mathbf{w}([v_2, v_3], :) \in \mathcal{E}^d_2
    \\
    \mathbf{w}([v_2, v_4], :) \in \mathcal{E}^d_2
    \\
    \mathbf{w}([v_3, v_4], :) \in \mathcal{E}^d_2
\end{pmatrix}.
\]

**Remark 5.** Let \((n, d_1, d_2)\) be an ordered tuple of nonnegative integers, and let \(\mathcal{V}\) and \(\mathcal{E}\) be discrete sets of edge and vertex features. In the definitions and exposition that follows, we will be considering \(\mathcal{G}_{n, \mathcal{V}, \mathcal{E}} - \text{valued random variables. Implicitly, we mean the following: letting } (\Omega, \mathcal{F}, \mathbb{P}) \text{ be a given probability space, } (G, \mathbf{X}, \mathbf{W}) : \Omega \rightarrow \mathcal{G}_{n, \mathcal{V}, \mathcal{E}} \text{ is a } \mathcal{G}_{n, \mathcal{V}, \mathcal{E}} - \text{valued random variable if it is } (\mathcal{F}, \mathcal{F}_{G_n} \otimes \mathcal{F}_{d_1} \otimes \mathcal{F}_{d_2}) - \text{measurable, where } \mathcal{F}_{G_n} \text{ is the total sigma field on } \mathcal{G}_n, \mathcal{F}_{d_1} \text{ is the total sigma field on } \mathcal{V}^{n \times d_1}, \text{ and } \mathcal{F}_{d_2} \text{ is the total sigma field on } \mathcal{E}^{N \times d_2}.

With Definition 1 in hand, lifting the definition of **Nominatable Distributions** first introduced in [29] to the attributed graph setting is relatively straightforward.

**Definition 6.** For a given \(n, m \in \mathbb{Z}_{>0}\) and given sets of discrete vertex and edge features \(\mathcal{V}\) and \(\mathcal{E}\), respectively, the set of **Richly Featured Nominatable Distributions** of order \((n, m)\) with feature sets \(\mathcal{V}\) and \(\mathcal{E}\), denoted \(\mathcal{F}_{\mathcal{V}, \mathcal{E}}^{(n, m)}\), is the collection of all families of distributions of the form

\[
\mathbf{F}^{(n, m)} = \left\{ F^{(n, m)}_{c, \theta, (d_1, e_1), (d_2, e_2)} \mid (c, \theta, (d_1, e_1), (d_2, e_2)) \in \mathbb{Z}_{\geq 0} \times \mathbb{R}^{d(n, m)} \times \mathbb{Z}^2_{\geq 0} \times \mathbb{Z}^2_{> 0}, \right. \\
\left. \text{and } 0 \leq c \leq \min(n, m) \right\},
\]

where \(F^{(n, m)}_{c, \theta, (d_1, e_1), (d_2, e_2)}\) is a distribution on \(\mathcal{G}_n \times \mathcal{V}^{n \times d_1} \times \mathcal{E}^{N \times e_1} \times \mathcal{G}_m \times \mathcal{V}^{m \times d_2} \times \mathcal{E}^{M \times e_2}\) (recalling that \(N = \binom{n}{2}, M = \binom{m}{2}\)), parameterized by \(\theta \in \mathbb{R}^{d(n, m)}\) satisfying the following conditions:

1. The vertex sets \(V_1 = \{v_1, v_2, ..., v_n\}\) and \(V_2 = \{u_1, u_2, ..., u_m\}\) satisfy \(v_i = u_i\) for \(1 \leq i \leq c\). We refer to \(C = \{v_1, v_2, ..., v_c\} = \{u_1, u_2, ..., u_c\}\) as the core vertices. These are the vertices that are shared across the two graphs and imbue the model with a natural vertex correspondence.

2. Vertices in \(J_1 = V_1 \setminus C\) and \(J_2 = V_2 \setminus C\), satisfy \(J_1 \cap J_2 = \emptyset\). We refer to \(J_1\) and \(J_2\) as junk vertices. These are the vertices in each graph that have no corresponding vertex in the other graph.
3. If \((G_1, X, W, G_2, Y, Z)\) is distributed according to \(F^{(n,m)}_{c,\theta, (d_1, e_1), (d_2, e_2)}\), then \((G_1, X, W)\) is a \(G_{d_1, e_1}^{d_1, e_1} \times V, E\)-valued random variable and \((G_2, Y, Z)\) is a \(G_{d_2, e_2}^{d_2, e_2} \times V, E\)-valued random variable. The edge features \(W \in \tilde{E}^{N \times e_1}\) and \(Z \in \tilde{E}^{M \times e_2}\) almost surely satisfy

\[
W[e, :] = \begin{cases} 
(\star, \star, \cdots, \star) & \text{if } e \notin E(G_1); \\
E^{e_1} & \text{if } e \in E(G_1);
\end{cases}
\]

and

\[
Z[e, :] = \begin{cases} 
(\star, \star, \cdots, \star) & \text{if } e \notin E(G_2); \\
E^{e_2} & \text{if } e \in E(G_2).
\end{cases}
\]

4. The richly featured subgraphs induced by the junk vertices,

\[
\left( G_1[J_1], X[J_1, :], W \left[ \left( J_1 \atop 2 \right) \right] \right) \text{ and } \left( G_2[J_2], Y[J_2, :], Z \left[ \left( J_2 \atop 2 \right) \right] \right)
\]

are conditionally independent given \(\theta\).

In Definition 6, the rows of \(X \in \mathcal{V}^{n \times d_1}\) are the vertex features of \(G_1\), with \(X[i, :]\) representing the feature associated with vertex \(i\) in \(G_1\). Similarly, the rows of \(Y \in \mathcal{V}^{n \times d_2}\) are the vertex features of \(G_2\), with \(Y[i, :]\) representing the vertex feature of vertex \(i\) in \(G_2\). We do not, a priori, assume that any vertex features are missing, although extending the definition to \(\tilde{V} = \mathcal{V} \cup \{\star\}\) is straightforward. With this definition in place, we are ready to define feature aware vertex nomination schemes.

**Note:** In order to ease notation moving forward, we will write

\[
\Theta := (c, \theta, (d_1, e_1), (d_2, e_2)),
\]

and accordingly write \(F^{(n,m)}_{c,\theta, (d_1, e_1), (d_2, e_2)}\) for \(F^{(n,m)}_{c,\theta, (d_1, e_1), (d_2, e_2)}\). In the sequel, we will assume that the feature sets \(\mathcal{E}\) and \(\mathcal{V}\) are given and satisfy \(|\mathcal{E}| = |\mathcal{V}| = \infty\). We will suppress the dependence of the family of richly featured nominatable distributions on the feature sets \(\mathcal{E}\) and \(\mathcal{V}\), writing \(F^{(n,m)} = F^{(n,m)}_{\mathcal{V}, \mathcal{E}}\).

### 2.2 Vertex Nomination Schemes

In vertex nomination, the labels of vertices in the second graph, \(g_2\), are assumed unknown a priori. In order to accomplish this in our Featured Nominatable Distribution framework, we introduce obfuscation functions as in [29]. Obfuscation functions serve to hide vertex labels, and can be interpreted as a non-probabilistic version of the vertex shuffling considered in [56, 26].
Definition 7. Consider graphs \((g_1, g_2) \in G_{m_1, n_1, \mathcal{E}} \times G_{m_2, n_2, \mathcal{E}}\) with vertex sets \(V_1\) and \(V_2\), respectively. An obfuscating set, \(H\), of \(V_1\) and \(V_2\) of order \(|V_2| = m\) is a set satisfying \(H \cap V_i = \emptyset\) for \(i = 1, 2\), and \(|H| = |V_2| = m\). Given obfuscating set \(H\), an obfuscating function \(\sigma : V_2 \to H\) is a bijection from \(V_2\) to \(H\). We denote by \(O_H\) the set of all such obfuscation functions. For a richly featured network \(g = (g, x, w) \in G_{m, n, \mathcal{E}}\), we will write \(\sigma(g) = (\sigma(g), \sigma(x), \sigma(w))\) where

i. \(\sigma(g)\) denotes the graph \(g = (V_g, E_g)\) with labels obfuscated by \(\sigma\). That is, \(\sigma(g) = (V_{\sigma(g)}, E_{\sigma(g)})\), where \(V_{\sigma(g)} = \{\sigma(v) : v \in V_g\}\) and \(E_{\sigma(g)}\) is such that \(\{u, v\} \in E_g\) if and only if \(\{\sigma(u), \sigma(v)\} \in E_{\sigma(g)}\).

ii. \(\sigma(x)\) is the vertex feature matrix associated with \(\sigma(g)\), so that for \(u \in H\),

\[
(\sigma(x))[u, \cdot] = x[\sigma^{-1}(u), \cdot].
\]

iii. \(\sigma(w)\) is the edge feature matrix associated with \(\sigma(g)\), so that for \(\{v, u\} \in (H/2)\),

\[
(\sigma(w)) \{[v, u], \cdot] = w \{[\sigma^{-1}(v), \sigma^{-1}(u)], \cdot]\).
\]

Note that we will assume that \(H\) is ordered (by an arbitrary but fixed ordering), and that the edges of \(\sigma(w)\) are ordered lexicographically according to the ordering on \(H\). We do not necessarily assume that the ordering of \(H\) is the ordering induced by \(V\). That is, we do not necessarily assume that \(u \leq v\) implies \(\sigma(u) \leq \sigma(v)\).

The purpose of the obfuscating function is to render the labels on the vertices in \(g_2\) uninformative. As such, it is sensible to require vertex nomination schemes (defined below) to be independent of labels in the following sense. Informally, if a set of vertices have identical features and edge structures, then their rankings in a VN scheme should be independent of the chosen obfuscation function \(\sigma \in O_H\). This is made precise in Definition 9 (and Assumption 10) below, but requires some preliminary definitions.

Definition 8. Let \(g = (g, x, w) \in G_{d_1, d_2}^{d_1, d_2}\) be a richly featured network. A permutation \(\sigma : [n] \to [n]\) acts on \(g\) to produce \(\sigma(g) = (g', x', w') \in G_{d_1, d_2}^{d_1, d_2}\), where

i. \(g' = \sigma(g)\) is the graph \(g\) with its vertex labels permuted by \(\sigma\).

ii. \(x'\) is the vertex feature matrix associated with \(g'\), so that for \(v \in [n]\),

\[
x'[v, \cdot] = x[\sigma^{-1}(v), \cdot].
\]

iii. \(w'\) is the edge feature matrix associated with \(g'\), so that for \(\{u, v\} \in ([n]/2)\),

\[
w'[[u, v], \cdot] = w[[\sigma^{-1}(u), \sigma^{-1}(v)], \cdot].
\]
We call a permutation $\sigma$ a feature-preserving automorphism (abbreviated $f$-automorphism) of $g$ if $g = \sigma(g)$. Similarly, we call a permutation $\sigma$ a feature-preserving isomorphism between $g$ and $g'$ (abbreviated $f$-isomorphism) if $g' = \sigma(g)$.

Let $g = (g, x, w) \in G^{d_1, d_2}_{n, V, E}$ be a richly featured network. For each $u \in V_g$, define

$$\mathcal{I}(u; g) := \{w \in V_g \text{ s.t. } \exists \text{ an } f\text{-automorphism } \sigma \text{ of } g \text{ s.t. } \sigma(u) = w\}.$$ 

With the above notation in hand, we are now ready to introduce the concept of a feature aware vertex nomination scheme. In the definition to follow, $V^*$ represents the set of vertices of interest in $g_1$. These are usually assumed to be in $V_1 \cap V_2$, and the goal of a vertex nomination scheme is to have $o(V^*)$ concentrate at the top of the produced rank list in $T_H$.

**Definition 9 (Feature-aware VN Scheme).** Let $n, m, d_1, e_1, d_2, e_2 \in \mathbb{Z}_{>0}$ and $V, E$ be given. Let $H$ be an obfuscating set of $V_1$ and $V_2$ of order $|V_2| = m$, and let $o \in \mathcal{O}_H$ be given. For a set $A$, let $\mathcal{T}_A$ denote the set of all total orderings of the elements of $A$.

A feature-aware vertex nomination scheme (FA-VN scheme) on $G^{d_1, e_1}_{n, V, E} \times o(G^{d_2, e_2}_{m, V, E})$ is a function

$$\Phi : G^{d_1, e_1}_{n, V, E} \times o(G^{d_2, e_2}_{m, V, E}) \times 2^{V_1} \to \mathcal{T}_H$$

satisfying the consistency criteria in Assumption 10. We let $\mathcal{N}^{(n, m)} = \mathcal{N}^{(d_1, e_1), (d_2, e_2)}$ denote the set of all such VN schemes.

The consistency criteria we require FA-VN schemes to satisfy essentially forces the schemes to be agnostic to the labels in the obfuscated $o(g_2)$. To accomplish this, we define the following.

**Assumption 10 (FA-VN Consistency criteria).** With notation as in Definition 9, for each $u \in V_2$ and $V^* \subseteq V_1$, define

$$\text{rank}_{\Phi(g_1, o(g_2), V^*)}(o(u))$$

to be the position of $o(u)$ in the total ordering provided by $\Phi(g_1, o(g_2), V^*)$. Further, define $\tau_{\Phi} : G^{d_1, e_1}_{n, V, E} \times G^{d_2, e_2}_{m, V, E} \times \mathcal{O}_H \times 2^{V_1} \times 2^{V_2} \to 2^m$ via

$$\tau_{\Phi}(g_1, g_2, o, V^*, S) = \{\text{rank}_{\Phi(g_1, o(g_2), V^*)}(o(u)) \text{ s.t. } u \in S\}.$$ 

For any $g_1 \in G^{d_1, e_1}_{n, V, E}$, $g_2 \in G^{d_2, e_2}_{m, V, E}$, $V^* \subseteq V_1$, obfuscating functions $o_1, o_2 \in \mathcal{O}_H$ and any $u \in V(g_2)$, we require

$$\tau_{\Phi}(g_1, g_2, o_1, V^*, \mathcal{I}(u; g_2)) = \tau_{\Phi}(g_1, g_2, o_2, V^*, \mathcal{I}(u; g_2))$$

$$\Leftrightarrow o_2 \circ o_1^{-1}(\mathcal{I}(\Phi(g_1, o_1(g_2), V^*)[k]; o_1(g_2)) = \mathcal{I}(\Phi(g_1, o_2(g_2), V^*)[k]; o_2(g_2))$$

for all $k \in [m]$. 

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The consistency property in Definition 9 requires that the ranking of \{2, 8\} must be the same under \(o_1\) and \(o_2\). This requirement is obeyed by the VN scheme illustrated in subplot (a), but is violated by the scheme illustrated in subplot (b).

where \(\Phi(g_1, o(g_2), V^*)[k]\) denotes the \(k\)-th element (i.e., the rank-\(k\) vertex) in the ordering \(\Phi(g_1, o(g_2), V^*)\).

Figure 1 gives a simple illustrative example of this consistency criterion (i.e., Eq. 1) in action. Note here that if \(\mathcal{I}(u; g_2) = \{u\}\) for all \(u \in V_2\), then the consistency criterion forces

\[
\Phi(g_1, \sigma(o(g_2)), V^*) = \sigma(\Phi(g_1, o(g_2), V^*))
\]

for any permutation \(\sigma\) and obfuscating \(o \in \mathcal{O}_H\).

2.2.1 Ties that bind

In VN and other IR ranking problems, ties due to identical structure (here represented by \(f\)-isomorphisms in \(g_1\) or \(g_2\)) cause theoretical complications. We refer the interested reader to \([29, 1]\) for examples of these complications and how they can be handled.

In order to avoid the additional notational and definitional burdens required to deal with tie-breaking in these situations, we will make the following assumption on the distributions considered in \(\mathcal{F}(n,m)\).

Assumption 11. Let \((G_1, G_2) \sim \mathcal{F}_\Theta(n,m) \in \mathcal{F}(n,m)\). Consider the events

\[
D_1 = \{ \text{the only } f\text{-automorphism of } G_1 \text{ is } \sigma = id_n \}
\]

\[
D_2 = \{ \text{the only } f\text{-automorphism of } G_2 \text{ is } \sigma = id_m \}
\]
\( F_{\Theta}^{(n,m)} \) satisfies \( \mathbb{P}_{F_{\Theta}^{(n,m)}}(D_1) = \mathbb{P}_{F_{\Theta}^{(n,m)}}(D_2) = 1 \).

This assumption is unrealistic if there are only a few categorical vertex features (for example, roles in a corporate hierarchy), but this assumption is less restrictive when there are a large number of available categorical features or the features are continuous. We stress that this assumption is made purely to ease the presentation of theoretical material, and the practical impact of this assumption being violated is easily overcome.

### 2.3 Loss and Bayes Loss

A vertex nomination scheme is, essentially, a semi-supervised IR system for querying large networks. Similar to the recommender system framework [43], a VN scheme is judged to be successful if the top of the nomination list contains a high concentration of vertices of interest from the second network. This motivates the definition of VN loss based on the concept of precision-at-\( k \).

**Definition 12.** Let \( \Phi \in \mathcal{N}^{(n,m)} = \mathcal{N}^{(n,m)}_{(d_1,e_1),(d_2,e_2)} \) be a vertex nomination scheme, \( H \) an obfuscating set of \( V_1 \) and \( V_2 \) of order \( |V_2| = m \), and \( \sigma \in \mathcal{D}_H \). Let \( (g_1,g_2) \) be realized from

\[
(G_1,X,W,G_2,Y,Z) \sim F_{\Theta}^{(n,m)} \in \mathcal{F}^{(n,m)}
\]

with a vertex of interest set \( V^* \subset \mathcal{C} = V_1 \cap V_2 \). For \( k \in \{m-1\} \), we define

(i) For \((g_1,g_2)\) realized as \((G_1,X,W,G_2,Y,Z)\), the level-\( k \) nomination loss

\[
\ell_k(\Phi,g_1,\sigma(g_2),V^*) := 1 - \frac{\sum_{v \in V^*} \mathbb{1}\{\text{rank}_{\Phi}(g_1,\sigma(g_2),V^*)(\sigma(v)) \leq k\}}{|k|}
\]

(ii) The level-\( k \) error of \( \Phi \) is defined as

\[
L_k(\Phi,V^*) = L_k(\Phi,V^*,\sigma) := \mathbb{E}_{(G_1,G_2) \sim F_{\Theta}^{(n,m)}}[\ell_k(\Phi,G_1,\sigma(G_2),V^*)]
\]

\[
= 1 - \frac{1}{k} \sum_{v \in V^*} \mathbb{P}_{F_{\Theta}^{(n,m)}}\left( \text{rank}_{\Phi}(G_1,\sigma(G_2),V^*)(\sigma(v)) \leq k \right),
\]

where \( G_1 = (G_1,X,W) \) and \( G_2 = (G_2,Y,Z) \).

The level-\( k \) Bayes optimal scheme for \( F_{\Theta}^{(n,m)} \) is defined as any element

\[
\Phi^*_{k,V^*} = \Phi^*_{k,V^*} \in \arg\min_{\Phi \in \mathcal{N}^{(n,m)}} L_k(\Phi,V^*),
\]

with corresponding Bayes error \( L^*_k \).

**Remark 13.** Note that we could have also defined a recall-based loss function via

\[
\ell^{(r)}_k(\Phi,g_1,g_2,V^*) := \frac{\sum_{v \in V^*} \mathbb{1}\{\text{rank}_{\Phi}(g_1,\sigma(g_2),V^*)(\sigma(v)) \geq k+1\}}{|V^*|}.
\]
We focus on the more natural precision-based loss function, but we note in passing that consistency and Bayes optimality with respect to these two loss functions is equivalent when $|V^*| = O(1)$.

3 Bayes Optimal VN schemes

In [29], a Bayes optimal VN scheme (i.e., one that achieves optimal expected VN loss) was derived in the setting where one observes a network without features. In the feature-rich setting, derivations are similar, though they require more nuance. After some preliminary work, this section culminates in the definition of the feature-aware Bayes optimal scheme in Section 3.2.

3.1 Obfuscating Features

How should we model the effect of the obfuscation function on features in the VN framework? If we observe $o(g_2)$, then we have no knowledge of which member of $[g_2] := \{g_2' : g_2 \simeq g_2'\}$ was obfuscated, but we do know what features are associated to each of the vertices and edges. That is, the features themselves are not obfuscated, merely the order in which they are observed. In order to model this setting, we adopt the following conventions.

Let $n, m, d_1, e_1, d_2, e_2 \in \mathbb{Z}_{>0}$ and $\mathcal{V}, \mathcal{E}$ be given. Furthermore, let the set of vertices of interest, $V^* \subset C = V_1 \cap V_2$, be fixed. Let $H$ be an obfuscating set of of $V_1$ and $V_2$ of order $|V_2| = m$, and $o \in \mathcal{O}_H$. Define $A_{n,m}^{d_1,e_1,d_2,e_2}$ to be the set of asymmetric richly featured graphs

$$A_{n,m} = A_{n,m}^{d_1,e_1,d_2,e_2} := \left\{(g_1, g_2) \in \mathcal{G}_n^{d_1,e_1} \times \mathcal{G}_m^{d_2,e_2} : \text{s.t. there are no non-trivial } f\text{-automorphisms of } g_1 \text{ or } g_2\right\}.$$ 

Under Assumption 11, $F_{\Theta}^{(n,m)}$ is supported on $A_{n,m}$.

For each $(g_1, g_2) \in \mathcal{G}_n^{d_1,e_1} \times \mathcal{G}_m^{d_2,e_2}$, define

$$(g_1, o(g_2)) = \left\{(g_1, g_2) \in \mathcal{G}_n^{d_1,e_1} \times \mathcal{G}_m^{d_2,e_2} : o(g_2) \simeq o(g_2)\right\} = \left\{(g_1, \hat{g}_2) \in \mathcal{G}_n^{d_1,e_1} \times \mathcal{G}_m^{d_2,e_2} : \hat{g}_2 \simeq g_2\right\}.$$ 

Note that if $(g_1, g_2) \in A_{n,m}$ the asymmetry of $g_2$ yields that

$$\left|\left(g_1, [o(g_2)]\right)\right| = m!.$$
In light of the action of the obfuscating function on the features and vertex labels of \(g_2\), we view \((g_1, [\sigma(g_2)])\) as the set of possible graph pairs that could have led to the observed graph pair \((g_1, \sigma(g_2))\).

For each \(u \in H\) and \(v \in V_2\), we also define the following restriction:

\[
(g_1, [\sigma(g_2)])_{u=\sigma(v)} = \left\{(g_1, \hat{g}_2) \in G_{n, V, E}^{(d_1, e_1)} \times G_{m, V, E}^{(d_2, e_2)} \text{ s.t. } \sigma(\hat{g}_2) = \sigma(\sigma(g_2)), \right. \\
\left. \text{where } \sigma \text{ is an } f\text{-isomorphism satisfying } \sigma(u) = \sigma(v) \right\}
\]

\[
= \left\{(g_1, \hat{g}_2) \in G_{n, V, E}^{(d_1, e_1)} \times G_{m, V, E}^{(d_2, e_2)} \text{ s.t. } \hat{g}_2 = \sigma(g_2), \right. \\
\left. \text{where } \sigma \text{ is an } f\text{-isomorphism satisfying } \sigma(\sigma^{-1}(u)) = v \right\}
\]

and for \(S \subseteq V_2\), define

\[
(g_1, [\sigma(g_2)])_{u \in \sigma(S)} = \bigcup_{v \in S} (g_1, [\sigma(g_2)])_{u=\sigma(v)}.
\]

### 3.2 Defining Bayes Optimality

We are now ready to define a Bayes optimal scheme \(\Phi^*\) for a given \(F_{\Theta}^{(n,m)} \in F^{(n,m)}\) satisfying Assumption 11. We will define the scheme element-wise on each asymmetric \((g_1, [\sigma(g_2)])\), and then systematically lift the scheme to all of \(\mathcal{A}_{n,m}^{d_1,e_1,d_2,e_2}\). To wit, let

\[
\left\{(g_1^{(i)}, g_2^{(i)})\right\}_{i \in I}
\]

be such that

\[
\left(g_1^{(i)}, [\sigma(g_2^{(i)})]\right) : i \in I
\]

is a partition \(G_{n, V, E}^{d_1,e_1} \times G_{m, V, E}^{d_2,e_2}\). To ease notation, we will from here forth adopt the following shorthand.

1. We use \((g_1^{(i)}, [\sigma(g_2^{(i)})]\right)\) to denote the event \(\{(G_1, \sigma(G_2)) \in (g_1^{(i)}, [\sigma(g_2^{(i)})]\right)\}\).
2. For \(u \in H\), we use \((g_1^{(i)}, [\sigma(g_2^{(i)})]_{u=\sigma(v)}\) to denote the event

\[
\left\{(G_1, \sigma(G_2)) \in (g_1^{(i)}, [\sigma(g_2^{(i)})]_{u=\sigma(v)}\right. \\
\left. \right\}.
\]

We will use this often with \(u = \Phi(g_1^{(i)}, \sigma(g_2^{(i)}), V^*)[j]\).
3. We use \((g_1^{(i)}, [\sigma(g_2^{(i)})]_{u=\sigma(V^*)}\) to denote the event

\[
\left\{(G_1, \sigma(G_2)) \in (g_1^{(i)}, [\sigma(g_2^{(i)})]_{u=\sigma(V^*)}\right. \\
\left. \right\}.
\]

We will use this often with \(u = \Phi(g_1^{(i)}, \sigma(g_2^{(i)}), V^*)[j]\).
Let \( S \) denote the set of indices \( i \) such that \((g_1^{(i)}, g_2^{(i)}) \in A_{n,m}; \) i.e., \( g_1^{(i)} \) and \( g_2^{(i)} \) are asymmetric as richly featured networks. For each \( i \in S \), writing \( \mathbb{P}(\cdot) \) for \( \mathbb{P}_{F_{\Theta}^{(n,m)}}(\cdot) \) to ease notation, define

\[
\Phi^* \left( g_1^{(i)}, o(g_2^{(i)}), V^* \right) \in \arg \max_{u \in H} \mathbb{P} \left( (g_1^{(i)}, [o(g_2^{(i)})])_{u \in o(V^*)} \mid (g_1^{(i)}, [o(g_2^{(i)})]) \right)
\]

For \( i \notin S \), any fixed and arbitrary definition of \( \Phi^* \) (subject to the consistency criterion in Definition 9) on \((g_1^{(i)}, [o(g_2^{(i)})])\) will suffice, as this set has measure 0 under \( F_{\Theta}^{(n,m)} \) by Assumption 11. Theorem 14 shows that \( \Phi^* \) defined above is indeed level-\( k \) Bayes optimal for all \( k \) for any nominatable distribution satisfying Assumption 11. A proof is given in Appendix B.1.

**Theorem 14.** Let \( F_{\Theta}^{(n,m)} \in \mathcal{F}^{(n,m)} \) satisfy Assumption 11, and let \( V^* \subset C = V_1 \cap V_2 \) be a given set of vertices of interest in \( G_1 \). The FA-VN scheme \( \Phi^* \) defined in Equation (2) is a level-\( k \) Bayes optimal scheme for \( F_{\Theta}^{(n,m)} \) for all \( k \in [m] \) and any obfuscating set \( H \) and obfuscating function \( o \in \mathcal{O}_H; \) i.e., \( \Phi^* \in \arg \min_{\Phi \in \mathcal{L}^{(n,m)}} L_k(\Phi, V^*) \) for all \( k \in [m] \).

## 4 The benefit of content and context

It is intuitively clear that incorporating features should improve VN performance, provided those features are correlated with vertex “interestingness”. Indeed, this is a common theme across many graph-based machine learning tasks (see, for example, [60, 5, 32]), and the same holds in the present VN setting. The combination of network structure and informative features can significantly improve the VN Bayes error. Consider, for instance, the following simple example set in the context of the stochastic blockmodel [18].
Definition 15. An undirected \( n \)-vertex graph \( G = (V, E) \) is an instantiation of a Stochastic Blockmodel with parameters \((K, b, \Lambda)\) (abbreviated \( G \sim \text{SBM}(K, b, \Lambda) \)) if:

1. The vertex set \( V \) is partitioned into \( K \) communities \( V = V_1 \sqcup V_2 \sqcup \ldots \sqcup V_K \);
2. The community membership function \( b : V \to [K] \) denotes the community of \( v \);
   i.e., \( v \in V_{b(v)} \);
3. \( \Lambda \) is a \( K \times K \) matrix of probabilities: for each \( \{u, v\} \in (V^2) \), we have that
   \[ 1 \{\{u, v\} \in E\} \sim \text{Bernoulli}(\Lambda(b(u), b(v))) \]
   and the collection of random variables
   \[ \{1 \{\{u, v\} \in E\} : \{u, v\} \in (V^2)\} \]
   are mutually independent.

Example 16. Let \( G_1, G_2 \) be independent \( 2n \)-vertex \( \text{SBM}(2, \Lambda, b) \) random graphs with

\[
\Lambda = \begin{pmatrix} a & b \\ b & c \end{pmatrix}, \quad b(v) = \begin{cases} 1 & \text{if } 1 \leq v \leq n \\ 2 & \text{if } n + 1 \leq v \leq 2n \end{cases},
\]

where \( b < a < c \) are fixed (i.e., do not vary with \( n \)). Edges in both \( G_1 \) and \( G_2 \) are independent and the probability of an edge between vertices \( \{u, v\} \) is equal to

\[
\mathbb{P}(\{u, v\} \in E(G_i)) = \begin{cases} a & \text{if } \{u, v\} \subset [n]; \\ c & \text{if } \{u, v\} \subset \{n + 1, \ldots, 2n\}; \\ b & \text{otherwise}. \end{cases}
\]

Take \( V^* = \{v_1\} \) with corresponding vertex of interest \( u^* = u_1 \in V_2 \) with \( b(v_1) = b(u_1) = 1 \). In the absence of features, \( L_k^* = (1 + o(1))(1 - \frac{\min(k,n)}{n}) \), owing to the fact that vertices in the same community are stochastically identical. If the graphs are endowed with edge features \( X, Y \in \mathbb{Z}^{2n} \),

\[
X^T = Y^T = \begin{bmatrix} 1, 1, & \cdots, & 1, 2, & 2, & \cdots, & 2, 1, & \cdots, & 1 \end{bmatrix}
\]

then these features provide significant information for identifying \( v_1 \in V(G_2) \); indeed, we see that a ranking scheme that ignores network structure, can do no better than randomly ranking the vertices with feature 1, and thus has a loss \( L_k^* = 1 - \frac{\min(k,n)}{n} \). In contrast, if one considers the richly attributed graphs \( (G_1, X) \) and \( (G_2, Y) \), the Bayes optimal loss is reduced to \( L_k^* = (1 + o(1))(1 - \frac{\min(k,n/2)}{n/2}) \) for all \( k, n \), as the network topology and vertex features offer complementary information, and taking both into account improves the Bayes optimal rate.

Can Bayes optimal performance in \( VN \) ever be improved by ignoring features? Subject to the consistency criteria in Definition 9, the answer is more nuanced, as defining a scheme that both ignores features and satisfies the consistency criteria in
Definition 9 is often not possible. A scheme \( \Phi \) that ignores features must have that for all \((g_1, g_2) \in \mathcal{G}_n \times \mathcal{G}_m \) and all features

\[
(x, w, y, z), (x', w', y', z') \in \mathcal{X}^{d_1} \times \mathcal{E}^{e_1} \times \mathcal{X}^{d_2} \times \mathcal{E}^{e_2}
\]

with \( \gamma(w) = \gamma(w') = g_1 \) and \( \gamma(z) = \gamma(z') = g_2 \),

\[
\Phi \left( (g_1, x, w), o(g_2, y, z), V^* \right) = \Phi \left( (g_1, x', w'), o(g_2, y', z'), V^* \right).
\]  

(2)

Now consider \( g_1 = (g_1, x, w) \) and \( g_2 = (g_2, y, z) \) that are asymmetric (i.e., have non-trivial f-automorphisms) as featured networks, but for which \( g_1 \) and \( g_2 \) have non-trivial automorphism groups. By assumption, there exists \( \sigma \neq \text{id} \) such that

\[
\sigma(o(g_2)) = o(g_2, y', z').
\]

Then the consistency criterion in Definition 9 requires

\[
\sigma(\Phi(g_1, o(g_2), V^*)) = \Phi(g_1, \sigma(o(g_2)), V^*),
\]

while Equation (2) requires \( \Phi(g_1, \sigma(o(g_2)), V^*) = \Phi(g_1, o(g_2), V^*), a contradiction.

For Equation (2) to hold in general, we need to consider a consistency criteria analogous to Equation (1) that is compatible with schemes that ignore the vertex features. The following definition, adapted from [1], suffices.

**Definition 17 (Feature Oblivious VN Scheme).** Let \( n, m, d_1, d_2, e_1, e_2 \in \mathbb{Z}_{\geq 0} \) and \( \mathcal{V}, \mathcal{E} \) be given. Let \( H \) be an obfuscating set of \( V_1 \) and \( V_2 \) of order \( |V_2| = m \), and let \( o \in \mathcal{O}_H \) be given. A feature oblivious vertex nomination scheme (FO-VN scheme) is a function

\[
\Psi : \mathcal{G}^{d_1, e_1}_{m, \mathcal{V}, \mathcal{E}} \times o(\mathcal{G}^{d_2, e_2}_{m, \mathcal{V}, \mathcal{E}}) \times 2^{V_1} \rightarrow \mathcal{T}_H,
\]

satisfying Equation (2) as well as the consistency criteria in Assumption 18.

Similar to the FA-VN consistency criteria, we require FO-VN schemes to be similarly label-agnostic for the obfuscated labels of the second graph.

**Assumption 18 (FO-VN Consistency Criteria).** With notation as in Definition 17, for each \( g_2 = (g_2, y, z) \in \mathcal{G}^{d_2, e_2}_{m, \mathcal{V}, \mathcal{E}} \) and \( u \in V_2 \), let

\[
\mathcal{J}(u; g_2) = \{ w \in V_2 \ s.t. \ \exists \ \text{an automorphism} \ \sigma \ \text{of} \ g_2, \ s.t. \ \sigma(u) = w \}.
\]

For any \( g_1 \in \mathcal{G}^{d_1, e_1}_{n, \mathcal{V}, \mathcal{E}}, g_2 \in \mathcal{G}^{d_2, e_2}_{m, \mathcal{V}, \mathcal{E}} \), \( V^* \subset V_1 \cap V_2 \), obfuscating functions \( o_1, o_2 \in \mathcal{O}_H \) and any \( u \in V_2 \), we require

\[
\tau_\Psi \left( g_1, g_2, o_1, V^*, \mathcal{J}(u; g_2) \right) = \tau_\Psi \left( g_1, g_2, o_2, V^*, \mathcal{J}(u; g_2) \right) \iff \forall k \in [m] : o_2 \circ o_1^{-1} \left( \mathcal{J}(\Psi(g_1, o_1(g_2), V^*)[k]) ; o_1(g_2) \right) = \mathcal{J}(\Psi(g_1, o_2(g_2), V^*)[k] ; o_2(g_2))
\]  

(3)
where $\Psi(g_1, o(g_2), V^*)[k]$ denotes the $k$-th element in the ordering $\Psi(g_1, o(g_2), V^*)$ (i.e., the rank-$k$ vertex).

The criterion in Equation (3) is less restrictive than that in Equation (1), and it is not immediate that incorporating features yields an FA-VN scheme with smaller loss than the Bayes optimal FO-VN scheme. We illustrate this in the following example.

**Example 19.** Let $F \in \mathcal{F}^{(n,m)}$ be a distribution such that $G_1 \overset{a.s.}{=} K_n$ and $G_2 \overset{a.s.}{=} K_m$, where $K_n$ denotes the complete graph on $n$ vertices. If the $f$-automorphism group of $G_1 G_2$ are a.s. trivial, then any given FA-VN scheme can be outperformed by a well-chosen FO-VN scheme. Indeed, if there is a single vertex of interest $v^*$ in $G_1$ with corresponding vertex $u^*$ in $G_2$, then there exists a FO-VN scheme $\Psi$ that satisfies $\Psi(g_1, o(g_2), v^*)[1] = o(u^*)$ for almost all $g_1, o(g_2)$. Such a $\Psi$ cannot satisfy Equation (1), and it is possible to have $L_K(\Phi^* V^*) > 0$ for FA-VN Bayes optimal $\Phi^*$.

However, consider distributions satisfying the following assumption.

**Assumption 20.** Let $(G_1 = (G_1, X, W), G_2 = (G_2, Y, Z)) \sim F_{\Theta}^{(n,m)}$ and consider the events

$$D_3 = \{ \text{the only automorphism of } G_1 \text{ is } \sigma = \text{id}_n \}$$

$$D_4 = \{ \text{the only automorphism of } G_2 \text{ is } \sigma = \text{id}_m \}$$

Under this assumption on $F_{\Theta}^{(n,m)}$, $\mathbb{P}_{\mathcal{F}_{\Theta}^{(n,m)}}(D_3) = \mathbb{P}_{\mathcal{F}_{\Theta}^{(n,m)}}(D_4) = 1$.

Under Assumption 20, we have that $\mathcal{I}(u; g_2) \overset{a.s.}{=} \mathcal{J}(u; g_2) \overset{a.s.}{=} \{ u \}$, and the consistency criteria in Assumptions 10 and 18 are almost surely equivalent. It is then immediate that Bayes optimality cannot be improved by ignoring features. That is, a FO-VN $\Psi$ scheme is almost surely a FA-VN scheme, and hence $L_K(\Psi, V^*) \geq L_K(\Phi^*, V^*)$ for all $k \in [m]$. This leads us to ask whether we can establish conditions under which ignoring features strictly decreases VN performance.

## 4.1 Feature oblivious Bayes optimality

We first establish the notion of a Bayes optimal FO-VN scheme for distributions satisfying Assumption 20. Defining

$$\mathfrak{G}_{n,m} = \{(g_1, o(g_2)) \in \mathcal{G}_n \times o(\mathcal{G}_m) \text{ s.t. } g_1, g_2 \text{ are asymmetric} \},$$

let $\{(g_1, g_2)\}_{i=1}^p$ be such that $\{(g_1, [o(g_2)])\}_{i=1}^p$ partitions $\mathfrak{G}_{n,m}$. For $F_{\Theta}^{(n,m)}$ supported on $\mathfrak{G}_{n,m}$, it follows from [1] that a Bayes optimal FO-VN scheme, $\Psi^*$, can be constructed as follows. If $(g_1^i, g_2^i) \in \{(g_1, g_2)\}_{i=1}^p$, and $(g_1^i, o(g_2^i))$ is any featured extension of
For each \((g_1^i, g_2^i)\) (note that this notation will be implicit moving forward), we sequentially define (breaking ties in a fixed but arbitrary manner and writing \(P(\cdot)\) for \(P_{F_{\Theta}^{(n,m)}}(\cdot)\) to ease notation)

\[
\Psi^*(g_1^i, o(g_2^i), V^*)[1] \in \arg \max_{u \in H} P\left( (g_1^i, [o(g_2^i)])_{u \in o(V^*)} \mid (g_1^i, [o(g_2^i)]) \right)
\]

\[
\Psi^*(g_1^i, o(g_2^i), V^*)[2] \in \arg \max_{u \in H \setminus \Psi^*[1]} P\left( (g_1^i, [o(g_2^i)])_{u \in o(V^*)} \mid (g_1^i, [o(g_2^i)]) \right)
\]

\[
\vdots
\]

\[
\Psi^*(g_1^i, o(g_2^i), V^*)[m] \in \arg \max_{u \in H \setminus \{\cup_{j=1}^{m-1}\Psi^*[j]\}} P\left( (g_1^i, [o(g_2^i)])_{u \in o(V^*)} \mid (g_1^i, [o(g_2^i)]) \right),
\]

where \((g_1, [o(g_2)])\) and \((g_1, [o(g_2)])_{u \in o(V^*)}\) (that is, the graphs without their features) are defined analogously to the featured \((g_1, [o(g_2)])\) and \((g_1, [o(g_2)])_{u \in o(V^*)}\) respectively:

\[
(g_1, [o(g_2)]) = \left\{ (g_1, \hat{g}_2) \in \mathcal{G}_{n,m} \text{ s.t. } o(\hat{g}_2) \simeq o(g_2) \right\}
\]

\[
(g_1, [o(g_2)])_{u = o(v)} = \left\{ (g_1, \hat{g}_2) \in \mathcal{G}_{n,m} \text{ s.t. } o(\hat{g}_2) = \sigma(o(g_2)), \text{ where } \sigma \text{ is an isomorphism satisfying } \sigma(u) = o(v) \right\}
\]

For each \((g_1^i, g_2^i) \in (g_1^i, [o(g_2^i)])\), choose the f-isomorphism \(\sigma\) such that \(o(g_2^i) = \sigma(o(g_2^i))\), and define

\[
\Psi^*(g_1^i, o(g_2^i), V^*) = \sigma(\Psi^*(g_1^i, o(g_2^i), V^*)).
\]

For elements \((g_1, o(g_2)) \notin \mathcal{G}_{n,m}\), any fixed and arbitrary definition of \(\Phi_{\Omega}^{(n,m)}\) satisfying Equation (3) suffices (as this set has measure 0 under \(P_{F_{\Theta}^{(n,m)}}\) by Assumption 20). Note that \(\Psi^*\) is almost surely well-defined, as the definition of \(\Psi^*\) on

\[
\mathcal{A}_{n,m} = \mathcal{A}_{n,m, n, \mathcal{E}}^{(d_1, e_1, d_2, e_2)} := \{(g_1 = (g_1, x, w), g_2 = (g_2, y, z)) \in \mathcal{G}_{n, \mathcal{Y}, \mathcal{E}}^{d_1, e_1} \times \mathcal{G}_{m, \mathcal{Y}, \mathcal{E}}^{d_2, e_2} \text{ s.t. } g_1, g_2 \text{ are asymmetric}\}
\]

is independent of the choice of the partition \(\{(g_1^i, g_2^i) : i = 1, 2, \ldots, p\}\).

### 4.2 The Benefit of Features

With the FO-VN scheme defined, we seek to understand when, for distributions \(F_{\Theta}^{(n,m)}\) supported on \(\mathcal{A}_{n,m}\), we have \(L_k(\Phi^*, V^*) < L_k(\Psi^*, V^*)\) where \(\Phi^*\) and \(\Psi^*\) are the Bayes optimal FA-VN and FO-VN schemes, respectively, under \(F_{\Theta}^{(n,m)}\). Toward this end, we first define the following \(\mathcal{T}_H\)-valued random variable.
Definition 21. Let $F_{\Theta}^{(n,m)} \in \mathcal{F}^{(n,m)}$ and let $V^* \subseteq V_1 \cap V_2$ be a given set of vertices of interest, and let $\sigma : V_2 \mapsto H$ be a given obfuscating function. Let $\Phi$ be a VN scheme (either feature-aware or feature-oblivious), and define, letting $\Omega$ be our sample space, the $\mathcal{T}_H$-valued random variable

$$X_\Phi : \Omega \mapsto \mathcal{T}_H$$

by $X_\Phi(\omega) = \Phi(G_1(\omega), \sigma(G_2(\omega)), V^*)$. For each $k \leq m$, define $X^k_\Phi = X_\Phi[1 : k] \in \mathcal{T}^k_H$, where we define $\mathcal{T}^k_H$ to be the set of all $k$-tuples of distinct elements of $H$ (each such tuple can be viewed as specifying a total ordering of $k$ distinct elements of $H$).

Remark 22. Note that in the setting of continuous features, the measurability of $X_\Phi$ is not immediate (and indeed, is non-trivial to establish); this technical hurdle is the main impetus for discretizing the feature space.

We can now characterize the conditions under which incorporating features strictly improves VN performance. A proof of Theorem 23 can be found in Appendix B.2.

Theorem 23. Let $F_{\Theta}^{(n,m)} \in \mathcal{F}^{(n,m)}$ be a richly featured nominatable distribution satisfying Assumption 20. Let $V^* \subseteq V_1 \cap V_2$ be a given set of vertices of interest, and let $H$ be an obfuscating set of $V_1$ and $V_2$ of order $|V_2| = m$ with $\sigma \in \mathcal{O}_H$. Letting $\Phi^*$ and $\Psi^*$ be Bayes optimal FA-VN and FO-VN schemes, respectively, under $F_{\Theta}^{(n,m)}$, we have that

$$L_k(\Phi^*, V^*) = L_k(\Psi^*, V^*)$$

if and only if there exists a Bayes optimal FA-VN scheme $\Phi^*$ with

$$\mathbb{I}(X^k_{\Phi^*}; (G_1, G_2)) = \mathbb{H}(X^k_{\Phi^*}),$$

where $\mathbb{I}$ is the mutual information and $\mathbb{H}$ the statistical entropy defined by

$$\mathbb{H}(X^k_{\Phi^*}) = - \sum_{\xi \in \mathcal{T}^k_H} \mathbb{P}(X^k_{\Phi^*} = \xi) \log(\mathbb{P}(X^k_{\Phi^*} = \xi))$$

$$\mathbb{I}(X^k_{\Phi^*}; (G_1, G_2)) = \sum_{\xi \in \mathcal{T}^k_H} \sum_{(g_1, g_2) \in \mathcal{G}_n \times \mathcal{G}_m} \mathbb{P}(\xi, (g_1, g_2)) \log \left( \frac{\mathbb{P}(\xi, (g_1, g_2))}{\mathbb{P}(\xi) \mathbb{P}((g_1, g_2))} \right),$$

where we have written $\mathbb{P}(\xi, (g_1, g_2))$ as shorthand for $\mathbb{P}(X^k_{\Phi^*} = \xi, (G_1, G_2) = (g_1, g_2))$.

We note that, since $\mathbb{I}(X^k_{\Phi^*}; (G_1, G_2)) \leq \mathbb{H}(X^k_{\Phi^*})$, Theorem 23 can be restated as $L_k(\Phi^*, V^*) < L_k(\Psi^*, V^*)$ if and only if for all Bayes optimal FA-VN schemes $\Phi^*$,

$$\mathbb{I}(X^k_{\Phi^*}; (G_1, G_2)) < \mathbb{H}(X^k_{\Phi^*}).$$

Stated succinctly, there is excess uncertainty in $X^k_{\Phi^*}$ after observing $(G_1, G_2)$; and $X^k_{\Phi^*}$ is not deterministic given $(G_1, G_2)$. 

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5 The benefit of context and content

In contrast to the feature-oblivious VN schemes considered in Section 4, one can also consider VN schemes that use only features and ignore network structure. Defining such a network-oblivious VN scheme (NO-VN scheme) is not immediately straightforward. Ideally, we would like to have that for all \((g_1, g_2), (g_1', g_2') \in \mathcal{G}_n \times \mathcal{G}_m\) and all edge features \((w, z), (w', z')\) compatible with \((g_1, g_2)\) and \((g_1', g_2')\) respectively,

\[
\Phi((g_1, x, w), o(g_2, y, z), V^*) = \Phi((g_1', x, w'), o(g_2', y, z'), V^*)
\]

for any choice of vertex features \(x, y\). As in the FO-VN scheme setting, this leads to potential violation of the internal consistency criteria of Equation (1). Indeed, consider \(g_1 = (g_1, x, w)\) and \(g_2 = (g_2, y, z)\) with asymmetric graphics but with symmetries in \(y\) (i.e., there exists non-identity permutation matrix \(P_\sigma\) such that \(P_\sigma y = y\)). On such networks, Equations (1) and (5) cannot both hold simultaneously. Thus, we consider a relaxed consistency criterion as in Assumption 18. We first define

\[
\mathcal{Y}(u; g_2) = \{w \in V(g_2) : \exists \text{ bijection } \sigma \text{ s.t. } P_\sigma y = y \text{ and } \sigma(u) = w\},
\]

and make the following consistency assumption.

**Assumption 24** (NO-VN Consistency Criteria). For any \(g_1 \in \mathcal{G}^{d_1,e_1}_{n,V,E}, g_2 \in \mathcal{G}^{d_2,e_2}_{m,V,E}\), letting \(H\) be an obfuscating set of \(V_1\) and \(V_2\) of order \(|V_2| = m\) with \(o_1, o_2 \in \mathcal{O}_H\), \(V^* \subset V_1 \cap V_2\) be the set of vertices of interest, and taking \(u \in V(g_2)\), if \(\Xi\) is a VN scheme satisfying this assumption, then

\[
r_\Xi(g_1, g_2, o_1, V^*, \mathcal{Y}(u; g_2)) = r_\Xi(g_1, g_2, o_2, V^*, \mathcal{Y}(u; g_2))
\]

\[
\Leftrightarrow o_2 \circ o_1^{-1}(\mathcal{Y}(\Xi(g_1, o_1(g_2), V^*)[k]); o_1(g_2)) = \mathcal{Y}(\Xi(g_1, o_2(g_2), V^*)[k]; o_2(g_2))
\]

for all \(k \in [m]\),

where \(\Xi(g_1, o(g_2), V^*)[k]\) denotes the \(k\)-th element in the ordering \(\Xi(g_1, o(g_2), V^*)\) (i.e., the rank-\(k\) vertex under \(\Phi\)).

A network-oblivious VN scheme \(\Xi\) is then a VN scheme as in Definition 9, where the consistency criterion of Equation (1) is replaced with that in Equation (6) and we further require Equation (5) to hold. As with FA-VN schemes, we consider distributions satisfying the following assumption.

**Assumption 25.** Let \((G_1 = (G_1, X, W), G_2 = (G_2, Y, Z)) \sim F^{(n,m)}_\Theta \in \mathcal{F}^{(n,m)}\). The events

\[
D_5 = \{X = P_\sigma X \implies \sigma = \text{id}\},
\]

\[
D_6 = \{Y = P_\sigma Y \implies \sigma = \text{id}\}
\]

satisfy \(\mathbb{P}_{F^{(n,m)}_\Theta}(D_5) = \mathbb{P}_{F^{(n,m)}_\Theta}(D_6) = 1\).
Under Assumption 25, we have that $\mathcal{I}(u; g_2) \cup \mathcal{Y}(u; g_2) \cup \{u\}$, and the consistency criteria are almost surely equivalent. As in Section 4, under this assumption, we have that Bayes optimality cannot be improved by ignoring the network. Indeed, one can show that the NO-VN scheme is almost surely a FA-VN scheme, and we are led once again to ask under what circumstances VN performance will be strictly worsened by ignoring the network (and subsequently, the edge features). To this end, we wish to compare Bayes optimality of NO-VN with that of FA-VN.

### 5.1 Network oblivious Bayes optimality

We first establish the notion of a Bayes optimal NO-VN scheme for distributions satisfying Assumption 25. Define

$$
\hat{\mathcal{F}}_{n,m} := \{ (x, y) \in \mathbb{R}^{n \times d_1} \times \mathbb{R}^{m \times d_2} \text{ s.t. } x, y \text{ have distinct rows} \},
$$

and for $(x, y) \in \hat{\mathcal{F}}_{n,m}$, define

$$
(x, [o(y)]) = \left\{ (x, \hat{y}) \in \hat{\mathcal{F}}_{n,m} \text{ s.t. there exists permutation } \sigma \text{ s.t. } P_\sigma y = \hat{y} \right\},
$$

and

$$
(x, [o(y)])_{u=o(v)} = \left\{ (x, \hat{y}) \in \hat{\mathcal{F}}_{n,m} \text{ s.t. there exists permutation } \sigma \text{ s.t. } P_\sigma y = \hat{y} \right\}.
$$

For a given $F_{\Theta}^{(n,m)}$ satisfying Assumption 25, we will define the Bayes optimal NO-VN scheme, $\Xi^*$, element-wise on vertex feature matrices with no row repetitions (similar to in Section 3.2), and then lift the scheme to all richly featured graphs with vertex features not in $\hat{\mathcal{F}}_{n,m}$. For $(x, w, y, z)$ with $x$ and $y$ having distinct rows, let $g_1$ and $g_2$ be the unique graphs with edge structure compatible with $w$ and $z$ respectively. Writing $g_1 = (g_1, x, w)$ and $g_2 = (g_2, y, z)$, we define, writing $\mathbb{P}(\cdot)$ for $\mathbb{P}_{F_{\Theta}^{(n,m)}}(\cdot)$ to ease notation

$$
\Xi^*(g_1, o(g_2), V^*|1) \in \arg \max_{u \in H} \mathbb{P}\left(F \left(\left(x, [o(y)]\right)_{u \in \Theta(V^*)}|(x, [o(y)])\right)\right),
$$

$$
\Xi^*(g_1, o(g_2), V^*|2) \in \arg \max_{u \in H \setminus \{\Xi[1]\}} \mathbb{P}\left(F \left(\left(x, [o(y)]\right)_{u \in \Theta(V^*)}|(x, [o(y)])\right)\right),
$$

$$
\vdots
$$

$$\Xi^*(g_1, o(g_2), V^*|m) \in \arg \max_{u \in H \setminus \{\cup_{j<m} \{\Xi[j]\}\}} \mathbb{P}\left(F \left(\left(x, [o(y)]\right)_{u \in \Theta(V^*)}|(x, [o(y)])\right)\right),
$$

where we write $(x, [o(y)])$ in the conditioning statement as shorthand for (writing $g_1 = (g_1, x, w)$ and $g_2 = (g_2, y, z)$)

$$(G_1, o(G_2)) \in \{((g_1, x, w), o((g_2, y, z))) \text{ s.t. } (x, y) \in (x, [o(y)])\}.$$
Note that once again, ties in the maximizations when constructing $\Xi^*$ are assumed to be broken in an arbitrary but nonrandom manner. For each element $(g'_1, g'_2) \in (g_1, o(g_2))$, choose the f-isomorphism $\sigma$ such that $o(g'_2) = \sigma(o(g'_2))$, and define

$$\Xi^*(g'_1, o(g'_2), V^*) = \sigma(\Xi^*(g_1, o(g_2), V^*)).$$ 

For elements $(x, y) \notin \mathcal{F}_{n,m}$ and arbitrary edge features $w, z$, any fixed and arbitrary definition of $\Xi^*$ on (well-defined) graphs in $G_n \times \{x\} \times \{w\} \times \{y\} \times \{z\}$ suffices, subject to the internal consistency criterion in Equation (6), as this set has measure 0 under $F_{F_{\Theta}}^{(n,m)}$ under Assumption 25.

### 5.2 The benefit of network topology

Once again, our aim is to understand, for distributions satisfying Assumption 25, when is $L_k(\Phi^*, V^*) < L_k(\Xi^*, V^*)$? That is, when does incorporating the network topology into the vertex-level features strictly improve VN performance? Theorem 26 characterizes these conditions. The proof is completely analogous to the proof of Theorem 2, and is included in Appendix B.3 for completeness.

**Theorem 26.** Let $F_{F_{\Theta}}^{(n,m)} \in \mathcal{F}^{(n,m)}$ be a richly featured nominatable distribution satisfying Assumption 25. Let $V^* \subseteq V_1 \cap V_2$ be a given set of vertices of interest and let $H$ be an obfuscating set of $V_1$ and $V_2$ of order $|V_2| = m$ with $o \in \mathcal{O}_H$. Let $\Phi^*$ and $\Xi^*$ be Bayes optimal FA-VN and NO-VN schemes, respectively, under $F_{F_{\Theta}}^{(n,m)}$. Then $L_k(\Phi^*, V^*) = L_k(\Xi^*, V^*)$ if and only if there exists a Bayes optimal FA-VN scheme $\Phi^*$ with

$$\mathbb{I}(X^k_{\Phi^*}; (X, Y)) = \mathbb{H}(X^k_{\Phi^*}).$$ 

Note that, since $\mathbb{I}(X^k_{\Phi^*}; (X, Y)) \leq \mathbb{H}(X^k_{\Phi^*})$, Theorem 26 can be equivalently stated as $L_k(\Phi^*, V^*) < L_k(\Xi^*, V^*)$ if and only if it holds all Bayes optimal FA-VN schemes $\Phi^*$ satisfy $\mathbb{I}(X^k_{\Phi^*}; (X, Y)) < \mathbb{H}(X^k_{\Phi^*})$. Said yet another way, there is excess uncertainty in $X^k_{\Phi^*}$ after observing vertex features $(X, Y)$, and $X^k_{\Phi^*}$ is not deterministic given $(X, Y)$.

### 6 Simulations and Experiments

We turn now to a brief experimental exploration of the vertex nomination problem as applied to both simulated and real data. We consider a VN scheme based on spectral clustering, which we denote VN $\circ$ GMM $\circ$ ASE. We refer the reader to [1] for details.
and a further exploration of this scheme in an adversarial version of vertex nomination without node or edge features.

In our experiments, edge features will appear as edge weights or edge directions, while vertex features will take the form of feature matrices $x$ and $y$, following the notation of previous sections. The scheme $\text{VN} \circ \text{GMM} \circ \text{ASE}$ proceeds as follows. Note that we have assumed $n = m$ for simplicity, but the procedure can be extended to pairs of differently-sized networks in a straight-forward manner.

i. Pass the edge weights to ranks, and augment the diagonal of the adjacency matrix by setting $A_{i,i} = \sum_{j \neq i} A_{i,j} / (n - 1)$ \cite{54}; see Appendix A.1 for detail.

ii. Embed the two networks into a common Euclidean space, $\mathbb{R}^d$ using Adjacency Spectral Embedding (ASE) \cite{50} (see Appendix A.2 for details). The embedding dimension $d$ is chosen by estimating the elbow in the scree plots of the adjacency matrices of the networks $G_1$ and $G_2$ \cite{62}, taking $d$ to be the larger of the two elbows. Applying ASE to an $n$-vertex graph results in a mapping of the $n$ vertices in the graph to points in $\mathbb{R}^d$. We denote the embeddings of graphs $G_1$ and $G_2$ by $\hat{X}_1, \hat{X}_2 \in \mathbb{R}^{n \times d}$, respectively, with the $i$-th row of each of these matrices corresponding to the embedding of the $i$-th vertex in its corresponding network.

iii. Given seed vertices $S$ (see Appendix A.3) whose correspondence is known a priori across networks, solve the orthogonal Procrustes problem \cite{46} (see Appendix A.4) to align the rows of $\hat{X}_1[S, :]$ and $\hat{X}_2[S, :]$. Apply this Procrustes rotation to the rows of $\hat{X}_2$, yielding $\hat{Y}_2 \in \mathbb{R}^{n \times d}$. If $p$-dimensional vertex features are available, append the vertex features to the embeddings as $Z_1 = [\hat{X}_1 \ | \ x] \in \mathbb{R}^{n \times (d+p)}$ and $Z_2 = [\hat{Y}_2 \ | \ y] \in \mathbb{R}^{n \times (d+p)}$.

iv. Cluster the rows of both $Z_1$ and $Z_2$ using a Gaussian mixture modeling-based clustering procedure (e.g., \texttt{mClust} in \texttt{R} \cite{15}). For each vertex $v$, let $\mu_v$ and $\Sigma_v$ be the mean and covariance of the normal mixture component containing $v$. For each $u \in V(G_2)$, compute the distances

$$D(V^*, u) = \min_{v^* \in V^*} \max \left\{ \sqrt{(v^* - u)^\top \Sigma_{u}^{-1}(v^* - u)}, \sqrt{(v^* - u)^\top \Sigma_{v^*}^{-1}(v^* - u)} \right\}.$$

v. Rank the unseeded vertices in $G_2$ so that the vertex $u$ minimizing $D(V^*, u)$ is ranked first, with ties broken in an arbitrary but fixed manner.

Below, we apply this VN scheme in an illustrative simulation and on a real data network pair derived from the a neuroscience application.
Figure 2: Improvement in vertex nomination performance under the stochastic block model specified above, as a function of $\epsilon \in (0,0.1,0.2,0.3,0.5)$ for fixed $\delta = 1$, based on 10 randomly chosen seeded vertices. The plot shows $r_{fg}(k) - r_f(k)$, as defined in Equation (1), for $k \in (1,10,20,30,40)$. Results are averaged over 100 Monte Carlo trials, with error bars indicating two standard errors of the mean.

### 6.1 Synthetic data

To further explore the complementary roles of network structure and features, we consider the following simulation, set in the context of the stochastic blockmodel [18], as described in Definition 15. We consider $G_1 \sim \text{SBM}(5,b,\Lambda_1)$ independent of $G_2 \sim \text{SBM}(5,b,\Lambda_2)$, with $V(G_i) = \{1,2,\ldots,250\}$, $b(v) = \lceil 250/v \rceil$, $\Lambda_1 = \text{diag}(\epsilon+0.05,\epsilon,\epsilon,\epsilon,\epsilon) + 0.3 * J_5$, and $\Lambda_2 = 0.8 * \Lambda_1 + 0.2 * J_5$, where $J_p$ denotes the $p$-by-$p$ matrix of all ones. We designate block 1 as the anomalous block, containing the vertices of interest across the two networks, with the signal in the anomalous block 1 dampened in $G_2$ compared to $G_1$ owing to the convex combination of $\Lambda_1$ and the “flat” matrix $J_5$. $v \in V$ such that $b(v) = 1$ will be considered the vertices of interest, and we consider vertex features $x,y \in \mathbb{R}^{250 \times 5}$ of the form (letting $I_d$ denote the $d$-by-$d$ identity matrix)

$$x(v) \sim \begin{cases} \text{Norm}(\delta\vec{1},I_5) & \text{if } b(v) = 1 \\ \text{Norm}(\vec{0},I_5) & \text{if } b(v) \neq 1 \end{cases}$$

$$y(v) \sim \begin{cases} \text{Norm}(\delta\vec{1},I_5) & \text{if } b(v) = 1 \\ \text{Norm}(\vec{0},I_5) & \text{if } b(v) \neq 1 \end{cases}$$

independently over all $v \in V$ and generating $x$ and $y$ independently of one another. Note that when applying VN$\circ$GMM$\circ$ASE to the above data, we set the parameters as the true $d = 5$, with the number of clusters in step (iv) set to 5 as well. In practice there are numerous principled heuristics to select this dimension parameter (e.g., USVT [6]...
or finding an elbow in the scree plot [62]) and the number of clusters (e.g., optimizing silhouette width or minimizing BIC [15]). We do not pursue these model selection problems further here.

We select 10 vertices at random from block 1 in $G_1$ and from block 1 in $G_2$ to serve as seeded vertices. The effects of $\epsilon$ and $\delta$ are as follows. Larger values of $\epsilon$ provide more separation between the blocks in the underlying SBM, making it easier to distinguish the vertices of interest from the seeded vertices. This is demonstrated in Figure 2, where we vary $\epsilon \in (0, 0.1, 0.2, 0.3, 0.5)$ with $\delta = 1$ held fixed. The figure shows, for different choices of number of seed vertices $x$, the gain in precision at $x$ achieved by incorporating the graph topology as compared to a nomination scheme based on features alone. Define $r_{fg}(k)$ to be the number of vertices of interest in $G_2$ nominated in the top $k$ by VN $\circ$ GMM $\circ$ ASE applied to $(G_1, x, G_2, y)$, and define $r_f(k)$ to be the number of vertices of interest in $G_2$ nominated in the top $k$ by VN $\circ$ GMM $\circ$ ASE applied to $(x, y)$, that is, step (iv) of the algorithm above applied only to the vertex features. Figure 2 plots $r_{fg}(k) - r_f(k)$ for $k \in (1, 10, 20, 30, 40)$. Note that we do not consider seeded vertices in our rank list, so the maximum value achievable by $r_{fg}$ or $r_f$ is 40. Results are averaged over 100 Monte Carlo replicates of the experiment, with error bars indicating 2 standard errors of the mean. Examining the figure, we see the expected phenomenon: as $\epsilon$ increases, the gain in VN precision from incorporating the network increases. For small values of $\epsilon$, the graphs are detrimental to performance when compared to using features alone, since the structure of $\Lambda_1$ and $\Lambda_2$ are such that it is difficulty to distinguish the communities from one another (and to distinguish the interesting community from the rest of the network). As $\epsilon$ increases, the community structure in networks $G_1$ and $G_2$ becomes easier to detect, and incorporating network structure into the vertex nomination procedure becomes beneficial to performance as compared to a procedure using only vertex features.

While $\epsilon$ controls the strength of the signal present in the network, $\delta$ controls the signal present in the features, with larger values of $\delta$ allowing stronger delineation of the block of interest from the rest of the graph based on features alone. To demonstrate this, we consider the same experiment as that summarized in Figure 2, but this time fixing $\epsilon = 0.25$ and varying $\delta \in (0, 0.5, 1, 1.5, 2)$. The results are plotted in Figure 3, where we plot $r_{fg}(k) - r_g(k)$ over $k \in (1, 10, 20, 30, 40)$ where $r_g(k)$ is the number of vertices of interest in $G_2$ nominated in the top $k$ by VN $\circ$ GMM $\circ$ ASE applied to $(G_1, G_2)$, that is, ignoring vertex features. As with Figure 2, we see that as $\delta$ increases, the gain in VN performance from incorporating vertex features increases. For small values of $\delta$, features are detrimental to performance, again owing to the fact that there is insufficient signal present in them to differentiate the vertices of interest from the
rest of the network.

In each of the above figures, using one of the two available data modalities (networks or features) gave performance that, while significantly better than chance, was suboptimal. These experiments suggest that combining informative network structure with informative features should yield better VN performance than utilizing either source in isolation.

6.2 C. Elegans

We next consider a real data example derived from the C. elegans connectome, as presented in [57, 55]. In this data, neurons in the C. elegans brain correspond to vertices in our network, and edges join pairs of neurons that form a synapse. The data capture the connectivity among the 302 labeled neurons in the hermaphroditic C. elegans brain for two different synapse types called electrical gap junctions and chemical synapses. These two different synaptic types yield two distinct connectomes (i.e., brain networks) capturing the two different kinds of interactions between neurons. After preprocessing the data, including removing neurons that are isolates in either connectome, symmetrizing the directed chemical connectome and removing self-loops (see [7] for details), we obtain two weighted networks on 253 shared vertices: $G_c$, capturing the chemical synapses, and $G_e$, capturing the electrical gap junction synapses. The graphs are further en-
Figure 4: Improvement in vertex nomination performance when using both network structure and neuronal type features, compared to (a) using network structure only and (b) using neuronal type features only. Performance was measured according to the number of vertices of interest whose corresponding match was ranked in the top $x$ (i.e., $y = |\{v \in V(G_c) \in \text{s.t.} \ rank_{\Phi}(v') \leq x\}|$) versus $x$. Each grey line corresponds to a single trial, and shows the improvement of this performance measure when using both network structure and vertex features as compared to the performance of its feature-oblivious (left) or network-oblivious (right) counterpart. We have highlighted in black a single “good” trial in each subplot.

This data provides a good setting for evaluating vertex nomination performance. Each of the 253 neurons in $G_c$ has a known true corresponding neuron in $G_e$. Thus, there is a sensible ground truth in a vertex nomination problem across $G_c$ and $G_e$, in the sense that each vertex in $G_c$ has one and only one corresponding vertex in $G_e$. We thus consider the following experiment. On each trial, one vertex $v$ in $G_c$ is chosen uniformly at random and is designated as the vertex of interest. An additional 20 vertices are sampled to serve as seeded vertices for the Procrustes alignment step, and the VN$\circ$GMM$\circ$ASE nomination scheme is applied as outlined previously. Performance was measured by computing the number of vertices of interest whose corresponding match was ranked in the top $x$, according to

$$y(x) = |\{u \in V(G_e) \in \text{s.t.} \ rank_{\Phi}(v) \leq x\}|, \ x = 1, 2, \ldots, 253.$$  

We denote by $y_{GF}$, $y_G$ and $y_F$, respectively, the performance of VN applied to both network and features, the network only, and the features only. Figure 4 summarizes the result of 100 independent Monte Carlo trials of this experiment. Each curve in the figure corresponds to one trial. In each trial, we compared the performance of
VN based on both network structure and vertex features against using either only
network structure (i.e., feature-oblivious VN) or only vertex features (i.e., network-
oblivious VN). Thus, the left panel of Figure 4 shows VN performance based on both
network structure and neuronal type features, which we append onto $\hat{X}_c$ and $\hat{Y}_e$ in step
(iii) above, minus performance of the scheme using the graph alone (i.e., $y_{GF} - y_G$).
Similarly, in the right panel of Figure 4, we consider VN performance based on the
graph with the neuronal type features minus performance of the scheme in the setting
with only neuronal features (i.e., $y_{GF} - y_F$). Each of the gray lines represents one trial
of this experiment, with one line rendered in black to highlight a single trial with a
comparatively “good” seed set. Note that same trial (and thus the same seed set) is
highlighted in both panels. Performance is also summarized in Table 2.

Using only the neuronal features for vertex nomination amounts to considering a
coarse clustering of the neurons into the three neuronal types. As such, recovering
correspondences across the two networks networks based only on this feature informa-
tion is thus effectively at chance, conditioned on the neuronal type. When $y_{GF} - y_F$ is
approximately 0, the graph is effectively providing only enough information to coarsely
cluster the vertices into their neuronal types. Examining Figure 4 and Table 2, it is
clear that incorporating features adds significant signal versus only considering network
structure (indeed $y_{GF} - y_G$ is uniformly positive).

Interestingly, here the right-hand panel suggests that adding the network topology
improves performance compared to a scheme that only uses features. While not usually
the case (we expect the graph to add significant signal to the features in general) this is
not unsurprising in the present setting. Here, the network topology across the graphs
differs dramatically (for example, $G_c$ has more than three times the edges of $G_e$),
and it is notoriously difficult to discover the vertex correspondence across this pair of
networks using only topology. Indeed, state-of-the-art network alignment algorithms
only recover approximately 5% of the correspondences correctly even using 50 a priori
known seeded vertices [39]. It is thus not immediate that there is sufficient signal in
the networks to identify individual neurons across networks beyond their vertex type
[39]. While the features add significant signal to the network, the graph also adds

| $k$ | $y_{GF} - y_F$ | $y_{GF} - y_G$ |
|-----|---------------|---------------|
| 1   | 1.73          | 1.53          |
| 5   | 4.76          | 7.94          |
| 10  | 7.60          | 15.55         |
| 15  | 7.83          | 22.31         |
| 20  | 8.12          | 28.30         |
| 25  | 7.25          | 34.42         |
| 30  | 6.14          | 41.35         |
| 50  | -1.29         | 73.43         |

Table 2: Mean values of $y_{GF} - y_G$ and $y_{GF} - y_F$ over the initial range of values of $x$ considered in the experiment. Note that the mean of $y_{GF} - y_F$ is less than 0 for $k$ sufficiently large.
signal to the features. For small $k$, which are typically most important for most vertex nomination problems, $y_{GF} - y_{F}$ is positive on average, and for well-chosen seed sets (see the black lines in the figure), this difference can be dramatic.

7 Discussion

It is intuitively clear that informative features and network topology will together yield better performance in most network inference tasks than using either mode in isolation. Indeed, in the context of vertex nomination, this has been established empirically across a host of application areas [10, 30]. However, examples abound where the underlying network does not offer additional information for subsequent information retrieval, and may even be detrimental; see, for example, [42]. In this paper, we establish the first (to our knowledge) theoretical exploration of the dual role of network and features, and we provide necessary and sufficient conditions under which VN performance can be improved by incorporating both network structure and features. Along the way, we have formulated a framework for vertex nomination in richly featured networks, and derived the analogue of Bayes optimality in this framework. We view this work as constituting an initial step towards a more comprehensive understanding of the benefits of incorporating features into network data and complementing classical data with network structure. A core goal of future work is to extend the framework presented here to incorporate continuous features; establish theoretical results supporting our empirical findings of the utility of features and network in the VN $\circ$ GMM $\circ$ ASE algorithm; understand the role of missing or noisily observed features; and develop a framework for adversarial attack analysis in this richly featured setting akin to that in [1].

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Algorithmic primitives

Here, we provide background information and technical details related to the algorithmic primitives involved in the VN $\circ$ GMM $\circ$ ASE scheme described in Section 6.

### A.1 Passing to ranks and diagonal augmentation

Consider a weighted adjacency matrix $A \in \mathbb{R}^{n \times n}$, and let $w \in \mathbb{R}^s$ be the vector of edge weights of $A$. Note that we are agnostic to the dimension of $w$, which will vary according to whether $A$ is symmetric, hollow, etc. Define $r \in \mathbb{R}^s$ by taking $r_i$ to be the rank of $w_i$ in the weight vector $w$, with ties broken by averaging ranks. By the pass-to-ranks operation, we mean to replace the edge weights in $w$ with the vector $2r/(s + 1)$. That is, replacing the weighted edges of $A$ by their ranks. Note that if $A$ is binary, the pass-to-ranks operation simply returns $A$ unchanged.

By diagonal augmentation we mean setting $A_{i,i} = \sum_{j \neq i} A_{i,j} / (n - 1)$ for each $i = 1, 2, \cdots, n$. In experiments, we find that these preprocessing steps are essential for robust and reliable performance on real network data [54].

### A.2 Adjacency Spectral Embedding

Given an undirected network with adjacency matrix $A \in \mathbb{R}^{n \times n}$, the $d$-dimensional Adjacency Spectral Embedding (ASE) of $A$ yields a mapping of the $n$ vertices in the network to points in $d$-dimensional space in such a way that vertices that play similar structural roles in the network are mapped to nearby points in $\mathbb{R}^d$ [49].

**Definition 27** (Adjacency spectral embedding). Given $d \in \mathbb{Z}_{>0}$, the adjacency spectral embedding (ASE) of $A$ into $\mathbb{R}^d$ is defined by $\hat{X} = U_A S_A^{1/2} \in \mathbb{R}^{n \times d}$ where

$$|A| = [U_A |U_A^T|][S_A \oplus S_A^\perp][U_A |U_A^T]$$

is the spectral decomposition of $|A| = (A^T A)^{1/2}$, $S_A \in \mathbb{R}^{d \times d}$ is the diagonal matrix with the $d$ largest eigenvalues of $|A|$ on its diagonal and $U_A \in \mathbb{R}^{n \times d}$ has columns which are the eigenvectors corresponding to the eigenvalues of $S_A$. The $i$-th row of $\hat{X}$ corresponds to the position in $d$-dimensional Euclidean space to which the $i$-th vertex is mapped.
A.3 Seeds

In vertex nomination, vertices in the core $C$ are shared across the two networks, although the correspondence between $C \cap V_1$ and $C \cap V_2$ is unknown owing to the obfuscation function. In many applications, however, some of these correspondences may be known ahead of time. We refer to vertices in $C$ for which this correspondence is known as seeded vertices, and denote them by $S \subseteq C$. Said another way, seeded vertices are vertices in $C$ whose labels are not obfuscated. In this case, the obfuscation function would take the form $\mathcal{O}_S : V_2 \mapsto S \cup H$ where

$$\mathcal{O}_S(u) = \begin{cases} u & \text{if } u \in S \\ h \in H & \text{if } u \in V_2 \setminus S \end{cases}$$

and $H$ is an obfuscating set of order $m - |S|$ satisfying $H \cap V_i = \emptyset$ for $i = 1, 2$. Seeded vertices, and the information they provide, have proven to be valuable resources across both VN (see, for example, [12, 28, 40]) and other network-alignment tasks (see, for example, [13, 27, 33]).

A.4 Orthogonal Procrustes

The $d$-dimensional adjacency spectral embedding of a network on $n$ vertices yields a collection of $n$ points in $\mathbb{R}^d$, one point for each vertex. A natural way to compare two networks on $n$ vertices is to compare the point clouds produced by their adjacency spectral embeddings (see, e.g., [52]). Approaches of this sort are especially natural in low-rank models, such as the random dot product graph [3, 45] and the stochastic block model. In such models, we can write the expectation of the adjacency matrix as $E A = XX^T$ for $X \in \mathbb{R}^{n \times d}$, and the adjacency spectral embedding of $A$ is a natural estimate of $X$, up to orthogonal rotation. That is, for some unknown orthogonal $Q \in \mathbb{R}^{d \times d}$, $X$ and $\tilde{X}Q$ are close. Non-identifiabilities of this sort are inherent to latent space network models, whereby transformations that preserve pairwise similarity of the latent positions lead to identical distributions over networks [47]. Owing to this non-identifiability, comparison of two networks via their adjacency spectral embeddings $\tilde{X}$ and $\tilde{Y}$ requires accounting for this unknown rotation.

Given matrices $X, Y \in \mathbb{R}^{n \times d}$, the orthogonal Procrustes problem seeks the orthogonal matrix $Q \in \mathbb{R}^{d \times d}$ that minimizes $\|XQ - Y\|_F$ (where $\|\cdot\|_F$ is the Frobenius norm). The problem is solved by computing the singular value decomposition $X^TY = U\Sigma V^T$, with the optimal $Q$ given then by $Q^* = UV^T$. We note that the orthogonal Procrustes problem is just one of a number of related alignment problems for point clouds [17].
B Proofs and supporting results

Below we provide proofs of our main theoretical results and supporting lemmas.

B.1 Proof of Theorem 14

Recall that $\mathcal{S}$ is the set of indices $i$ such that $g_1^{(i)}$ and $g_2^{(i)}$ are asymmetric as richly featured networks (i.e., for $j = 1, 2$ there are no non-trivial $f$-automorphisms of $g_j^{(i)}$).

To compare the VN loss of $\Phi^*$ to that of an arbitrary VN scheme $\Phi$, we will proceed as follows. Let $k \leq m - 1$ be fixed. With

$$(G_1, G_2) = ((G_1, X, W), (G_2, Y, Z)) \sim F^{(n,m)}_{\Theta},$$

define $A_j^i := \{\text{rank}_{\Phi(g_1, \sigma(g_2), V^*)}(\sigma(v)) = j\}$ for each $j \in [k]$. Then we have that

$$\mathbb{P}(A_j^i) = \sum_{i \in \mathcal{S}} \mathbb{P}[A_j^i | (g_1^{(i)}, [\sigma(g_2^{(i)})]) \mathbb{P}((g_1^{(i)}, [\sigma(g_2^{(i)})])).$$

Next, note that for each $v \in V^*$ and $i \in \mathcal{S},$

$$\{ (g_1, g_2) \in ((g_1^{(i)}, [\sigma(g_2^{(i)})]) : \text{rank}_{\Phi(g_1, \sigma(g_2), V^*)}(\sigma(v)) = j \}$$

$$= \{ (g_1, g_2) \in ((g_1^{(i)}, [\sigma(g_2^{(i)})]) : \Phi(g_1, \sigma(g_2), V^*)[j] = \sigma(v) \}$$

$$= \{ (g_1, g_2) \in ((g_1^{(i)}, [\sigma(g_2^{(i)})]) : \exists f\text{-isomorphism } \sigma \text{ s.t. } \sigma(\sigma_2^{(i)}) = \sigma(g_2)$$

and $\sigma(\Phi(g_1^{(i)}, \sigma(g_2^{(i)}), V^*)[j]) = \sigma(v)$

$$= (g_1^{(i)}, [\sigma(g_2^{(i)})])_{\Phi(g_1^{(i)}, \sigma(g_2^{(i)}), V^*)[j] = \sigma(v)}.$$ 

To ease notation moving forward, we define the following key term for the support of $F^{(n,m)}_{\Theta}$ satisfying Assumption 11; i.e., on all $(g_1, g_2) \in \bigcup_{i \in \mathcal{S}} (g_1^{(i)}, [\sigma(g_2^{(i)})]),$

$$R_k(\Phi, g_1, g_2, V^*) := \sum_{j \leq k} \sum_{v \in V^*} \mathbb{P}[A_j^i | (g_1, [\sigma(g_2)])]$$

$$= \sum_{j \leq k} \sum_{v \in V^*} \mathbb{P}[(g_1, [\sigma(g_2)]) \Phi(g_1, \sigma(g_2), V^*)[j] = \sigma(v) | (g_1, [\sigma(g_2)])]$$

$$= \sum_{j \leq k} \mathbb{P}[(g_1, [\sigma(g_2)]) \Phi(g_1, \sigma(g_2), V^*)[j] = \sigma(v^*) | (g_1, [\sigma(g_2)])],$$

and note that, by definition of $\Phi^*$ as the optimal nomination scheme, for any $i \in \mathcal{S},$

$$R_k(\Phi, g_1^{(i)}, g_2^{(i)}, V^*) \leq R_k(\Phi^*, g_1^{(i)}, g_2^{(i)}, V^*).$$
Thus, for any FA-VN scheme $\Phi$, we have

$$1 - L_k(\Phi, V^*) = \frac{1}{k} \sum_{v \in V^*} \mathbb{P}(\text{rank}_{\Phi(G_1, o(G_2), V^*)}(o(v)) \leq k) = \frac{1}{k} \sum_{j \leq k} \sum_{v \in V^*} \mathbb{P}(A^j_v)$$

$$= \frac{1}{k} \sum_{i \in S} R_k(\Phi, g^1_i, g^2_i, V^*) \mathbb{P}\left((g^1_i, [o(g^2_i)])\right)$$

$$\leq \frac{1}{k} \sum_{i \in S} R_k(\Phi^*, g^1_i, g^2_i, V^*) \mathbb{P}\left((g^1_i, [o(g^2_i)])\right) = 1 - L_k(\Phi^*, V^*),$$

from which we deduce that $L_k(\Phi^*, V^*) \leq L_k(\Phi, V^*)$, completing the proof.

### B.2 Proof of Theorem 23

Suppose that $\mathbb{I}(X^k_{\Phi^*}; (G_1, G_2)) = \mathbb{H}(X^k_{\Phi^*})$, whence $\mathbb{H}(X^k_{\Phi^*}; (G_1, G_2)) = 0$ and thus for each $(g_1, g_2)$ with $\mathbb{P}((G_1, G_2) = (g_1, g_2)) > 0$ it holds for all $\xi \in \mathcal{T}^k_H$ that

$$\mathbb{P}(X^k_{\Phi^*} = \xi | (G_1, G_2) = (g_1, g_2)) \in \{0, 1\}.$$

For each $(g_1, g_2)$, let $\xi_{g_1, g_2}$ denote the unique element in the support of $X^k_{\Phi^*} | (G_1, G_2) = (g_1, g_2)$. With this notation in hand, we define the FO-VN scheme $\Psi$ as follows. For $g_1 = (g_1, x, w)$ and $g_2 = (g_2, y, z)$, take

$$\Psi(g_1, o(g_2), V^*) = \tilde{\xi}_{g_1, g_2},$$

where $\tilde{\xi}_{g_1, g_2} \in \mathcal{T}_H$ satisfies

i. $\tilde{\xi}_{g_1, g_2}[1 : k] = \xi_{g_1, g_2};$

ii. $\tilde{\xi}_{g_1, g_2}[k + 1 : m]$ is ordered lexicographically according to some predefined total ordering of $H$.

Then $\Psi$ is an FO-VN scheme by construction, and

$$\Psi(G_1, o(G_2), V^*)[1 : k] \overset{a.s.}{=} \Phi^*(G_1, o(G_2), V^*)[1 : k],$$

from which $L_k(\Phi^*, V^*) = L_k(\Psi, V^*) \geq L_k(\Psi^*, V^*) \geq L_k(\Phi^*, V^*)$ and therefore $L_k(\Phi^*, V^*) = L_k(\Psi^*, V^*)$, as desired.

To prove the other half of the Theorem, we proceed as follows. The assumption that $L_k(\Phi^*, V^*) = L_k(\Psi^*, V^*)$ implies that (with notation as in Section B.1),

$$0 = L_k(\Phi^*, V^*) - L_k(\Psi^*, V^*)$$

$$= \frac{1}{k} \sum_{i \in S} \left[ R_k(\Psi^*, g^1_i, g^2_i, V^*) - R_k(\Phi^*, g^1_i, g^2_i, V^*) \right] \mathbb{P}\left((g^1_i, [o(g^2_i)])\right),$$
and therefore, since
\[ R_k(\Psi^*, g_1^{(i)}, g_2^{(i)}, V^*) \leq R_k(\Phi^*, g_1^{(i)}, g_2^{(i)}, V^*) \]
for all \( i \in S \), we conclude that
\[ R_k(\Psi^*, g_1^{(i)}, g_2^{(i)}, V^*) = R_k(\Phi^*, g_1^{(i)}, g_2^{(i)}, V^*). \]

Therefore, there exists a tie-breaking scheme in the definition of \( \Phi^* \) that yields
\[ \Psi^*(g_1^{(i)}, o(g_2^{(i)}), V^*)[1 : k] = \Phi^*(g_1^{(i)}, o(g_2^{(i)}), V^*)[1 : k] \]
for all \( i \in S \), and hence
\[ \Psi^*(G_1, o(G_2), V^*)[1 : k] \overset{a.s.}{=} \Phi^*(G_1, o(G_2), V^*)[1 : k]. \]

We therefore have that \( \mathbb{H}(X_{\Phi^*}^k | (G_1, G_2)) = \mathbb{H}(X_{\Psi^*}^k | (G_1, G_2)) \). Since \( \Psi^* \) is a constant given \((G_1, G_2)\), we have \( \mathbb{H}(X_{\Phi^*}^k | (G_1, G_2)) = 0 \), and therefore \( \mathbb{H}(X_{\Phi^*}^k | (G_1, G_2)) = 0 \), completing the proof.

### B.3 Proof of Theorem 26

We assume throughout that \( F \) satisfies Assumption 25. We begin by assuming that \( \mathbb{I}(X_{\Phi^*}^k : (X, Y)) = \mathbb{I}(X_{\Phi^*}^k) \), which implies that \( \mathbb{H}(X_{\Phi^*}^k | (X, Y)) = 0 \). Therefore, for each \((x, y)\) satisfying \( \mathbb{P}((X, Y) = (x, y)) > 0 \) and each \( \xi \in \mathcal{T}_H^k \), we have
\[ \mathbb{P}(X_{\Phi^*}^k = \xi | (X, Y) = (x, y)) \in \{0, 1\}. \]

For each \((x, y)\), let \( \xi_{x,y} \) be the unique element in the support of \( X_{\Phi^*}^k | (X, Y) = (x, y) \). We define the NO-VN scheme \( \Xi \) as follows. For \( g_1 = (g_1, x, w) \) and \( g_2 = (g_2, y, z) \), we take
\[ \Xi(g_1, o(g_2), V^*) = \widehat{\xi}_{x,y}, \]
where \( \widehat{\xi}_{x,y} \in \mathcal{T}_H \) satisfies
i. \( \widehat{\xi}_{x,y}[1 : k] = \xi_{x,y} \);
ii. \( \widehat{\xi}_{x,y}[k + 1 : m] \) is ordered lexicographically according to some predefined total ordering of \( H \).

\( \Xi \) is an NO-VN scheme by construction, and
\[ \Xi(G_1, o(G_2), V^*)[1 : k] \overset{a.s.}{=} \Phi^*(G_1, o(G_2), V^*)[1 : k], \]
from which \( L_k(\Phi^*, V^*) = L_k(\Xi, V^*) \geq L_k(\Xi^*, V^*) \geq L_k(\Phi^*, V^*) \), and we conclude that \( L_k(\Phi^*, V^*) = L_k(\Xi^*, V^*). \)
To prove the other half of the theorem, we note that \( L_k(\Phi^*, V^*) = L_k(\Xi^*, V^*) \) implies that (with notation as in Section B.1),

\[
0 = L_k(\Phi^*, V^*) - L_k(\Xi^*, V^*)
\]

\[
= \frac{1}{k} \sum_{i \in S} \left[ R_k(\Xi^*, g_1^{(i)}, g_2^{(i)}, V^*) - R_k(\Phi^*, g_1^{(i)}, g_2^{(i)}, V^*) \right] P \left( g_1^{(i)}, \sigma(g_2^{(i)}) \right),
\]

since

\[
R_k(\Xi^*, g_1^{(i)}, g_2^{(i)}, V^*) \leq R_k(\Phi^*, g_1^{(i)}, g_2^{(i)}, V^*)
\]

for all \( i \in S \), we conclude that

\[
R_k(\Xi^*, g_1^{(i)}, g_2^{(i)}, V^*) = R_k(\Phi^*, g_1^{(i)}, g_2^{(i)}, V^*).
\]

Thus, there exists a tie-breaking scheme in the definition of \( \Phi^* \) such that

\[
\Xi^*(g_1^{(i)}, \sigma(g_2^{(i)}), V^*)[1 : k] = \Phi^*(g_1^{(i)}, \sigma(g_2^{(i)}), V^*)[1 : k]
\]

for all \( i \in S \), and hence

\[
\Xi^*(G_1, \sigma(G_2), V^*)[1 : k] \overset{a.s.}{=} \Phi^*(G_1, \sigma(G_2), V^*)[1 : k].
\]

We then have that \( \mathbb{H}(X_{\Phi^*}^k, |(X, Y)) = \mathbb{H}(X_{\Xi^*}^k, |(X, Y)) \). Since \( \Xi^* \) is a constant given \( (X, Y) \), we have \( \mathbb{H}(X_{\Xi^*}^k, |(X, Y)) = 0 \), whence we conclude that \( \mathbb{H}(X_{\Phi^*}^k, |(X, Y)) = 0 \), which completes the proof.

### B.4 Supporting lemmas

The following lemma follows from our assumption of asymmetry.

**Lemma 28.** If \( (g_1, g_2) \in (g_1^{(i)}, [\sigma(g_2^{(i)})]) \) for \( i \in S \), then

\[
(g_1, [\sigma(g_2)])_{\Phi(g_1, \sigma(g_2), V^*)[j] = \sigma(v)} = (g_1^{(i)}, [\sigma(g_2^{(i)})])_{\Phi(g_1^{(i)}, \sigma(g_2^{(i)}), V^*)[j] = \sigma(v)}.
\]

**Proof.** By the assumption that \( (g_1, g_2) \in (g_1^{(i)}, [\sigma(g_2^{(i)})]) \), we have that \( g_1 = g_1^{(i)} \), and there exists an isomorphism \( \tau \) such that \( g_2 = \tau(g_2^{(i)}) \). From our assumption that \( i \in S \) and the consistency criteria in Definition 9,

\[
\Phi(g_1, \sigma(g_2), V^*) = \tau(\Phi(g_1^{(i)}, \sigma(g_2^{(i)}), V^*)).
\]

A similar argument shows that \( (g_1, [\sigma(g_2)]) = (g_1^{(i)}, [\sigma(g_2^{(i)})]) \). We then have that

\[
(g_1, [\sigma(g_2)])_{\Phi(g_1, \sigma(g_2), V^*)[j] = \sigma(v)}
\]

\[
= \left\{ (g_1', g_2) \in (g_1, [\sigma(g_2)]) \text{ s.t. rank}_{\Phi(g_1', \sigma(g_2), V^*)}[\sigma(v)] = j \right\}
\]

\[
= \left\{ (g_1', g_2') \in (g_1^{(i)}, [\sigma(g_2^{(i)})]) \text{ s.t. rank}_{\Phi(g_1', \sigma(g_2'), V^*)}[\sigma(v)] = j \right\}
\]

\[
= (g_1^{(i)}, [\sigma(g_2^{(i)})])_{\Phi(g_1^{(i)}, \sigma(g_2^{(i)}), V^*)[j] = \sigma(v)}
\]

as we wished to show. \( \square \)
The following Lemma is straightforward, but is key to proving Bayes optimality.

**Lemma 29.** Let $\Phi^*$ be a Bayes optimal VN scheme, and let $\Phi$ be any other VN scheme. For any $(g_1, g_2) \in \bigcup_{i \in S} (g_1^{(i)}, [o(g_2^{(i)})]),$

$$R_k(\Phi, g_1, g_2, V^*) \leq R_k(\Phi^*, g_1, g_2, V^*).$$

**Proof.** If there exists an $i \in S$ such that $(g_1, g_2) = (g_1^{(i)}, g_2^{(i)}),$ the result follows from the definition of $\Phi^*.$ Consider then

$$(g_1, g_2) \in \left\{ \bigcup_{i \in S} (g_1^{(i)}, [o(g_2^{(i)})]) \right\} \setminus \left\{ [g_1^{(i)}, g_2^{(i)}] \right\}_{i \in S},$$

and let $i' \in S$ be such that $(g_1, g_2) \in (g_1^{(i')}, [o(g_2^{(i')})]).$ We have that

$$R_k(\Phi, g_1, g_2, V^*) = \sum_{j \leq k} \mathbb{P}\left( (g_1, [o(g_2)]) \mid \Phi(g_1, o(g_2), V^*), j \in o(V^*) \right| (g_1, [o(g_2)]) \right)$$

$$= \sum_{j \leq k} \mathbb{P}\left( (g_1^{(i')}, [o(g_2^{(i')})]) \mid \Phi(g_1^{(i')}, o(g_2^{(i')}), V^*), j \in o(V^*) \right| (g_1^{(i')}, [o(g_2^{(i')})]) \right)$$

$$\leq \sum_{j \leq k} \mathbb{P}\left( (g_1^{(i')}, [o(g_2^{(i')})]) \mid \Phi^*(g_1^{(i')}, o(g_2^{(i')}, V^*), j \in o(V^*) \right| (g_1^{(i')}, [o(g_2^{(i')})]) \right)$$

$$= \sum_{j \leq k} \mathbb{P}\left( (g_1, [o(g_2)]) \mid \Phi^*(g_1, o(g_2), V^*), j \in o(V^*) \right| (g_1, [o(g_2)]) \right)$$

$$= R_k(\Phi^*, g_1, g_2, V^*),$$

where the inequality follows from the optimality of $\Phi^*.$

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