VERTEX NOMINATION SCHEMES FOR MEMBERSHIP PREDICTION¹

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Suppose that a graph is realized from a stochastic block model where one of the blocks is of interest, but many or all of the vertices' block labels are unobserved. The task is to order the vertices with unobserved block labels into a "nomination list" such that, with high probability, vertices from the interesting block are concentrated near the list's beginning. We propose several vertex nomination schemes. Our basic—but principled—setting and development yields a best nomination scheme (which is a Bayes–Optimal analogue), and also a likelihood maximization nomination scheme that is practical to implement when there are a thousand vertices, and which is empirically nearoptimal when the number of vertices is small enough to allow comparison to the best nomination scheme. We then illustrate the robustness of the likelihood maximization nomination scheme to the modeling challenges inherent in real data, using examples which include a social network involving human trafficking, the Enron Graph, a worm brain connectome and a political blog network.

1. Article overview. In a stochastic block model, the vertices of the graph are partitioned into blocks, and the existence/nonexistence of an edge between any pair of vertices is an independent Bernoulli trial, with the Bernoulli parameter being a function of the block memberships of the pair of vertices. We are concerned here with a graph realized from a stochastic block model such that many or all of the vertices' block labels are hidden (i.e., unobserved). Suppose that one particular block is of interest, and the task is to order the vertices with a hidden block label into a "nomination list" with the goal of having vertices from the interesting block concentrated near the beginning of the list. Forming such a nomination list can be assisted by any available knowledge about the underlying model parameters, as well as by utilizing knowledge of block membership for any of the vertices for which such block labels are observed. A vertex nomination scheme is a function that, to each such possible observed graph, assigns an associated nomination list. In this paper we present, analyze, and illustrate the effectiveness of several vertex nomination schemes. Some of these vertex nomination schemes uti-

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lize graph matching and spectral partitioning machinery. See Coppersmith (2014), Coppersmith and Priebe (2012) and Lee and Priebe (2012) for recent work on vertex nomination, as well as a survey of closely related problems.

One illustrative example of vertex nomination would be a social network with vertices representing people, some of whom are engaged in human trafficking, the rest of whom are not engaged in human trafficking, and with edges representing a working relationship between the individuals. Law enforcement may have as a priority separating human trafficking from mundane sex work, because not all illegal acts represent the same level of overall coercion. If several of these people are known to law enforcement as human traffickers, several are known to law enforcement to not be human traffickers, and there are very limited resources to scrutinize the remainder as yet ambiguous people to see if they are human traffickers, then a task would be to use the available information and the adjacencies so as to order the as yet ambiguous vertices into a nomination list that would prioritize these vertices for this further scrutiny through other investigative means. In particular, the nomination task here is a task which is not simply classification—it is prioritization. Later, in Section 9, we highlight a much more elaborate real-data application of vertex nomination in a social network involving actual human trafficking.

In Section 2 we formally and carefully define the setting and the concept of a vertex nomination scheme. Although prioritization is a ubiquitous need that can be treated in an ad hoc fashion specific to individual applications, we here formally set the problem in the stochastic block model setting, which has gained so much popularity in recent literature [e.g., see Airoldi et al. (2009), Bickel and Chen (2009), Nowicki and Snijders (2001)] and is a useful model for real data. This formal setting will be useful for principled development of techniques that have solid theoretical foundations and are also robust to the modeling challenges inherent in real data.

In Section 3 we introduce the canonical vertex nomination scheme. It is analogous to the Bayes classifier in the setting of classification. Indeed, we prove in Proposition 1 that the canonical vertex nomination scheme is at least as effective as every other vertex nomination scheme, and it thus serves the valuable role of a "gold standard" with which to gauge the success of other vertex nomination schemes. However, it is computationally practical to implement only when there are on the order of a very few tens of vertices.

In Section 4 we introduce the likelihood maximization vertex nomination scheme, which fundamentally utilizes graph matching machinery. The graph matching problem is to find a bijection between the vertex sets of two graphs that minimizes the number of induced adjacency disagreements; there is a vast literature dedicated to this problem, for example, see the article Thirty Years of Graph Matching in Pattern Recognition [Conte et al. (2004)] for an excellent survey. Although graph matching is intractable in theory, there have been recent advances in approximate graph matching algorithms that are both tractable and effective; for example, see Lyzinski, Fishkind and Priebe (2014), Vogelstein et al. (2015) and Zaslavskiy, Bach and Vert (2009). In particular, the very recent SGM algorithm of

Lyzinski, Fishkind and Priebe (2014) has been shown in Lyzinski et al. (2015b) to be theoretically and practically superior to convex relaxation approaches. Using the SGM algorithm of Lyzinski, Fishkind and Priebe (2014) for approximate graph matching, the likelihood maximization vertex nomination scheme is practical to implement for on the order of 1000 vertices. In Sections 8.1, 8.2 and 8.3, we illustrate the robustness of the likelihood maximization vertex nomination scheme to the model misspecifications inherent in real data. Furthermore, we demonstrate in Section 7 that likelihood maximization performs nearly as well as the canonical "gold standard"—on graphs that have few enough vertices so that canonical is indeed computable.

In Section 5 we introduce the spectral partitioning vertex nomination scheme; it is practical to implement for tens of thousands of vertices or more. Based on the results in Sussman et al. (2012) and Fishkind et al. (2013), then followed up in Lyzinski et al. (2014b), the spectral partitioning vertex nomination scheme nominates perfectly as the number of vertices goes to infinity, under mild conditions.

In Section 7 we perform illustrative simulations at three different scales, that is, a "small scale" experiment with ten ambiguous vertices, a "medium scale" experiment with 500 ambiguous vertices, and a "large scale" experiment with 10,000 ambiguous vertices. With respect to nomination effectiveness and practicality of implementation, the canonical vertex nomination scheme dominates at the small scale, the likelihood maximization scheme dominates at the medium scale, and the spectral partitioning scheme dominates at the large scale.

In Section 8.1 we illustrate our vertex nomination schemes on the "Enron Graph," a graph with email addresses of former employees of the failed Enron Corporation as vertices, and edges indicating email contact between the associated vertices over a time interval. Our vertex nomination schemes are used to nominate higher-echelon former Enron employees. Then, in Sections 8.2 and 8.3 we illustrate on examples with a worm-brain connectome (to nominate motor neurons) and a blog network (to nominate political affiliation).

In Section 9 we illustrate the impact of our vertex nomination machinery on a real-data social network involving human trafficking. The data are associated with the DARPA Memex and XDATA programs. We have a graph of web advertisements, some of them with known association to human trafficking. Using the machinery developed in this manuscript, we were able to nominate ambiguous advertisements for human trafficking in a manner that was operationally significant.

2. Vertex nomination schemes; setting and definition. In this article we assume for simplicity that graphs are simple (i.e., edges are not directed, there are no parallel edges and no single-edge loops), but much of what we do is generalizable.

We begin by describing the stochastic block distribution $SB(K, m, n, b, \Lambda)$, which will be our random graph setting; its parameters are a positive integer *K* (the number of *blocks*), a nonnegative integer *m* (the number of *seeds*), a positive integer *n* (the number of *ambiguous vertices*), an arbitrary but fixed function $b: \{1, 2, ..., m + n\} \rightarrow \{1, 2, ..., K\}$ (the *block membership function*) and a symmetric matrix $\Lambda \in [0, 1]^{K \times K}$ (the *adjacency probabilities*). A random graph with distribution SB(K, m, n, b, Λ) has the vertex set $W := \{1, 2, ..., m + n\}$ and, for each unordered pair of distinct vertices $\{w, w'\} \in {W \choose 2}$, w is adjacent to $w' (w \sim w')$ according to an independent Bernoulli trial with parameter $\Lambda_{b(w), b(w')}$.

The vertex set *W* is partitioned into two sets, the set $U := \{1, 2, ..., m\}$ (the *seeds*) and the set $V := \{m + 1, m + 2, ..., m + n\}$ (the *ambiguous vertices*). For each i = 1, 2, ..., K, define $m_i := |\{u \in U : b(u) = i\}|$ and $n_i := |\{v \in V : b(v) = i\}|$. The function *b* is only partially observed; its values are known on *U*, but not on *V*. In other words, the block memberships of the seeds are known, and the block memberships of the ambiguous vertices are unknown, but we will assume for simplicity that Λ is known, and that $n_1, n_2, ..., n_K$ are known. Given a random graph from SB(K, m, n, b, Λ), the most general inferential task would be to estimate *b* on *W*, but we will fine tune this task very soon. (Note that if Λ and $n_1, n_2, ..., n_K$ were not known then, if there are enough seeds, Λ could be approximated from edge densities of subgraphs induced by various subsets of the seeds and, in addition, the values of $n_1, n_2, ..., n_K$ might be approximated if it just so happens to be known that they are roughly proportional to the respective values of $m_1, m_2, ..., m_K$. Of course, $m_1, m_2, ..., m_K$ are known by virtue of the fact that *b* is known on *U*.)

Define Ξ to be the set of bijective functions from W to W that fix the elements of U; of course, $|\Xi| = n!$. Any two graphs G and H on the vertex set W are called *equivalent* if G is isomorphic to H under some function $\xi \in \Xi$; if G is also asymmetric (i.e., its automorphism group is trivial), then such a ξ is unique to G, H, denote it $\xi_{G,H}$. For any graph G on vertex set W, the equivalence class of equivalent-to-G graphs on vertex set W will be denoted $\langle G \rangle$; in particular, $\langle G \rangle$ is an event. The set of all such equivalence classes is denoted Θ ; the events in Θ partition the sample space.

A vertex nomination scheme Φ is a mapping that, to each asymmetric graph G with vertex set W, associates a linear ordering of the vertices in V—called the nomination order, and denoted as a list $(\Phi_G(1), \Phi_G(2), \dots, \Phi_G(n))$ —such that for every H equivalent to G it holds that $(\xi_{G,H}(\Phi_G(1)), \xi_{G,H}(\Phi_G(2)), \dots, \xi_{G,H}(\Phi_G(n))) = (\Phi_H(1), \Phi_H(2), \dots, \Phi_H(n))$. In other words, and described somewhat informally, if each equivalence class of graphs is viewed as a (single) graph whose vertex set is comprised of labeled vertices U and unlabeled vertices V, then to each equivalence class (i.e., partially vertex-labeled graph) Φ associates a list of unlabeled vertices of V.

Note that the fraction of all graphs on vertex set W which are symmetric goes very quickly to zero as |W| goes to infinity [Erdős and Rényi (1963), Pólya (1937)]. Although symmetric graphs are thus negligibly many, it is helpful for notation to extend the domain of Φ to include symmetric graphs, and this can be done in many different ways. For simplicity of analysis we will simply say for

now that, to every symmetric graph G on the vertex set W, the associated nomination list is declared to be (m + 1, m + 2, ..., m + n) (and we do not require the nomination list in this case to meet the property mentioned above).

In this article, we assume that only membership in the first block is of interest; the specific task we are concerned with is to find vertex nomination schemes under which there will be, with high probability, an abundance of members of the first block that are near the beginning of the nomination list. As an illustrative example related to the Enron Graph example in Section 8.1, consider a corporation with $m + n = m_1 + m_2 + n_1 + n_2$ employees, of which $m_1 + n_1$ are involved in fraud and $m_2 + n_2$ are not involved in fraud. The probability of communication between fraudsters is fixed, as is the probability of communication between nonfraudsters, as is the probability of communication between any fraudster and any nonfraudster. Of the $m_1 + n_1$ fraudsters, m_1 have been identified as fraudsters. Based on observing all of the employee communications (together with knowledge of the identities of m_1 fraudsters and m_2 nonfraudsters), we wish to draw up a nomination list of the $n_1 + n_2$ ambiguous employees so that there are many fraudsters early in the list.

The effectiveness of a vertex nomination scheme Φ is quantified in the following manner. For any graph G with vertex set W, and for any integer j such that $1 \leq j$ $j \le n$, the precision at depth j of Φ for G is defined to be $\frac{|\{1 \le i \le j: b(\Phi_G(i))=1\}|}{i}$; for the corporate illustration, this represents the fraction of the first j employees on the nomination list that are actual fraudsters in truth. The *average precision* of Φ for G is defined to be $\frac{1}{n_1} \sum_{j=1}^{n_1} \frac{|\{1 \le i \le j: b(\Phi_G(i))=1\}|}{j}$; it has a value between 0 (per the corporate example, if none of the first n_1 nominated employees are fraudsters) and 1 (if all of the first n_1 nominated employees are fraudsters). Note that the average precision of Φ for G is equal to $\sum_{i=1}^{n_1} (\frac{1}{n_1} \sum_{j=i}^{n_1} \frac{1}{j}) \delta_{b(\Phi_G(i))=1}$, where δ is the usual indicator function. In particular, the average precision of Φ for G is a convex combination of the indicators $\delta_{b(\Phi_G(i))=1}$, with more weight in this convex combination for indicators associated with lower values of *i*. The mean average *precision* of the vertex nomination scheme Φ is the expected value of the average precision for a random graph G distributed $SB(K, m, n, b, \Lambda)$. The closer that this number is to 1, the more effective a vertex nomination scheme Φ is deemed. Note that a "chance" vertex nomination scheme would have the value $\frac{n_1}{n}$ as its mean average precision.

We point out that our definition of average precision is slightly different than a definition commonly used in the information retrieval community; our definition is a pure average precision, whereas the other definition is actually an integral of the precision over recall.

3. The canonical vertex nomination scheme. In this section we define the canonical vertex nomination scheme, which is analogous to the Bayes classifier in

the Bayes classifier's setting of classification. Indeed, we prove in Proposition 1 that the mean average precision of the canonical vertex nomination scheme is greater than or equal to the mean average precision of every other vertex nomination scheme. Unfortunately, because of its computational intractability (a visibly exponential runtime as the number of vertices increases), the canonical vertex nomination scheme is only practical to implement for up to a few tens of vertices. Nonetheless, because of Proposition 1, the canonical vertex nomination scheme serves as a valuable "gold standard" to evaluate the performance of other more computationally tractable vertex nomination schemes. (This is analogous to the role of the Bayes classifier in the classification setting.) Our ongoing research seeks to approximate the canonical vertex nomination scheme in a scalable fashion.

3.1. Definition of the scheme. Consider the random graph G distributed $SB(K, m, n, b, \Lambda)$. When G is asymmetric then, for any $v \in V$, the conditional probability

(1)
$$\mathbb{P}[\{H \in \langle G \rangle : b(\xi_{G,H}(v)) = 1\} | \langle G \rangle]$$

may be described as the probability, given the event that we observe a graph equivalent to *G*, that the vertex corresponding to *v* would be in the first block. The *canonical vertex nomination scheme*, which we denote as Φ^C , orders the vertices of *V* as $\Phi^C_G(1), \Phi^C_G(2), \ldots, \Phi^C_G(n)$ in decreasing order of this conditional probability; that is, we define Φ^C so that, for all $i = 1, 2, \ldots, n-1$,

(2)

$$\mathbb{P}[\{H \in \langle G \rangle : b(\xi_{G,H}(\Phi_G^C(i))) = 1\} | \langle G \rangle] \\
\geq \mathbb{P}[\{H \in \langle G \rangle : b(\xi_{G,H}(\Phi_G^C(i+1))) = 1\} | \langle G \rangle].$$

To more easily compute the conditional probability in equation (1), let $\binom{V}{n_1,n_2,...,n_K}$ denote the collection of all the $\binom{n}{n_1,n_2,...,n_k}$ partitions of the elements of V into subsets called $V_1, V_2, ..., V_K$ with respective cardinalities $n_1, n_2, ..., n_K$. Given any such partition $(V_1, V_2, ..., V_K) \in \binom{V}{n_1,n_2,...,n_K}$, let us create the following notation. For any k = 1, 2, ..., K and $\ell = k + 1, k + 2, ..., K$, let $e_{k,\ell}$ denote the number of edges in G with one endpoint in $V_k \cup \{u \in U : b(u) = k\}$ and the other endpoint in $V_\ell \cup \{u \in U : b(u) = \ell\}$, and define $c_{k,\ell} := (m_k + n_k)(m_\ell + n_\ell) - e_{k,\ell}$. Let $e_{k,k}$ denote the number of edges in G with both endpoints in $V_k \cup \{u \in U : b(u) = k\}$, and define $c_{k,k} := \binom{m_k + n_k}{2} - e_{k,k}$. Then, in the stochastic block model, the conditional probability in equation (1) can be computed as

(3)
$$\frac{\sum_{(V_1, V_2, \dots, V_K) \in \binom{V}{n_1, n_2, \dots, n_K}} \text{ such that } v \in V_1 \prod_{k=1}^K \prod_{\ell=k}^K (\Lambda_{k,\ell})^{e_{k,\ell}} (1 - \Lambda_{k,\ell})^{c_{k,\ell}}}{\sum_{(V_1, V_2, \dots, V_K) \in \binom{V}{n_1, n_2, \dots, n_K}} \prod_{k=1}^K \prod_{\ell=k}^K (\Lambda_{k,\ell})^{e_{k,\ell}} (1 - \Lambda_{k,\ell})^{c_{k,\ell}}}$$

Although we are not able to evaluate the probability of *G* since the block membership function *b* is not fully observed, nonetheless, the conditional probabilities in equation (1) can indeed be evaluated via equation (3) by just knowing the values of the parameters n_1, n_2, \ldots, n_K and Λ .

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3.2. Optimality of the canonical vertex nomination scheme.

THEOREM 1. For any vertex nomination scheme Φ , the mean average precision of the canonical vertex nomination scheme Φ^C is greater then or equal to the mean average precision of Φ .

PROOF. For each $i = 1, 2, ..., n_1$, define $\alpha_i := \frac{1}{n_1} \sum_{j=i}^{n_1} \frac{1}{j}$ and, for each $i = n_1 + 1, n_1 + 2, ..., n$, define $\alpha_i := 0$. The sequence $\alpha_1, \alpha_2, ..., \alpha_n$ is clearly a non-negative, nonincreasing sequence. Note that if $a_1, a_2, ..., a_n$ is any (other) nonincreasing, nonnegative sequence of real numbers, and $a'_1, a'_2, ..., a'_n$ is any permutation of the sequence $a_1, a_2, ..., a_n$, then

(4)
$$\sum_{i=1}^{n} \alpha_i a'_i \leq \sum_{i=1}^{n} \alpha_i a_i.$$

Indeed, this is easily verified by first considering particular sequences a_1, a_2, \ldots, a_n of the form $1, 1, \ldots, 1, 0, \ldots, 0, 0$ (i.e., *j* consecutive 1's followed by n - j consecutive 0's, for different values of $j = 1, 2, \ldots, n$) and then noting that the nonnegative combinations of such particular sequences indeed comprise all non-increasing, nonnegative sequences with *n* entries.

Consider the random graph *G* distributed $SB(K, m, n, b, \Lambda)$. Recall that Θ denotes the set of equivalence classes of graphs on the vertex set *W*.

Expanding the mean average precisions of Φ , then bounding and simplifying, yields

$$\mathbb{E}\left(\sum_{i=1}^{n} \alpha_{i} \delta_{b(\Phi_{G}(i))=1}\right) = \sum_{i=1}^{n} \alpha_{i} \mathbb{P}(b(\Phi_{G}(i))=1)$$

$$= \sum_{i=1}^{n} \alpha_{i} \left(\sum_{\mathcal{G} \in \Theta} \mathbb{P}(\mathcal{G}) \mathbb{P}(b(\Phi_{G}(i))=1 \middle| \mathcal{G})\right)$$

$$(5) \qquad = \sum_{\mathcal{G} \in \Theta} \mathbb{P}(\mathcal{G}) \left(\sum_{i=1}^{n} \alpha_{i} \mathbb{P}(b(\Phi_{G}(i))=1 \middle| \mathcal{G})\right)$$

$$\leq \sum_{\mathcal{G} \in \Theta} \mathbb{P}(\mathcal{G}) \left(\sum_{i=1}^{n} \alpha_{i} \mathbb{P}(b(\Phi_{G}^{C}(i))=1 \middle| \mathcal{G})\right)$$

$$= \sum_{i=1}^{n} \alpha_{i} \mathbb{P}(b(\Phi_{G}^{C}(i))=1) = \mathbb{E}\left(\sum_{i=1}^{n} \alpha_{i} \delta_{b(\Phi_{G}^{C}(i))=1}\right),$$

where the inequality in equation (5) follows from equations (4) and (2), (and from our assumption that all nomination schemes agree when G is symmetric). The desired result is shown. \Box

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4. Likelihood maximization vertex nomination scheme. In this section we define the likelihood maximization vertex nomination scheme. It will be practical to implement even when there are on the order of a thousand vertices. We will see in Section 7 that it is a very effective vertex nomination scheme, when compared to the canonical vertex nomination scheme "gold standard" on graphs small enough to make the comparison. In Sections 8.1, 8.2 and 8.3 we will see that likelihood maximization appears to be nicely robust to the modeling challenges inherent in real data.

4.1. Definition of the scheme. Suppose the random graph G is distributed $SB(K, m, n, b, \Lambda)$. There are two stages in defining—and computing—the likelihood maximization vertex nomination scheme.

The first stage is concerned with estimating the block assignment function *b*. Let \mathfrak{B} denote the set of functions $\mathfrak{b}: W \to \{1, 2, ..., K\}$ such that \mathfrak{b} agrees with *b* on *U*, and such that it also holds, for all i = 1, 2, ..., K, that $|\{v \in V : \mathfrak{b}(v) = i\}| = n_i$. For any $\mathfrak{b} \in \mathfrak{B}$, and for all k = 1, 2, ..., K and $\ell = k + 1, k + 2, ..., K$, let $e_{k,\ell}(\mathfrak{b})$ denote the number of edges in *G* with one endpoint in $\{w \in W : \mathfrak{b}(w) = k\}$ and the other endpoint in $\{w \in W : \mathfrak{b}(w) = \ell\}$, and also denote $c_{k,\ell}(\mathfrak{b}) := (m_k + n_k)(m_\ell + n_\ell) - e_{k,\ell}(\mathfrak{b})$. For all k = 1, 2, ..., K, let $e_{k,k}(\mathfrak{b})$ denote the number of edges in *G* with both endpoints in $\{w \in W : \mathfrak{b}(w) = k\}$, and also denote $c_{k,k}(\mathfrak{b}) := \binom{m_k + n_k}{2} - e_{k,k}(\mathfrak{b})$. In the SB(K, m, n, b, Λ) distribution, if *b* had been replaced with $\mathfrak{b} \in \mathfrak{B}$, then the probability of realizing the graph *G* would have been

(6)
$$p(\mathfrak{b},G) := \prod_{k=1}^{K} \prod_{\ell=k}^{K} (\Lambda_{k,\ell})^{e_{k,\ell}(\mathfrak{b})} (1 - \Lambda_{k,\ell})^{c_{k,\ell}(\mathfrak{b})}$$

Define \hat{b} , the maximum likelihood estimator of b, to be the member of \mathfrak{B} such that the probability of G is maximized. In other words (then taking logarithms and ignoring additive constants),

(7)

$$\hat{b} := \arg\max_{\mathfrak{b}\in\mathfrak{B}} p(\mathfrak{b}, G) = \arg\max_{\mathfrak{b}\in\mathfrak{B}} \sum_{k=1}^{K} \sum_{\ell=k}^{K} e_{k,\ell}(\mathfrak{b}) \log\left(\frac{\Lambda_{k,\ell}}{1 - \Lambda_{k,\ell}}\right)$$

$$= \arg\max_{\mathfrak{b}\in\mathfrak{B}} \sum_{\{w,w'\}\in\binom{W}{2}} \delta_{w\sim_G w'} \log\left(\frac{\Lambda_{\mathfrak{b}(w),\mathfrak{b}(w')}}{1 - \Lambda_{\mathfrak{b}(w),\mathfrak{b}(w')}}\right).$$

The optimization problem in equation (7) is an example of seeded graph matching, and we can efficiently and effectively approximate its solution. The details of this are deferred to the next section, Section 4.2, and we now continue on to the second stage of defining and computing the likelihood maximization vertex nomination scheme, assuming that we have computed \hat{b} .

For any $v, v' \in V$ such that $\hat{b}(v) = 1$ and $\hat{b}(v') \neq 1$, define $\hat{b}_{v \leftrightarrow v'} \in \mathfrak{B}$ such that $\hat{b}_{v \leftrightarrow v'}$ agrees with \hat{b} for all $w \in W$ except that $\hat{b}_{v \leftrightarrow v'}(v') = 1$ and $\hat{b}_{v \leftrightarrow v'}(v) = \hat{b}(v')$.

For any $v, v' \in V$ such that $\hat{b}(v) = 1$ and $\hat{b}(v') \neq 1$, we can interpret a low/high value of the quantity $\frac{p(\hat{b}_{v \leftrightarrow v'}, G)}{p(\hat{b}, G)}$ as a measure of our conviction/lack-of-conviction that \hat{b} should be used to estimate b, as opposed to estimating b with specifically $\hat{b}_{v \leftrightarrow v'}$. In this spirit, for all $v \in V$ such that $\hat{b}(v) = 1$, a low/high value of the geometric mean

(8)
$$\left(\prod_{v'\in V:\hat{b}(v')\neq 1} \frac{p(\hat{b}_{v\leftrightarrow v'}, G)}{p(\hat{b}, G)}\right)^{1/(n-n_1)}$$

can be interpreted as a measure (for the purpose of ordering) of our conviction/lackof-conviction in our estimation that b(v) is 1. Also, for all $v' \in V$ such that $\hat{b}(v') \neq 1$, a low/high value of the geometric mean

(9)
$$\left(\prod_{v \in V: \hat{b}(v)=1} \frac{p(\hat{b}_{v \leftrightarrow v'}, G)}{p(\hat{b}, G)}\right)^{1/n_1}$$

can be interpreted as a measure (just for the purpose of ordering) of our conviction/lack-of-conviction in our estimation that b(v') is not 1.

We now define the *likelihood maximization vertex nomination scheme* Φ^L to be such that it satisfies $\Phi^L_G(1), \Phi^L_G(2), \ldots, \Phi^L_G(n_1)$ are the $v \in V$ such that $\hat{b}(v) = 1$, listed in increasing order of the geometric mean in equation (8), and $\Phi^L_G(n_1 + 1), \Phi^L_G(n_1 + 2), \ldots, \Phi^L_G(n)$ are the $v' \in V$ such that $\hat{b}(v') \neq 1$, listed in decreasing order of the geometric mean in equation (9).

4.2. Solving the seeded graph matching problem. In this section we discuss how to compute \hat{b} in the likelihood maximization vertex nomination scheme Φ^L defined in the previous section. Given any $A, B \in \mathbb{R}^{(m+n) \times (m+n)}$, the quadratic assignment problem is to mini-

Given any $A, B \in \mathbb{R}^{(m+n)\times(m+n)}$, the *quadratic assignment problem* is to minimize $||A - PBP^T||_F^2$ over all permutation matrices $P \in \{0, 1\}^{(m+n)\times(m+n)}$, where $|| \cdot ||_F$ denotes the Frobenius matrix norm. If A and B are, respectively, adjacency matrices for two graphs, then this is called the *graph matching problem*; it is clearly equivalent to finding a bijection from the vertex set of one graph to the vertex set of the other graph so as to minimize the number of adjacency disagreements induced by the bijection. If P is further constrained so that the upper left corner is the $m \times m$ identity matrix, then the problem is called the *seeded quadratic assignment problem/seeded graph matching problem*; for graphs, this further restriction just means that part of the bijection between the vertex sets is fixed.

Note that the objective function can be simplified (under the restriction that *P* is a permutation matrix) as $||A - PBP^T||_F^2 = ||A||_F^2 + ||B||_F^2 - 2\langle A, PBP^T \rangle$, where $\langle \cdot, \cdot \rangle$ is the usual inner product $\langle C, D \rangle := \sum_{i,j} C_{ij} D_{ij}$. Thus, the above problems can be phrased as maximize $\langle A, PBP^T \rangle$ over all permutation matrices *P*.

The optimization problem in equation (7), for which \hat{b} is the solution, is precisely the seeded quadratic assignment problem above, where $A \in \mathbb{R}^{(m+n)\times(m+n)}$ is the adjacency matrix for the graph G, that is, $A_{i,j} := \delta_{i\sim Gj}$ for all $i, j \in$ $W \equiv \{1, 2, ..., m + n\}$, and $B \in \mathbb{R}^{(m+n)\times(m+n)}$ is the matrix wherein $B_{i,j} := \log(\frac{\Lambda_{\mathfrak{b}'(i),\mathfrak{b}'(j)}}{1-\Lambda_{\mathfrak{b}'(i),\mathfrak{b}'(j)}})$ for all $i, j \in W$, where \mathfrak{b}' is the member of \mathfrak{B} for which the sequence $\mathfrak{b}'(m+1), \mathfrak{b}'(m+2), \ldots, \mathfrak{b}'(m+n)$ are 1's contiguously, then 2's contiguously, ..., then K's contiguously. The $\mathfrak{b} \in \mathfrak{B}$ —over which the objective function in equation (7) is maximized—correspond precisely to the permutation matrices P in the seeded quadratic assignment problem, where the upper left corner of P is restricted to be the $m \times m$ identity matrix. We will call this problem a seeded graph matching problem because A is an adjacency matrix. (And we can also choose to think of B as a weighted adjacency matrix for a graph.)

The seeded graph matching problem is computationally hard; indeed, the quadratic assignment problem is NP-hard, and even deciding if two graphs are isomorphic is notoriously of unknown complexity [Garey and Johnson (1979), Read and Corneil (1977)]. However, approximate solutions can be found efficiently with the SGM (Seeded Graph Matching) Algorithm of Lyzinski, Fishkind and Priebe (2014), which is a seeded version of the FAQ algorithm of Vogelstein et al. (2015). [Indeed, SGM is more effective than convex relaxation techniques, as was recently shown in Lyzinski et al. (2015b).] We employ the SGM algorithm to obtain an approximate solution to \hat{b} for use in the likelihood maximization vertex nomination scheme. It runs in time $O(n^3)$, and can be implemented even when *n* is approximately 1000.

5. The spectral partitioning vertex nomination scheme. In this section we introduce the *spectral partitioning vertex nomination scheme*. Suppose *G* is distributed SB(K, m, n, b, Λ). We do not need to assume here that we know n_1, n_2, \ldots, n_K , nor the entries of Λ ; we just need to know the value of *K* and d := the rank of Λ . [Indeed, by the results in Fishkind et al. (2013), even just knowing an upper bound on *d* will be sufficient to obtain good performance.]

Say that the adjacency matrix for *G* is $A \in \{0, 1\}^{(m+n)\times(m+n)}$, that is, $A_{i,j} := \delta_{i\sim_G j}$ for all $i, j \in W \equiv \{1, 2, ..., m+n\}$. Compute *d* eigenvectors associated, respectively, with the *d* largest-modulus eigenvalues of *A*. Scale these eigenvectors so that their respective lengths are the square roots of the absolute values of their corresponding eigenvalues, and define $X \in \mathbb{R}^{(m+n)\times d}$ to have these scaled eigenvectors as its respective columns. The rows of *X* are low-dimensional embeddings of the corresponding vertices. Now, cluster the rows of *X* into *K* clusters; that is, solve the problem minimize $||X - C||_F$ over all matrices $C \in \mathbb{R}^{(m+n)\times d}$ with the property that each row of *C* is equal to one of just *K* row vectors, and the values of these *K* row vectors are also variables to be optimized over.

Say that c is the most frequent value of row vector in the optimal C among the rows corresponding to the vertices $\{u \in U : b(u) = 1\}$. (In other words, c is

the centroid associated with the most vertices known to be in the first block.) The spectral partitioning vertex nominating scheme, denoted by Φ^S , associates with *G* the ordering (of vertices in *V*) $\Phi^S_G(1), \Phi^S_G(2), \ldots, \Phi^S_G(n)$ in increasing order of Euclidean distance between *c* and their corresponding row in *X*.

Suppose we consider a sequence of graphs realized from the distributions SB(K, m, n, b, Λ) for, successively, m + n = 1, 2, 3, ..., where K and Λ are fixed, and Λ is positive semi-definite with the property that no two of its rows are equal. Also, assume that $m_1 \ge 1$, and there exists a positive constant γ such that, for all i = 1, 2, ..., K, it holds that $m_i + n_i \ge \gamma (m + n)^{3/4+\gamma}$. It was recently shown in Lyzinski et al. (2014b) [following the work in Sussman et al. (2012) and Fishkind et al. (2013)] that almost surely there are no incorrectly clustered vertices in the limit. This implies that the mean average precision of Φ^S converges to 1 as $m + n \to \infty$.

It will be computationally convenient to approximately (but very quickly) solve the clustering subproblem. This approximate clustering can be done with the kmeans algorithm or with the mclust procedure [Fraley and Raftery (1999), Fraley and Raftery (2003)]. In both cases, the vertices are nominated based on distance to cluster centroids; in k-means this amounts to the usual Euclidean distance, while for mclust this amounts to nominating based on the Mahalonobis distance.

6. The OTS vertex nomination scheme. The chief contribution of this manuscript is the formulation of the likelihood maximization vertex nomination scheme, along with our demonstration of its effectiveness; indeed, it is comparably effective to the "gold standard" canonical vertex nomination scheme (on graphs small enough to practically make this comparison, as we demonstrate in Section 7) and it is relatively robust to pathologies inherent in real data (as we demonstrate later in Section 8).

However, it is worthwhile to point out that classification algorithms for stochastic block models can often be naturally modified for use in nomination, by utilizing algorithm-inherent numeric scores to perform vertex ranking. For an excellent survey of the literature on community detection in networks—including the setting of stochastic block models—and available algorithms, see the very comprehensive survey article Fortunato (2010) and the papers cited therein, such as Newman and Girvan (2004) and the classic article Nowicki and Snijders (2001). Also, see Latent Dirichlet Allocation (LDA) [Blei, Ng and Jordan (2003)]. Because of the vast number of citations to it in the literature, we next choose to focus on the paper Airoldi et al. (2009), titled "Mixed membership stochastic blockmodels," and the associated R code which we call "MMSB" located at http://cran.r-project.org/web/packages/lda/lda.pdf [Chang and Dai (2010)]; in the setting of a mixed membership block model, MMSB assigns to each vertex a posterior probability of block membership in each of the various blocks. With this, we now define the *OTS vertex nomination scheme*, denoted Φ^O , which uses MMSB to order the vertices of V in decreasing order of posterior probability of membership in the specific block indicated by the most seeds.

We call this nomination scheme OTS "Off The Shelf" to emphasize that we use MMSB as a black box without getting under the hood of the code; as such, the use of the seeds is only to identify the block of interest. Indeed, under the hood modifications of existing community detection algorithms such as MMSB and LDA and LDA-based methodologies are expected to yield new vertex nomination schemes that will be increasingly effective and fast. We also expect even more effective vertex nomination schemes to come from merging vertex nomination techniques, perhaps similar in spirit to the work in Lyzinski et al. (2015a), where graph matching and spectral partitioning are merged into a more effective avenue of graph matching for large graphs.

7. Simulations: Comparing the vertex nomination schemes at three different scales. In this section we compare and contrast these vertex nomination schemes using three simulation experiments—essentially the same experiment at three different scales, "small scale," "medium scale" and "large scale." For each of the three experiments, we have K = 3 blocks in the stochastic block model. The matrix of Bernoulli parameters Λ is

$$\Lambda(\vartheta) := \vartheta \begin{bmatrix} 0.5 & 0.3 & 0.4 \\ 0.3 & 0.8 & 0.6 \\ 0.4 & 0.6 & 0.3 \end{bmatrix} + (1 - \vartheta) \begin{bmatrix} 0.5 & 0.5 & 0.5 \\ 0.5 & 0.5 & 0.5 \\ 0.5 & 0.5 & 0.5 \end{bmatrix},$$

with the value $\vartheta = 1$ for the small scale experiment, $\vartheta = 0.3$ for the medium scale experiment, and $\vartheta = 0.1$ for the large scale experiment, in order to decrease the signal when the number of vertices is larger.

Specifically, the matrix Λ for the small scale experiment, for the medium scale experiment and for the large scale experiment are, respectively,

$$\Lambda(1) = \begin{bmatrix} 0.5 & 0.3 & 0.4 \\ 0.3 & 0.8 & 0.6 \\ 0.4 & 0.6 & 0.3 \end{bmatrix}, \qquad \Lambda(0.3) = \begin{bmatrix} 0.50 & 0.44 & 0.47 \\ 0.44 & 0.59 & 0.53 \\ 0.47 & 0.53 & 0.44 \end{bmatrix},$$
$$\Lambda(0.1) = \begin{bmatrix} 0.50 & 0.48 & 0.49 \\ 0.48 & 0.53 & 0.51 \\ 0.49 & 0.51 & 0.48 \end{bmatrix},$$

so that as the number of vertices increases we have that ϑ gets closer to zero, which means that the blocks become less and less stochastically differentiable one from the other. Another notable feature of the Λ here is that the block of interest—the first block—is the intermediate density block, that is, the Bernoulli adjacency parameter for vertices in the first block is between the Bernoulli adjacency parameter.

eter for vertices in the second block and in the third block. This makes it more challenging to identify the vertices of the first block, which is the block of interest.

The values of (n_1, n_2, n_3) are taken to be multiples of (4, 3, 3), specifically, in the small-scale experiment $(n_1, n_2, n_3) = (4, 3, 3)$, in the medium-scale experiment $(n_1, n_2, n_3) = (200, 150, 150)$ and in the large-scale experiment $(n_1, n_2, n_3) = (4000, 3000, 3000)$. As for the seeds, the values of (m_1, m_2, m_3) in the respective experiments were taken as (4, 0, 0), (20, 0, 0) and (40, 0, 0).

These three experiments were performed as follows. We independently realized 50,000 graphs from the associated distribution of the small-scale experiment, 200 graphs in the medium-range experiment and 100 graphs in the large-scale experiment. To each observed graph we applied each of the following: the canonical vertex nomination scheme Φ^C , the likelihood maximization vertex nomination scheme Φ^L , the OTS vertex nomination scheme Φ^O and the spectral partitioning vertex nomination scheme Φ^S . Then, for each vertex nomination scheme, we recorded the fraction of the realizations for which the first nominee of the nomination list was a member of the block of interest, the fraction of the realizations for which the second nominee was a member of the block of interest, ..., the fraction of the realizations for which the realizations for which the nominet of the block of interest. In Figure 1(a), (b) and (c) these empirical probabilities are plotted against nomination list position, for the three respective experiments and the nomination schemes.

In the small-scale experiment, where n = 10, the likelihood maximization nomination scheme performed about as well as the ("gold standard") canonical nomination scheme, and the spectral partitioning nomination scheme performed very poorly—near chance. Then, in the medium-scale experiment, where n = 500, the canonical nomination scheme was no longer practical to compute, and the OTS and the spectral partitioning nomination scheme performed nearly as well as the likelihood maximization nomination scheme. For a few thousand vertices it was not practical to implement the likelihood maximization nomination scheme nor OTS, so in the large-scale experiment, where n = 10,000, the only nomination scheme that could be implemented was the spectral partitioning nomination scheme.

The empirical mean average precision for the canonical, likelihood maximization and spectral partitioning vertex nomination schemes in the three experiments were as follows (note that the mean average precision for chance is 0.4):

Mean average precision	Canonical	Likeli-max	OTS	Spectral
Small-scale exper., $n = 10, \vartheta = 1$	0.6958	0.6725	0.4763	0.3993
Medium-scale exper., $n = 500$, $\vartheta = 0.3$	*	0.9543	0.7846	0.7330
Large-scale exper., $n = 10,000, \vartheta = 0.1$	*	*	*	0.9901

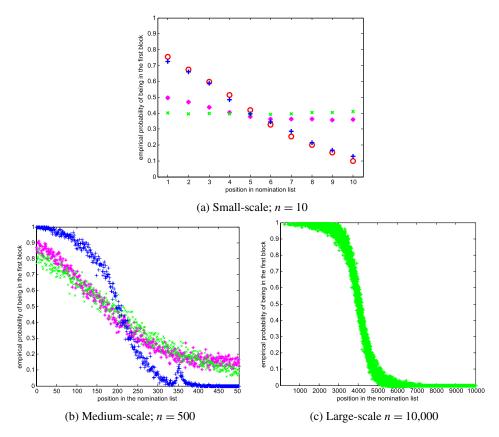


FIG. 1. The canonical vertex nomination scheme is in red, the likelihood maximization vertex nomination scheme is in blue, the OTS vertex nomination scheme is in purple, and the spectral partitioning vertex nomination scheme is in green. (Canonical scheme not shown in medium- and large-scale figures, liklihood maximization and OTS schemes not shown in large-scale figure.)

The running times in seconds were as follows:

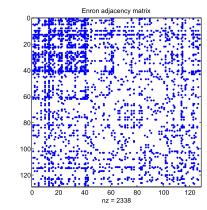
Running time per simulation	Canonical	Likeli-max.	OTS	Spectral
Small-scale experiment, $n = 10$	≈ 0.52	≈ 0.03	≈ 0.30	≈ 0.01
Medium-scale experiment, $n = 500$	*	≈ 332	≈ 58	≈ 0.17
Large-scale experiment, $n = 10,000$	*	*	*	≈ 106

Indeed, each of the canonical, likelihood maximization and spectral vertex nomination schemes is superior (in the sense of effectiveness, given practical computability limitations) to the other two at one of the three scales. At a small scale you should use the canonical vertex nomination scheme, at a medium scale you should use the likelihood maximization vertex nomination scheme, and at a large scale you should use the spectral partitioning vertex nomination scheme. **8. Real data examples.** While the stochastic block model is often useful for modeling real data, many times real data does not fit the model particularly well. In the following real-data experiments we see that the likelihood maximization vertex nomination scheme is robust to the lack of idealized conditions hypothesized and other pathologies inherent in real data. All of the data and code used in these experiments can be accessed at http://www.cis.jhu.edu/~parky/vn/.

8.1. *Example: The enron graph.* The Enron Corporation was a highly regarded, large energy company that went spectacularly bankrupt in the early 2000s amid systemic internal fraud. Enron has since become a popular exemplar of corporate fraud and corruption. In the wake of Enron's collapse, the US Energy Regulatory Commission collected a corpus of more than 600,000 emails sent between Enron employees, and this corpus was made public by the US Department of Justice and is available online at a number of websites, including http://research.cs.queensu.ca/home/skill/siamworkshop.html.

In Priebe et al. (2005), the authors restrict their attention to a 189 week period from the year 1998 through the year 2002; they identify 184 distinct email addresses in the Enron email corpus over this time interval, and they identify the pairs of these email addresses that had email communication with each other. Our "Enron Graph" that we use here is based on the graph in Priebe et al. (2005); our vertex set W consists of the 128 active email addresses for which the employee's job title in Enron was known. For every pair of such vertices, the pair of vertices are declared adjacent to each other when there was at least one email sent from either of the email addresses to the other. We then divided the vertices into two blocks: The "upper-echelon" set of vertices $\{w \in W : b(w) = 1\}$ are the vertices whose job titles were designated as CEO, president, vice president, chief manager, company attorney and chief employee. The "lower-echelon" set of vertices $\{w \in W : b(w) = 2\}$ are the vertices whose job titles were designated as employee, employee administrative, specialist, analyst, trader, director and manager (besides chief manager, which we designated upper echelon). We chose to group the job titles of manager and director with lower-echelon because a by-eye assessment of the graph indicated that their adjacency affinity was closer to the rest of the lower-echelon vertices. Indeed, this graph is certainly not a realization of an actual two-block stochastic block model, but for the purpose of illustration we will view it as very roughly having some two-block structure. The adjacency matrix is pictured in Figure 2(a).

We consider the following experiment. From the 43 upper-echelon vertices $\{w \in W : b(w) = 1\}$, discrete-uniform randomly select $m_1 = 10$ to have their block labels known, and the remaining $n_1 = 33$ have their block labels obscured. From the 85 lower-echelon vertices $\{w \in W : b(w) = 2\}$, independently, discrete-uniform randomly select $m_2 = 20$ to have their block labels known, and the remaining $n_2 = 65$ have their block labels obscured. Then compute $\hat{\Lambda}_{1,1}$, $\hat{\Lambda}_{2,2}$ and $\hat{\Lambda}_{1,2}$ as, respectively, the number of edges in the graph induced by the known





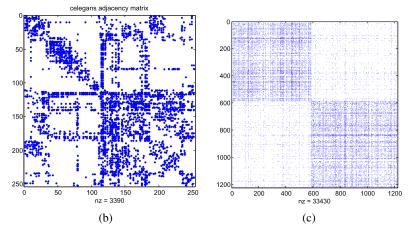


FIG. 2. Adjacency matrices for the real-data examples of Section 8. (a) Vertices partitioned into the 43 upper-echelon employees, then the 85 lower-echelon employees. (b) Vertices partitioned into the 110 motor neurons, 76 interneurons, then 67 sensory neurons. (c) Vertices partitioned into the 588 liberal blogs, then the 636 conservative blogs.

upper-echelon vertices, the number of edges in the graph induced by the known lower-echelon vertices, and the number of edges in the bipartite graph induced by the known upper-echelon and the known lower-echelon vertices, divided, respectively, by $\binom{n_1}{2}$, $\binom{n_2}{2}$ and n_1n_2 . Then perform likelihood maximization and spectral partitioning vertex nomination on this graph, using $\hat{\Lambda}$ as a substitute for Λ .

We independently repeated this experiment 30,000 times; Figure 3 plots the empirical probabilities of vertex membership in the upper echelon for the respective 98 positions in the nomination list, using the likelihood maximization vertex nomination scheme (in blue), the OTS vertex nomination scheme (in purple) and the spectral partitioning vertex nomination schemes (in green). These three vertex nomination schemes had empirical mean average precisions 0.7779 (likelihood

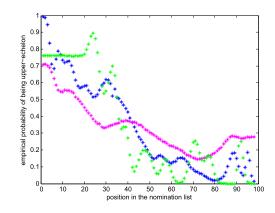


FIG. 3. Vertex nomination in the Enron Graph. The likelihood maximization, spectral partitioning and OTS vertex nomination schemes are, respectively, in blue, green and purple.

maximization), 0.7619 (spectral partitioning) and 0.5970 (OTS). For comparison, the mean average precision of chance is 0.3367.

Note here that the overall classification success of spectral partitioning (i.e., the nominating success averaged over the first 33 positions of the nomination list) is seen in Figure 3 as being comparable to the classification success of likelihood maximization. Also, here the mean average precision of spectral partitioning nomination is comparable to that of likelihood maximization nomination. However, here, very near the top of the nomination list, there is a visible plateau in the spectral partitioning nomination success, whereas maximum-likelihood is nominating very well; indeed, the first few nominees are nearly always from the block of interest.

8.2. Example: The caenorhabditis elegans connectome. The Caenorhabditis elegans (C.elegans) is a small roundworm whose connectome (neural-wiring) has been completely mapped out; see http://www.openconnectomeproject.org/#! celegans/c5tg. Our graph here has vertex set W consisting of the 253 nonisolated neurons and, for every pair of vertices, the two vertices are defined to be adjacent to each other if they are adjoined by a chemical synapse. Each neuron (i.e., vertex) is exactly one of the following neuron types: motor neuron, interneuron, or sensory neuron. For each $w \in W$, we define the block membership b(w) to be 1, 2, 3, respectively, according to whether the neuron is a motor neuron (there are 110 of these), interneuron (there are 76 of these) or sensory neuron (there are 67 of these). The adjacency matrix is pictured in Figure 2(b).

Consider the following experiment. Block membership is revealed for 30 discrete-uniformly selected motor neurons, 20 discrete-uniformly selected interneurons and 10 discrete-uniformly selected sensory neurons. We are interested in forming a nomination list out of the remaining 193 ambiguous neurons so that

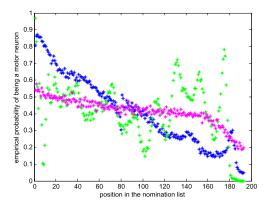


FIG. 4. Vertex nomination for motor neurons in C. Elegans: Likelihood maximization is colored blue, OTS is colored purple, spectral partitioning is colored green.

the beginning of the nomination list has an abundance of (the remaining 80) ambiguous motor neurons.

Perhaps the story behind your desire for this nomination list might be that you wish to study motor neurons, but have limited resources to biochemically test neuron type for the ambiguous neurons. The nomination list would be used to order the ambiguous neurons for the testing, to identify as many motor neurons as possible from the ambiguous neurons before your resources are depleted.

We repeated this experiment 1000 times, each time nominating for motor neurons using the likelihood maximization, the spectral partitioning vertex nomination scheme and the OTS vertex nomination scheme. In each repetition, we estimated Λ with $\hat{\Lambda}$, whose entries reflect the edge densities in the subgraphs induced by the various blocks intersecting the seeds. The empirical mean average precision for the likelihood maximization, spectral partitioning and OTS vertex nomination schemes were, respectively, 0.7272, 0.5096 and 0.5041; the mean average precision of chance is 0.4145. Figure 4 shows that empirical probability of being a motor neuron at every position in the vertex nomination list, for the likelihood maximization (blue), OTS (purple) and spectral partitioning (green) vertex nomination schemes.

Note that here spectral partitioning performed very erratically and (overall) poorly. This might be attributed to a lack of our idealized three-block structure here; that is to say, this graph does not appear to be an instantiation of monolithic stochastic behavior for vertices within the respective three blocks. In this case here, likelihood maximization was seen to be more robust to the lack of idealized block model setting, and still maintained a steady and very pronounced slope in Figure 4.

8.3. *Example: A political blog network*. The political blogosphere data in our next example was collected in Adamic and Glance (2005) around the time of the US presidential election in 2004. This data set consists of 1224 weblogs ("blogs"),

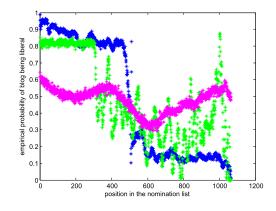


FIG. 5. Nominating blogs; likelihood maximization vertex nomination scheme is colored blue, OTS vertex nomination scheme is colored purple, and spectral partitioning vertex nomination scheme is colored green.

each of which web-links to—or is web-linked from—at least one other of these blogs. These blogs form the vertex set W of our graph. Each of the blogs was classified by Adamic and Glance (2005) as being either liberal or conservative; for each $w \in W$ we define b(w) to be 1 or 2, according to whether w was classified as liberal or conservative. There are 588 liberal blogs and 636 conservative blogs here. For each pair of vertices/blogs, the pair is adjacent if at least one of the blogs links to the other. The adjacency matrix is pictured in Figure 2(c).

Consider the following experiment. Discrete-uniform randomly select 80 liberal and 80 conservative blogs to have their political orientation revealed, and create a nomination list for the remaining 1064 ambiguous blogs. The story could be that you work for a political action committee and want to make a report summarizing liberal blog views on some current event. You have a limited amount of blogreading time and only know the content and political affiliations of a few of the blogs. Thus, you want to create a nomination list which will provide the order for your reading the ambiguous blogs, so that you read many liberal blogs in your limited time.

We repeated this experiment 1000 times and calculated the likelihood maximization, spectral partitioning and OTS vertex nomination schemes for each repetition. See the results in Figure 5. The mean average precision for the likelihood maximization, spectral partitioning and OTS vertex nomination schemes were, respectively, 0.8922, 0.7856 and 0.5429; the mean average precision for chance nomination was 0.4774.

9. Real-data example: Memex and human-trafficking. The Defense Advanced Research Projects Agency (DARPA) is an agency of the United States Department of Defense which, historically, was responsible for developing computer networking and NLS (an acronym for "oN-Line System"), which was the first

hypertext system and an important precursor to the contemporary graphical user interface (Wikipedia, The Free Encyclopedia, "DARPA", accessed February 15, 2015).

Today's web searches use a centralized, one-size-fits-all approach, which is very successful for everyday, common use. DARPA launched the Memex (a contraction of "Memory Extender") Program to create domain-specific index and search, which promises to be a substantially more powerful search tool, due to its domain specificity. The first domain that Memex has addressed is the general domain of human trafficking, which is an important problem for law enforcement, as well as the military and national intelligence services. Forums, chats, advertisements, job postings, hidden services, etc., on the web continue to enable a growing industry of modern slavery. The index curated by Memex for the counter-trafficking domain includes a rich set of data with millions of attributes that, when analyzed with technology, can show linkages between content that are not easily discoverable by a human analyst.

The graph G that we now consider can be accessed at http://www.cis.jhu.edu/ ~parky/vn/ and is associated with the DARPA Memex and XDATA programs. It has 31,248 vertices; each vertex corresponds to a web advertisement. For each pair of vertices, the pair are defined to be adjacent if the return contact information of the respective advertisements either share a return phone number or share a return address region (i.e., city/municipality/metropolitan area). There were 12,387 nodes whose advertisements had a particular string in the web URL which was ubiquitous to activities associated with human trafficking; these vertices were designated "red." The remaining 18,861 vertices were designated "nonred," and it remains unknown if the associated advertisements have any association whatsoever with human trafficking.

The broad goal is, of course, to identify nonred vertices/advertisements that have association with human trafficking. The direct approach of forming one large nomination list of the 18,861 nonred vertices is complicated; among the vertex nomination schemes introduced here, only the spectral partitioning nomination scheme is practical to directly compute for a graph this large, and the spectral partitioning is almost entirely ineffective (the adjusted rand index [Hubert and Arabie (1985)] between red/nonred and k-means on a two-dimensional embedding was 0.00707). Also, keeping in mind the benefits of model averaging, we decided to perform 10,000 independent replicates of the following smaller-scale procedure, using likelihood maximization nomination:

We discrete-uniformly randomly sampled 125 red vertices from among the 12,387 red vertices, and then discrete-uniformly sampled 50 of these 125 red vertices to be seeds (their status as red revealed for what follows) and the other 75 to be ambiguous (their status as red deliberately and temporarily obscured for what follows). We then also discrete-uniformly randomly sampled 125 nonred vertices from among the 18,861 nonred vertices, and then discrete-uniformly sampled 50 of these 125 nonred vertices to be seeds (their status as nonred revealed for what

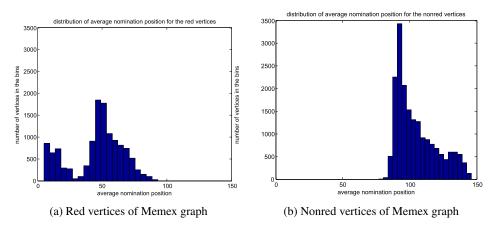


FIG. 6. Histograms of average nomination position for red vertices and nonred vertices in Memex.

follows) and the other 75 to be ambiguous (their status as nonred deliberately and temporarily obscured for what follows). We then used the likelihood maximization vertex nomination scheme to nominate the 150 ambiguous vertices (among the 250 selected).

For each of the 10,000 replications of the procedure described in the preceding paragraph, we noted the nomination position (from 1 to 150) of each of the ambiguous vertices and, for each of the 31,248 vertices of the graph, we averaged the vertex's nomination position over the many times that the vertex was selected to be ambiguous. In Figure 6(a) we plotted a histogram of the 12,387 red vertices, binned according to average nomination position, and in Figure 6(b) we plotted a histogram of the 18,861 nonred vertices, binned according to average nomination position. Note that some of the nonred vertices are much more likely to appear higher in the nomination lists than other nonred vertices; the left spike in the histogram of Figure 6(b) identifies nonred vertices that should have a higher priority for scrutiny to ascertain if they are associated with human trafficking. This outcome is of operational significance.

10. Discussion. In this paper the currently-popular stochastic block model setting enables the principled development of vertex nomination schemes. We introduced several vertex nomination schemes: the canonical, likelihood maximization, spectral partitioning and OTS vertex nomination schemes. In Section 7 we compared and contrasted the effectiveness and runtime of these vertex nomination schemes at small, medium and large scales. In Proposition 1 we proved that the canonical vertex nomination schemes, and thus it should be used as long as it is computationally feasible, which is up to a few tens of vertices. (The runtime visibly grows exponentially in the number of vertices.) The likelihood maximization

vertex nomination scheme, which utilizes state-of-the-art graph matching machinery, should be used next (i.e., when the canonical vertex nomination scheme can not be used), as long as it is computationally feasible, which is up to around 1000 or 1500 vertices. Sections 8.1, 8.2 and 8.3 then feature illustrations with real data and illustrate robustness of maximum-likelihood nomination to model pathology inherent in real data. Section 9 highlights an important contemporary application to stopping human trafficking.

These vertex nomination schemes are simple, yet effective. The likelihood maximization, spectral partitioning and OTS vertex nomination schemes are grown from basic block estimation strategies. Going forward, we expect to see the next generation of vertex nomination schemes build on similar such adaptations of block estimation strategies.

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