Graph link prediction in computer networks using Poisson matrix factorisation

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Abstract: Graph link prediction is an important task in cyber-security: relationships between entities within a computer network, such as users interacting with computers, or system libraries and the corresponding processes that use them, can provide key insights into adversary behaviour. Poisson matrix factorisation (PMF) is a popular model for link prediction in large networks, particularly useful for its scalability. In this article, PMF is extended to include scenarios that are commonly encountered in cyber-security applications. Specifically, an extension is proposed to explicitly handle binary adjacency matrices and include known covariates associated with the graph nodes. A seasonal PMF model is also presented to handle seasonal networks. To allow the methods to scale to large graphs, variational methods are discussed for performing fast inference. The results show an improved performance over the standard PMF model and other statistical network models.

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1. Introduction

In recent years, there has been a significant increase in investment from both government and industry in improving cyber-security using statistical and machine learning techniques on a wide range of data collected from computer networks (Heard et al., 2018; Jeske et al., 2018). One significant research challenge associated with these networks is link prediction, defined as the problem of predicting the presence of an edge between two nodes in a network graph, based on observed edges and attributes of the nodes (Liben-Nowell and Kleinberg, 2007). Adversaries attacking a computer network often affect relationships (links) between nodes within these networks, such as users authenticating to computers, or clients connecting to servers. New links (previously unobserved relationships) are of particular interest, as many attack behaviours such as lateral movement (Neil et al., 2013), phishing, and data retrieval, can create new edges between network entities (Metelli and Heard, 2019). In practical cyber applications, it is necessary to use relatively simple and scalable statistical methods, given the size and inherently dynamic nature of these networks.

Away from cyber applications, the link prediction problem has been an active field of research (see, for example, Dunlavy, Kolda and Acar, 2011; Lü and Zhou, 2011; Menon and Elkan, 2011), being similar, especially in its static formulation, to recommender systems (Adomavicius and Tuzhilin, 2005). Static link prediction (for example, Clauset, Moore and

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Newman, 2008) aims at filling in missing entries in a single incomplete graph adjacency matrix, as opposed to temporal link prediction (for example, Dunlavy, Kolda and Acar, 2011), which aims at predicting future snapshots of the graph given one or more fully observed snapshots. Static link prediction problems have been successfully tackled using probabilistic matrix factorisation methods, especially classical Gaussian matrix factorisation (Salakhutdinov and Mnih, 2007), and are currently widely used in the technology industry (see, for example, Agarwal, Zhang and Mazumder, 2011; Khanna et al., 2013; Paquet and Koenigstein, 2013). For dyadic count data, Poisson matrix factorisation (PMF) (Canny, 2004; Dunson and Herring, 2005; Cemgil, 2009; Gopalan, Hofman and Blei, 2015) emerged as a suitable model in the static link prediction framework. This work mainly focuses on temporal link prediction, showing that PMF is also useful for link prediction in this context, and it seems to be particularly well-suited for cyber-security applications.

The methodological contribution of this article is to present extensions of the PMF model, suitably adapted to scenarios which are commonly encountered in cyber-security applications. Traditionally, Poisson matrix factorisation methods are used on partially observed adjacency matrices of natural numbers representing, for example, ratings of movies provided by different users. In cyber-security applications, the matrix is fully observed, and the counts associated with network edges are complicated by repeated observations, polling at regular intervals, and the intrinsic burstiness of the events (Heard, Rubin-Delanchy and Lawson, 2014). Hence, each edge is usually represented by a binary indicator expressing whether at least one connection between the corresponding nodes was observed. Consequently, the standard PMF model, where counts associated with links are assumed to follow a Poisson distribution with unbounded support, cannot be applied directly. Instead, indicator functions are applied, leading to an extension for PMF on binary adjacency matrices. Next, a framework for including categorical covariates within the PMF model is introduced, which also allows for modelling of new nodes appearing within a network. Finally, extensions of the PMF model to incorporate seasonal dynamics are presented.

The rest of the article is organised as follows: Section 2 presents the computer network data which are to be analysed. Section 3 formally introduces Poisson matrix factorisation for network link prediction, and Section 4 discusses the proposed PMF model for binary matrices and labelled nodes. A seasonal extension is described in Section 5. Finally, results of the analysis are presented in Section 6.

2. LANL computer network data

The methodologies in this article have been developed to provide insight into authentication data extracted from the publicly released “Unified Host and Network Dataset” from Los Alamos National Laboratory (LANL) (Turcotte, Kent and Hash, 2018).

The data contain authentication logs collected over a 90-day period from computers in the Los Alamos National Laboratory enterprise network running a Microsoft Windows operating system. An example record is:

```json
{"UserName": "User865586", "EventID": 4624, "LogHost": "Comp256596", "LogonID": "0x5a3bdf", "DomainName": "Domain001", "LogonTypeDescription": "Network", "Source": "Comp782342", "AuthenticationPackage": "Kerberos", "Time": 87264, "LogonType": 3}.
```
Fig 1: Number of links per day (top), and proportion of those that are new (bottom), after 20 days of observation of the LANL computer network. Solid red curve: User – Source. Dashed blue curve: User – Destination.

From each authentication record, the following fields are extracted for analysis: the user credential that initiated the event (UserName), the computer where the authentication originated (Source), and the computer the credential was authenticating to (most often LogHost). Two bipartite graphs are then generated: first, the network users and the computers from which they authenticate, denoted User – Source; second, the same users and the computers or servers they are connecting to, denoted User – Destination. The two graphs are first analysed separately, before a joint model is explored.

As generic notation, let $G = (U, V, E)$ represent one of these bipartite graphs, where $U = \{u_1, u_2, \ldots \}$ is the set of users and $V = \{v_1, v_2, \ldots \}$ a set of computers (sometimes referred to as hosts). The set $E \subseteq U \times V$ represents the observed edges, such that $(u, v) \in E$ if user $u \in U$ connected to host $v \in V$ in a given time interval. A finite set of edges $E$ can be represented as a rectangular $|U| \times |V|$ binary adjacency matrix $A$, where $A_{ij} = 1_{E}(\{u_i, v_j\})$.

For each user and computer, a list of categorical covariates were also obtained: 6 covariates are available for the users, and 3 for the computers. In total, there are $K = 1,064$ factor levels available for the user credentials and $H = 735$ factor levels for the computers. One objective of this article is to present methodology for incorporating such covariates within Poisson matrix factorisation.

As mentioned in Section 1, for cyber-security applications it would be valuable to accurately predict and assess the significance of new links. Importantly, many new links are formed each day as part of normal operating behaviour of a computer network; to demonstrate this, Figure 1 shows the the total number of edges formed each day and the percentage of those that are new for the User – Source and User – Destination graphs. Even though the relative percentage is small, this would still provide many more alerts than could be practically acted upon each day.
3. Background on Poisson matrix factorisation

Let $N \in \mathbb{N}^{[U] \times [V]}$ be a matrix of non-negative integers $N_{ij}$. For recommender system applications, $N_{ij}$ could represent information about how a user $i$ rated an item $j$, or a count of the times they have clicked on or purchased the item. The cyber-security application has a major difference: in recommender systems, if user $i$ never interacted with the item $j$, then $N_{ij}$ is considered as a missing observation, implying that the number of observations is a possibly very small fraction of $|U||V|$. On the other hand, in cyber-security, the absence of a link from $i$ to $j$ is itself an observation, namely $N_{ij} = 0$, and $|U||V|$ data points are observed. Such a difference has practical consequences, particularly regarding scalability in cyber-security of models borrowed from the recommender systems literature.

The hierarchical Poisson factorisation model (Gopalan, Hofman and Blei, 2015) specifies a distribution for $N_{ij}$ using a Poisson link function with rate given by the inner product between user-specific latent features $\alpha_i \in \mathbb{R}_+^R$ and host-specific latent features $\beta_j \in \mathbb{R}_+^R$, for a positive integer $R \geq 1$:

$$N_{ij} \sim \text{Pois}(\alpha_i^\top \beta_j) = \text{Pois} \left( \sum_{r=1}^R \alpha_{ir} \beta_{jr} \right).$$

(3.1)

If two latent features are close in the latent space, the corresponding nodes are expected to exhibit similar connectivity patterns. The specification of the model is completed with gamma hierarchical priors:

$$\alpha_{ir} \sim \Gamma(a^{(\alpha)}, c^{(\alpha)}), \quad i = 1, \ldots, |U|, \quad r = 1, \ldots, R,$$

$$\beta_{jr} \sim \Gamma(a^{(\beta)}, c^{(\beta)}), \quad j = 1, \ldots, |V|, \quad r = 1, \ldots, R,$$

$$\zeta_i^{(\alpha)} \sim \Gamma(b^{(\alpha)}, d^{(\alpha)}), \quad \zeta_j^{(\beta)} \sim \Gamma(b^{(\beta)}, d^{(\beta)}).$$

(3.2)

Each of the gamma distribution parameters $a^{(\alpha)}, b^{(\alpha)}, c^{(\alpha)}, a^{(\beta)}, b^{(\beta)}, c^{(\beta)}$ are positive real numbers which must be specified.

In the cyber-security context there are no missing observations in the matrix $N$. Consequently, an advantage of PMF over other models for link prediction (for example, Salakhutdinov and Mnih, 2007) is that the likelihood function only depends on the observed links, meaning evaluating the likelihood is $\Theta(\text{nnz}(N))$, where $\text{nnz}(\cdot)$ is the number of non-zero elements in the matrix, compared to $\Theta(|U||V|)$ for most statistical network models. In cyber-security, networks tend to be very large in the number of nodes, but extremely sparse: $\text{nnz}(N) \ll |U||V|$. Hence, PMF appears to be a particularly appealing modelling framework for this application.

The PMF model has been used as a building block for multiple extensions. For example, Chaney, Blei and Eliassi-Rad (2015) developed social Poisson factorisation to include latent social influences in personalised recommendations. Gopalan, Charlin and Blei (2014) developed collaborative topic Poisson factorisation, which adds a document topic offset to the standard PMF model to provide content-based recommendations and thereby tackle the challenge of recommending new items, referred to in the literature as cold starts. These ideas of combining collaborative filtering and content-based filtering are further developed in Zhang and Wang (2015), Singh and Gordon (2008) and da Silva, Langseth and Ramampiaro (2017), where social influences are added as constraints in the latter.
In general, most PMF-based methods presented in this section model binary adjacency matrices using the Poisson link function for convenience. This approach is computationally advantageous, but implies an incorrect model for the range: the entries $A_{ij}$ of the adjacency matrix are binary, whereas the Poisson distribution has support over the natural numbers.

It must be noted that many other models besides PMF have been proposed in the literature to tackle the link prediction task and for graph inference. Comprehensive surveys of the most popular statistical network models are given in Goldenberg et al. (2010) and Fienberg (2012). The problem of link prediction is also studied in other disciplines, for example physics (Lü and Zhou, 2011), or computer science, where graph neural networks (Zhang and Chen, 2018; Wu et al., 2020) have recently gained popularity. The model presented in this article can be classified as a latent feature model (LFM, Hoff, Raftery and Handcock, 2002). For a bipartite graph $G = (U, V, E)$ with adjacency matrix $A$, the LFM assumes that the nodes have $R$-dimensional latent representations $u_i \in \mathbb{R}^R$, $i \in U$ and $v_j \in \mathbb{R}^R$, $j \in V$. The entries of the adjacency matrix are then obtained independently as $P(A_{ij} = 1) = \kappa(u_i, v_j)$, where $\kappa : \mathbb{R}^R \times \mathbb{R}^R \rightarrow [0, 1]$ is a kernel function. A popular special case of LFM is the random dot product graph (RDPG, Athreya et al., 2018), where $\kappa(\cdot)$ is chosen to be the inner product between the latent positions. The extended PMF model proposed in this article is also a special case of LFM, assuming a particular form of kernel function with nodal covariates.

Dynamical extensions to PMF have also been studied. Charlin et al. (2015) use Gaussian random walk updates on the latent features to dynamically correct the rates of the Poisson distributions. Schein et al. (2015, 2016) propose a temporal version of PMF using the two main tensor factorisation algorithms: canonical polyadic and Tucker decompositions. Hoseini et al. (2018) combine the PMF model with the Poisson process to produce dynamic recommendations. Dynamic network models have also been widely studied outside the domain of matrix factorisation techniques (for a survey, see Kim et al., 2017). For example, Sewell and Chen (2015) extend LFM to a temporal setting. The dynamic models described above could handle generic network dynamics, but seasonality, a special case of temporal structure, has not been explicitly accounted for in the PMF literature. This article further aims to fill this gap and propose a viable seasonal PMF model.

4. PMF with labelled nodes and binary adjacency matrices

Suppose that there are $K$ covariates associated with each user and $H$ covariates for each host. Let the value of the covariate $k$ for user $i$ be denoted as $x_{ik}$. Similarly, let the value of the covariate $h$ for host $j$ be $y_{jh}$. In cyber-security applications, most available information types are categorical, indicating memberships of known groupings or clusters of nodes. For the remaining of this article, the covariates will be assumed to be binary indicators representing categorical variables. This type of encoding of categorical variables is commonly known in the statistical literature as dummy variable encoding, whereas the term one-hot encoding is used in the machine learning community. Several approaches for including nodal covariates in recommender systems using non-probabilistic matrix factorisation methods such as the Singular Value Decomposition (SVD) have been discussed in the literature (for some examples, see Nguyen and Zhu, 2013; Fithian and Mazumder, 2018; Dai et al., 2019). Regression methods for network data with covariates are also studied in Hoff (2005). In Section 1 and 3, it has been remarked that, for binary adjacency matrices, the standard PMF model for count data cannot be applied directly, since the observations are binary, whereas the Poisson dis-
distribution has support on the natural numbers. To model binary links, it is assumed here that the count \( N_{ij} \) is a latent random variable, and the binary indicator \( A_{ij} = 1_{N_{ij}}(N_{ij}) \) is a censored Poisson draw with a corresponding Bernoulli distribution. This type of link has been referred to in the literature as the Bernoulli-Poisson (BerPo) link (Acharya et al., 2015; Zhou, 2015). The full extended model is

\[
A_{ij} | N_{ij} = 1_{N_{ij}}(N_{ij}),
\]

\[
N_{ij} | \alpha_i, \beta_j, \Phi \sim \text{Pois}\left( \alpha_i^T \beta_j + 1_{K}^T(\Phi \odot x_i y_j^T)1_H \right)
\]

\[
= \text{Pois}\left( \sum_{r=1}^{R} \alpha_{ir} \beta_{jr} + \sum_{k=1}^{K} \sum_{h=1}^{H} \phi_{kh} x_{ik} y_{jh} \right), \quad (4.1)
\]

where \( 1_n \) is a vector of \( n \) ones, \( \odot \) is the Hadamard element-wise product, and \( x_i \) and \( y_j \) are \( K \) and \( H \)-dimensional binary vectors of covariates. The \( R \)-dimensional latent features \( \alpha_i \) and \( \beta_j \) appear in the traditional PMF model given in (3), and \( \Phi = \{ \phi_{kh} \} \in \mathbb{R}^{K \times H} \) is a matrix of interaction terms for each combination of the covariates. Under model (4),

\[
P(A_{ij} = 1) = 1 - \exp\left( -\sum_{r=1}^{R} \alpha_{ir} \beta_{jr} - \sum_{k=1}^{K} \sum_{h=1}^{H} \phi_{kh} x_{ik} y_{jh} \right) . \quad (4.2)
\]

To provide intuition for these extra terms, assume for the cyber-security application that a binary covariate for job title manager is provided for the users, and that a binary covariate for the location research lab for the hosts. If user \( i \) is a manager and host \( j \) is located in a research lab, then \( \phi_{kh} \) expresses a correction to the rate \( \alpha_i^T \beta_j \) for a manager connecting to a machine in a research lab. The covariate term is inspired by the bilinear mixed-effects models for network data in Hoff (2005).

The same hierarchical priors (3) are used for \( \alpha_i \) and \( \beta_j \) and the following prior distribution completes the specification of the model:

\[
\phi_{kh} \mid c^{(\phi)} \sim \Gamma(a^{(\phi)}, c^{(\phi)}), \quad k = 1, \ldots, K, \ h = 1, \ldots, H,
\]

\[
\zeta^{(\phi)} \sim \Gamma(b^{(\phi)}, c^{(\phi)}).
\]

Note that this model provides a natural way for handling what the literature commonly refers to as cold starts, where new users or hosts appear in the network. Provided that covariate-level information is known about new entities, then the estimates for \( \Phi \) can be used to make predictions about links where \( \alpha_i \) and \( \beta_j \) for new user \( i \) or new host \( j \) could be initialised from the prior or some other global statistic based on other users and hosts.

Another significant advantage of the model proposed in (4) is that the likelihood is \( \Theta(\text{nnz}(A)) \), analogously to the standard PMF model in (3), implying that the model scales well to large sparse networks. From (4):

\[
\log L(A) = \sum_{i,j: A_{ij} > 0} \log (e^{\psi_{ij}} - 1) - \left( \sum_i \alpha_i \right)^T \left( \sum_j \beta_j \right) - \sum_{k,h} \phi_{kh} x_k y_h ,
\]

where \( \psi_{ij} = \alpha_i^T \beta_j + 1_{K}^T(\Phi \odot x_i y_j^T)1_H \), \( x_k = \sum_{i=1}^{U} x_{ik} \), and \( y_h = \sum_{j=1}^{V} y_{jh} \).
4.1. Bayesian inference

Given an observed matrix $A$, inferential interest is on the marginal posterior distributions of the parameters $\alpha_i$ and $\beta_j$ for all the users and hosts, and the parameters $\Phi$ for the covariates, since these govern the predictive distribution for the edges observed in the future.

A common approach for performing inference is adopted, where additional latent variables are introduced. Given the (assumed) unobserved count $N_{ij}$, a further set of latent counts $Z_{ijl}$, $l = 1, \ldots, R + KH$, are used to represent the contribution of each component $l$ to the total latent count, such that $N_{ij} = \sum_l Z_{ijl}$. For $l \leq R$, $Z_{ijl} \sim \text{Pois}(\alpha_i \beta_j)$. Otherwise, $l$ refers to a $(k, h)$ covariate pair, and $Z_{ijl} \sim \text{Pois}(\phi_{kh})$. This construction ensures that $N_{ij}$ has precisely the Poisson distribution specified in (4).

Inference using Gibbs sampling is straightforward, as the full conditionals all have closed form expressions, but sampling-based methods do not scale well with network size. Instead, a variational inference procedure is proposed. Variational inference schemes have already been commonly and successfully used in the literature for network models (Nakajima, Sugiyama and Tomioka, 2010; Seeger and Bouchard, 2012; Salter-Townshend and Murphy, 2013; Hernández-Lobato, Houlsby and Ghahramani, 2014), despite the issue of introducing bias and potentially reducing estimation accuracy, in particular on the posterior variability (see, for example, Huggins et al., 2019).

Gibbs sampling also presents an additional difficulty in PMF models: the inner product $\alpha_i^T \beta_j$ is invariant to permutations of the latent features. In particular, $(Q\alpha_i)^T (Q\beta_j) = \alpha_i^T \beta_j$ for any permutation matrix $Q \in \mathbb{R}^{R \times R}$, which makes the posterior invariant under such transformation. This implies that the posterior is highly multimodal, a well-known burden for MCMC-based inference in Bayesian factor models (Papastamoulis and Ntzoufras, 2020). Hence, parameter estimates obtained as averages from MCMC samples from the posterior could be meaningless, since the algorithm could have switched among different modes. On the other hand, variational inference is well understood to be a “mode-seeking” algorithm, a desirable property for this problem. A practical comparison of the estimates of the inner products for prediction purposes will be briefly illustrated in Section 6.2.

4.2. Variational inference

Variational inference (see, for example, Blei, Kucukelbir and McAuliffe, 2017) is an optimisation based technique for approximating intractable distributions, such as the joint posterior density $p(\alpha, \beta, \Phi, \zeta, N, Z | A)$, with a proxy $q(\alpha, \beta, \Phi, \zeta, N, Z)$ from a given distributional family $Q$, and then finding the member $q^* \in Q$ that minimises the Kullback-Leibler (KL) divergence to the true posterior. Usually the KL-divergence cannot be explicitly computed, and therefore an equivalent objective, called the evidence lower bound (ELBO), is maximised instead:

$$\text{ELBO}(q) = \mathbb{E}_q[\log p(\alpha, \beta, \Phi, \zeta, N, Z, A)] - \mathbb{E}_q[\log q(\alpha, \beta, \Phi, \zeta, N, Z)],$$

(4.3)

where the expectations are taken with respect to $q(\cdot)$. The proxy distribution $q(\cdot)$ is usually chosen to be of much simpler form than the posterior distribution, so that maximising the ELBO is tractable. As in Gopalan, Hofman and Blei (2015) the mean-field variational family is used, where the latent variables in the posterior are considered to be independent and
governed by their own distribution, so that:

\[
q(\alpha, \beta, \zeta, \Phi, N, Z) = \prod_{i,r} q(\alpha_{ir}|\lambda^{(\alpha)}_{ir}, \mu^{(\alpha)}_{ir}) \times \prod_{j,r} q(\beta_{jr}|\lambda^{(\beta)}_{jr}, \mu^{(\beta)}_{jr}) \\
\times \prod_{k,h} q(\phi_{kh}|\lambda^{(\phi)}_{kh}, \mu^{(\phi)}_{kh}) \times \prod_{i} q(\zeta_{i}|\mu^{(\alpha)}_{i}, \xi^{(\alpha)}_{i}) \times \prod_{j} q(\zeta_{j}|\mu^{(\beta)}_{j}, \xi^{(\beta)}_{j}) \\
\times q(\zeta^{(\phi)}|\mu^{(\phi)}_{i}, \xi^{(\phi)}_{i}) \times \prod_{i,j} q(N_{ij}, Z_{ij}|\theta_{ij}, \chi_{ij}).
\] (4.4)

The objective function (4.2) is optimised using coordinate ascent mean field variational inference (CAVI), whereby each density or variational factor is optimised while holding the others fixed (see Bishop, 2006; Blei, Kucukelbir and McAuliffe, 2017, for details). Using this algorithm the optimal form of each variational factor is:

\[
q^*(v_j) \propto \exp \left\{ \mathbb{E}_{v_{-j}} [\log p(v_j|v_{-j}, A)] \right\},
\] (4.5)

where \(v_j\) is an element of a partition of the full set of parameters \(v\), and the expectation is taken with respect to the variational densities that are currently held fixed for \(v_{-j}\), defined as \(v\) excluding the parameters in the subset \(v_j\). Convergence of the CAVI algorithm is determined by monitoring the change in the ELBO over subsequent iterations.

Since the prior distributions are chosen to be conjugate, the full conditionals in (4.2) are all available analytically. Full details are given in Appendix A. Also, since all the conditionals are exponential families, each \(q(v_j)\) obtained from (4.2) is from the same exponential family (Blei, Kucukelbir and McAuliffe, 2017). Hence, with the exception of \(q(N_{ij}, Z_{ij}|\theta_{ij}, \chi_{ij})\), the proxy distributions in (4.2) are all gamma; for example, \(q(\alpha_{ir}|\lambda^{(\alpha)}_{ir}, \mu^{(\alpha)}_{ir}) = \Gamma(\lambda^{(\alpha)}_{ir}, \mu^{(\alpha)}_{ir})\). The update equations for the parameters \(\{\lambda, \mu, \nu, \xi, \theta, \chi\}\) of the variational approximation can be obtained using (4.2), which is effectively the expected parameter of the full conditional with respect to \(q\). The full variational inference algorithm is detailed in Algorithm 1. Note that each update equation only depends upon the elements of the matrix where \(A_{ij} > 0\), providing computational efficiency for large sparse matrices. Further details concerning the update equations for the Poisson and multinomial parameters \(\theta\) and \(\chi\) are also given in Appendix B.

### 4.3. Link prediction

Given the optimised values of the parameters of the variational approximation \(q^*(\cdot)\) to the posterior, a Monte Carlo posterior model estimate of \(P(A_{ij} = 1)\) can be obtained by averaging (4) over \(M\) samples from \(q^*(\alpha_{ir}|\lambda^{(\alpha)}_{ir}, \mu^{(\alpha)}_{ir})\), \(q^*(\beta_{jr}|\lambda^{(\beta)}_{jr}, \mu^{(\beta)}_{jr})\), and \(q^*(\phi_{kh}|\lambda^{(\phi)}_{kh}, \mu^{(\phi)}_{kh})\):

\[
\hat{P}(A_{ij} = 1) = 1 - \frac{1}{M} \sum_{m=1}^{M} \exp \left( - \sum_{r=1}^{R} \alpha^{(m)}_{ir} \beta^{(m)}_{jr} - \sum_{h,k} \phi^{(m)}_{kh} x_{ikh} y_{jh} \right).
\] (4.6)

Alternatively, a computationally fast way to approximate \(P(A_{ij} = 1)\) plugs in the parameters of the estimated variational distributions:

\[
\tilde{P}(A_{ij} = 1|\hat{\alpha}_{ir}, \hat{\beta}_{jr}, \hat{\phi}_{kh}) = 1 - \exp \left( - \sum_{r=1}^{R} \hat{\alpha}_{ir} \hat{\beta}_{jr} - \sum_{h,k} \hat{\phi}_{kh} x_{ikh} y_{jh} \right),
\] (4.7)
Algorithm 1: Variational inference for binary PMF with covariates.

1. initialise $\lambda, \mu$ and $\xi$ from the prior,
2. set $\nu_i^{(\alpha)} = b^{(\alpha)} + Ra^{(\alpha)}$, $\nu_j^{(\beta)} = b^{(\beta)} + Ra^{(\beta)}$, $\nu^{(\phi)} = b^{(\phi)} + KH^{(\phi)}$,
3. calculate $\hat{x}_k = \sum_{i=1}^{|U|} x_{ik}$, $k = 1, \ldots, K$ and $\hat{y}_h = \sum_{j=1}^{|V|} y_{jh}$,
4. repeat
   
   for each entry of $A$ such that $A_{ij} > 0$, update the rate $\theta_{ij}$:
   
   $\theta_{ij} = \sum_{r=1}^R \exp \left\{ \psi(\lambda_{ir}^{(\alpha)}) - \log(\mu_{ir}^{(\alpha)}) + \psi(\lambda_{jr}^{(\beta)}) - \log(\mu_{jr}^{(\beta)}) \right\} + \sum_{k=1}^K \sum_{h=1}^H x_{ik} y_{jh} \exp \left\{ \psi(\lambda_{kh}^{(\phi)}) - \log(\mu_{kh}^{(\phi)}) \right\}$,
   
   where $\psi(\cdot)$ is the digamma function,
   
   for each entry of $\mathbf{A}$ such that $A_{ij} > 0$, update $\chi_{ijl}$:
   
   $\chi_{ijl} \propto \exp \left\{ \psi(\lambda_{il}^{(\alpha)}) - \log(\mu_{il}^{(\alpha)}) + \psi(\lambda_{jl}^{(\beta)}) - \log(\mu_{jl}^{(\beta)}) \right\}$ $l \leq R$,
   
   $x_{ik} y_{jh} \exp \left\{ \psi(\lambda_{kh}^{(\phi)}) - \log(\mu_{kh}^{(\phi)}) \right\}$ $l > R$,
   
   where, for $l > R$, $l$ corresponds to a covariate pair $(k, h)$,
   
   update the user-specific first-level parameters:
   
   $\lambda_{ir}^{(\alpha)} = a^{(\alpha)} + \sum_{j=1}^{|V|} A_{ij} \theta_{ij} \chi_{ijl} / (1 - e^{-\theta_{ij}})$, $\mu_{ir}^{(\alpha)} = \nu_i^{(\alpha)} / \xi_i^{(\alpha)} + \sum_{j=1}^{|V|} \lambda_{jr}^{(\beta)} / \mu_{jr}^{(\beta)}$,$^{(\phi)}$
   
   update the host-specific first-level parameters:
   
   $\lambda_{jr}^{(\beta)} = a^{(\beta)} + \sum_{i=1}^{|U|} A_{ij} \theta_{ij} \chi_{ijl} / (1 - e^{-\theta_{ij}})$, $\mu_{jr}^{(\beta)} = \nu_j^{(\beta)} / \xi_j^{(\beta)} + \sum_{i=1}^{|U|} \lambda_{ir}^{(\alpha)} / \mu_{ir}^{(\alpha)}$,$^{(\phi)}$
   
   update the covariate-specific first-level parameters:
   
   $\lambda_{kh}^{(\phi)} = a^{(\phi)} + \sum_{i,j=1}^{|U||V|} A_{ij} \theta_{ij} \chi_{ijl} / (1 - e^{-\theta_{ij}})$, $\mu_{kh}^{(\phi)} = \nu^{(\phi)} / \xi^{(\phi)} + \hat{x}_k \hat{y}_h$,$^{(\phi)}$
   
   update the second-level parameters:
   
   $\xi_i^{(\alpha)} = c^{(\alpha)} + \sum_{r=1}^R \lambda_{ir}^{(\alpha)} / \mu_{ir}^{(\alpha)}$, $\xi_j^{(\beta)} = c^{(\beta)} + \sum_{r=1}^R \lambda_{jr}^{(\beta)} / \mu_{jr}^{(\beta)}$, $\xi^{(\phi)} = c^{(\phi)} + \sum_{k,h} \lambda_{kh}^{(\phi)} / \mu_{kh}^{(\phi)}$
   
11. until convergence;
where, for example, \( \hat{\alpha}_{ir} = \lambda_{ir}^{(\alpha)} / \mu_{ir}^{(\alpha)} \), the mean of the gamma proxy distribution. Note that (4.3) clearly gives a biased estimate, and by Jensen’s inequality \( \hat{P}(A_{ij} = 1) \leq \tilde{P}(A_{ij} = 1) \) in expectation, but it carries a much lower computational burden. The approximation in (4.3) has been successfully used for link prediction and network anomaly detection purposes in Turcotte et al. (2016).

5. Seasonal PMF

The previous sections have been concerned with making inference from a single adjacency matrix \( A \). Now, consider observing a sequence of adjacency matrices \( A_1, \ldots, A_T \), representing snapshots of the same network over time. Further, suppose this time series of adjacency matrices has seasonal dynamics with some known fixed seasonal period, \( P \); for example, \( P \) could be one day, one week or one year. To recognize time dependence, a third index \( t \) is required, such that \( A_{ijt} \) denotes the \((i,j)\)-th element of the matrix \( A_t, t = 1, \ldots, T \).

As in Section 4, there are assumed to be underlying counts \( N_{ijt} \) which are treated as latent variables, and the sequence of observed adjacency matrices is obtained by \( A_{ijt} = 1_{N_{ijt}}(\Phi \odot x_i y_j) \). To account for seasonal repetition in connectivity patterns, the model proposed for the latent counts is:

\[
N_{ijt} \sim \text{Pois} \left( \sum_{r=1}^{R} \alpha_{ir} \gamma_{it' r} \beta_{jr} \delta_{jt' r} + \sum_{k=1}^{K} \sum_{h=1}^{H} \phi_{kh} x_{ik} y_{jh} \right) \quad (5.1)
\]

where, for example, \( t' = 1 + (t \mod P) \). In general, more complicated functions for \( t' \) might be required, as in Section 6.7.

The priors on \( \alpha_{ir} \) and \( \beta_{jr} \) are those given in (3); these parameters represent a baseline level of activity, which is constant over time. The two additional parameters \( \gamma_{it' r} \) and \( \delta_{jt' r} \) represent corrections to these rates for seasonal segment \( t' \in \{1, \ldots, P\} \). Note that for some applications, it may be anticipated that there is a seasonal adjustment to the rate for the interaction terms of the covariates, in which case temporal adjustments could be also added to \( \Phi \). For identifiability, it is necessary to impose constraints on the seasonal adjustments so that, for example, for all \( i, j, r, \gamma_{i1r} = \delta_{j1r} = 1 \).

For \( t' > 1 \), the following hierarchical priors are placed on \( \gamma_{it' r} \) and \( \delta_{jt' r} \):

\[
\gamma_{it' r} \sim \Gamma(a^{(\gamma)}, c^{(\gamma)}), \quad \delta_{jt' r} \sim \Gamma(b^{(\gamma)}, c^{(\gamma)}),
\]

\[
\gamma_{it' r} \sim \Gamma(a^{(\delta)}, c^{(\delta)}), \quad \delta_{jt' r} \sim \Gamma(b^{(\delta)}, c^{(\delta)}).
\]

Inference for the seasonal model can be performed following the same principles of Section 4.2; full details are given in Appendix C. The constraint is implemented in the variational inference framework by setting the variational approximation to \( \gamma_{i1r} \) and \( \delta_{j1r} \) to a delta function centred at 1.

6. Results

The extensions to the PMF model detailed in Sections 4 and 5 are now used to analyse the LANL authentication data described in Section 2. In order to assess the predictive performance of the models, the data are split into a training set corresponding to the first 56
days of activity, and a test set corresponding to days 57 through 82. During the latter time period, LANL conducted a red-team exercise, where the security team test the robustness of the network by attempting to compromise other network hosts; labels of known compromised authentication events will be used for evaluating the model performance in anomaly detection. The parameters are estimated from the training set adjacency matrix, constructed by setting $A_{ij} = 1$ if a connection from user $i$ to host $j$ is observed during the training period, and $A_{ij} = 0$ otherwise. The predictive performance of the model is then evaluated on the test set adjacency matrix, constructed similarly using the connections observed in the last 25 days.

Summary statistics about the data are provided in Table 1, where “cold starts” refer to links originating from new users and hosts in the test data. Figure 2 shows binary heat map plots of the adjacency matrices obtained from the training period for each the two graphs, User – Source and User – Destination. In all analyses, variational inference is used to estimate the parameters based on the the training data, with a threshold for convergence being $10^{-5}$ for relative difference between two consecutive values of the ELBO (4.2). The prior hyperparameters are set to $a^* = b^* = 1$ and $c^* = 0.1$, although the algorithm is fairly robust to the choice of these parameters. The number of latent features $R = 20$ and was chosen using the criterion of the elbow in the scree-plot of singular values.

| Table 1 | Summary of training and test sets for User – Destination and User – Source. |
|---------|--------------------------------------------------------------------------------|
|         | User – Destination            | User – Source            |
|         | Training set | Test set | Training set | Test set |
| Users   | 11,688        | 534 new  | 12,027       | 507 new  |
| Hosts   | 3,801         | 1,246 new | 15,881       | 1,236 new |
| Links   | 82,517        | 76,240   | 60,059       | 50,412   |
| New links | 11,418      | 12,080   |             |          |
| Cold starts | 3,401       | 3,014    |             |          |

(A) User – Source   
(B) User – Destination

Fig 2: Training set adjacency matrices for the two graphs (spy-plot). Nodes are sorted by in-degree and out-degree.
6.1. Including covariates

First, results are presented for the extended PMF (EPMF) model with covariates, discussed in Section 4. Performance is evaluated by the receiver operating characteristic (ROC) curve and the corresponding area under the curve (AUC). The AUC is used as a measure of quality of classification and will allow for the predictive power of the different models to be ranked. Due to the large computational effort of scoring all entries in the adjacency matrix for EPMF, mostly due to the calculation of $\text{1}_K^\top (\Phi \odot x_i y_j^\top) \text{1}_H$, the AUC is estimated by subsampling the negative class at random from the zeros in the adjacency matrix formed from the test data; the sample sizes is chosen to be three times the size of the number of edges in the test set. In general, if the sample size is chosen to be at least on the same order of magnitude as $\text{nnz}(A)$, this procedure leads to reliable estimates of the AUC, as demonstrated via simulation at the end of this subsection. The estimated AUC scores are summarised in Table 2. For evaluating the AUC scores for new links (edges in the test set not present in the training set), the negative class was also restricted to entries in the training adjacency matrix for which $A_{ij} = 0$.

Table 2 shows that the AUC for User – Destination does not change significantly when the extended model is used; however, for User – Source, the extended PMF model offers a significant improvement. The difference in the results between the two networks can be explained by the contrasting structures of the adjacency matrices. The edge density for User

| Feature          | User – Destination | User – Source |
|------------------|--------------------|--------------|
|                  | PMF                | EPMF         | PMF          | EPMF          |
| All links        | 0.98479            | 0.98707      | 0.85797      | 0.96602       |
| New links        | 0.95352            | 0.95474      | 0.89759      | 0.95260       |

![ROC curve](image)

**Fig 3**: ROC curves for standard PMF and extended PMF on User – Source, $R = 20$. 

**Table 2**: AUC scores for prediction of all and new links using standard and extended PMF. Number of latent features: $R = 20$. 

- **All links, PMF**: 0.98479
- **All links, EPMF**: 0.98707
- **New links, PMF**: 0.85797
- **New links, EPMF**: 0.96602
– Destination is 0.184% and for User – Source, 0.031%. However, despite User – Destination having a higher density, the links are concentrated on a small number of dominant nodes, as can be seen in Figure 2b. Therefore, the prediction task is relatively easy: the probability of a link is roughly approximated by a function of the degree of the node, and adding additional information is not particularly beneficial. For User – Source, as can be seen by Figure 2a, the links are more evenly distributed between the nodes, and the prediction task is more difficult. Hence, in this setting, including additional information about known groupings is crucial to improve the predictive capability of the model. The ROC curves for the User – Source graph are shown in Figure 3.

Some of the covariates might be more predictive than others. To evaluate such differences, the AUC for all links on User – Source have been recalculated excluding each user and host covariate in turn. The difference between the AUC for EPMF fitted with all the covariates, and for EPMF with covariate \( k \) removed, could then be used to quantify the predictive power of covariate \( k \). According to this methodology, the most relevant user covariates (using the covariate codes in the anonymised publicly released version of the dataset) are Covariate 1, with a loss in AUC of 0.05442 when it is removed from the model, followed by Covariate 2, with 0.03001. Similarly, for the hosts, the most predictive covariates appear to be Covariate 2, with score 0.05761, and Covariate 0, with 0.03116.

In order to assess the accuracy of the AUC approximation obtained from a subsample of the negative class, 500 simulations have been carried out. For standard PMF on User – Destination, estimates of the AUC for all links across different subsampled negative classes had standard deviation \( \approx 4.3 \cdot 10^{-5} \) for a sample size of 3nnz(\( A \)). If \( \text{nnz}(A) \) or 0.1\( \text{nnz}(A) \) are used, the standard deviation increases to \( \approx 7.6 \cdot 10^{-5} \) and \( \approx 2.4 \cdot 10^{-4} \) respectively, whereas using 5nnz(\( A \)) gives a value of \( \approx 3.5 \cdot 10^{-6} \).

### 6.2. Comparison with Gibbs sampling

As discussed in Section 4.1, a possible drawback of variational inference is the introduction of bias in the posterior estimates, in particular regarding the variability. Therefore, it is necessary to assess the loss in predictive performance caused by switching to the proposed variational approximation to the posterior. This task is not straightforward, since performing full Bayesian inference on the standard PMF and EPMF model is computationally extremely demanding when the graph is large, because many posterior samples (usually in the order of tens of thousands) are required to confidently estimate the parameters.

Appendix A gives details about the conditional distributions required to develop a Gibbs sampler. Table 3 presents the results obtained from 10,000 posterior samples with burnin 1,000. The link probabilities have been estimated using the unbiased score (4.3). No issues with convergence of the Markov chain were observed, and the performance seems comparable to the results obtained using variational inference, demonstrating that the loss in performance due to the variational approximation seems to be minimal.

It must be noted that variational inference converges in our application in less than 200 iterations. For example, for PMF on User – Source IP, the computation time is \( \approx 4.5 \) seconds per iteration on a MacBook Pro 2017 with a 2.3GHz Intel Core i5 dual-core processor. On the other hand, Gibbs sampling, despite the lower cost of \( \approx 2.6 \)s per iteration, requires many more posterior samples. Hence, the computational advantages guaranteed by the variational inference procedure are particularly relevant in this context.
Table 3
AUC scores for prediction of all and new links using Gibbs sampling. Number of latent features: \( R = 20 \).

|                  | User – Destination | User – Source | PMF   | EPMF   | PMF   | EPMF   |
|------------------|--------------------|---------------|-------|--------|-------|--------|
| All links        | 0.98737            | 0.98835       | 0.87130 | 0.95809 |
| New links        | 0.94311            | 0.94768       | 0.83979 | 0.92723 |

Table 4
AUC scores for prediction of cold starts.

|                  | User – Destination | User – Source | PMF   | EPMF   | PMF   | EPMF   |
|------------------|--------------------|---------------|-------|--------|-------|--------|
| New Users        | 0.96826            | 0.97785       | 0.73362 | 0.93148 |
| New Hosts        | 0.81789            | 0.82715       | 0.79541 | 0.91138 |

6.3. Cold starts
As discussed in Section 4, the extended PMF model allows for prediction of new entities or nodes in the network (cold starts). To assess performance on links in the test set involving new users or hosts, the estimates of the covariate coefficients \( \hat{\phi}_{kh} = \lambda_{kh} \mu_{kh} \) from the training period are used. The latent feature values are set equal to the mean of all users and hosts observed in the training set. For comparison against a baseline model, the regular PMF model is used where the latent features are set as above; this has the effect of comparing against the global mean.

Cold starts can be divided between new users and new hosts, and the AUC scores for prediction for each case are presented in Table 4. To calculate the AUC, the negative class is randomly sampled from the rows and columns corresponding to the new users and hosts, respectively. Again, there are only minor performance gains for User – Destination, and the regular PMF model using the global average of the latent features provides surprisingly good results. As discussed above, this can be explained by the prediction task being much simpler, and well approximated by a simple degree-based model. In contrast, for the User – Source graph the extended PMF model shows very good predictive performance for cold starts.

6.4. Red-team
The motivation for this work is the detection of cyber attacks; to assess performance from an anomaly detection standpoint, the event labels from the red-team attack are used as a binary classification problem. Figure 4 plots the ROC curves and AUC scores from the standard and extended PMF models, and improvements in detection capability are obtained using EPMF. Similarly to the previous cases, the predictive performance gain is most notable for User – Source.

6.5. Comparisons with alternative prediction methods
The results in Table 2 are compared in this section with alternative link prediction methods:
• **Probabilistic matrix factorisation** (Salakhutdinov and Mnih, 2007): \( A_{ij} \sim \alpha_i^\top \beta_j + \varepsilon_{ij} \), with \( \alpha_{ir} \sim N(0, \sigma_i^2) \) and \( \beta_{jr} \sim N(0, \sigma_j^2) \), where \( N(\cdot) \) denotes a normal distribution. The parameters were obtained by maximum a posteriori estimation using gradient ascent optimisation techniques.

• **Logistic matrix factorisation** (Johnson, 2014): \( A_{ij} \sim \text{Bernoulli}(p_{ij}) \) where \( \text{logit}(p_{ij}) = \alpha_i^\top \beta_j \), with \( \alpha_{ir} \sim N(0, \sigma_i^2) \) and \( \beta_{jr} \sim N(0, \sigma_j^2) \). The parameters were estimated using the same procedure described for probabilistic matrix factorisation.

• **Bipartite random dot product graph** (Athreya et al., 2018): \( A_{ij} \sim \text{Bernoulli}(\alpha_i^\top \beta_j) \). The latent positions \( \alpha_i \) and \( \beta_j \) can be estimated using tSVD (Dhillon, 2001). Assume \( A = UDV^\top + U_\perp D_\perp V_\perp^\top \), where \( D \in \mathbb{R}^{R \times R} \) is diagonal matrix containing the top \( R \) singular values in decreasing order, \( U \in \mathbb{R}^{|U| \times R} \) and \( V \in \mathbb{R}^{|V| \times R} \) contain the corresponding left and right singular vectors, and the matrices \( D_\perp, U_\perp, \) and \( V_\perp \) contain the remaining singular values and vectors. The tSVD estimates of \( \alpha_i \) and \( \beta_j \) are respectively the \( i \)-th and \( j \)-th row of \( UD^{1/2} \) and \( VD^{1/2} \). A comparison with tKatz (Dunlavy, Kolda and Acar, 2011) is also provided. The scores are estimated similarly to tSVD, replacing the diagonal entries of the matrix \( D \) with a transformation of the top \( R \) singular values \( d_1, ..., d_R \) of \( A \): \( f(d_i) = (1 - \eta d_i)^{-1} - 1 \), with \( \eta = 10^{-4} \).

• **Non-negative matrix factorisation** (for example, see Chen et al., 2017): nodes are assigned features \( W \in \mathbb{R}_{+}^{|U| \times R} \) and \( H \in \mathbb{R}_{+}^{|V| \times R} \) obtained as solutions to \( \|A - WH^\top\|_F \), where \( \| \cdot \|_F \) is the Frobenius norm. The score associated with any link \((i, j)\) is then obtained as \( w_i^\top h_j \), where \( w_i^\top \) and \( h_j^\top \) are respectively the \( i \)-th and \( j \)-th row of \( W \) and \( H \).

• **Degree-based model**, where the probability of a link is approximated as \( P(A_{ij} = 1) = 1 - \exp(-d_i^\text{out}d_j^\text{in}) \), where \( d_i^\text{out} \) and \( d_j^\text{in} \) are the out-degree and in-degree of each node.

The results are presented in Table 5. Overall, when compared to the results of PMF with Ber-Po link in Table 2, the PMF models achieve better results compared to other popular techniques, especially for new link prediction. Non-negative matrix factorisation and random
with minor differences in the updates for the covariate term. Variational inference for the joint model proceeds similarly to Algorithm 1, similarly, a standard joint PMF model would have the same structure as (6.6), without the two graphs. In particular, assume that $A$ separately. In this section, the predictive performance of the two individual models is compared. On the other hand, fitting EPMF in (4) only requires to calculate $x_iy_j^\top$ for all pairs such that $A_{ij} > 0$, which is $O(nnz(A)KH)$. This operation only takes 6.5 megabytes in memory for $User − Source$, since $A$ is extremely sparse in the cyber-security application. This is a significant practical advantage of the proposed model.

### 6.6. Comparison with a joint model

In the previous sections, the graphs $User − Source$ and $User − Destination$ were analysed separately. In this section, the predictive performance of the two individual models is compared to a joint PMF model, where the user-specific latent features are shared between the two graphs. In particular, assume that $A \in \{0, 1\}^{U \times V}$ represents the adjacency matrix for $User − Source$, and $A' \in \{0, 1\}^{U' \times V'}$ for $User − Destination$. The users are assigned latent positions $\alpha_i$, $i = 1, \ldots, |U|$ and covariates $x_i$, whereas the source and destination hosts are given latent positions $\beta_j$, $j = 1, \ldots, |V|$ and $\beta'_j$, $j = 1, \ldots, |V'|$ respectively, and covariates $y_j$ and $y'_j$. The joint extended PMF model (JEPMF) assumes:

$$A_{ij} = 1_{N_i} (N_{ij}), \ N_{ij} \sim \text{Poisson} \left( \alpha_i^\top \beta_j + 1_K (\Phi \odot x_iy_j^\top)1_H \right),$$

$$A'_{ij} = 1_{N'_i} (N'_{ij}), \ N'_{ij} \sim \text{Poisson} \left( \alpha_i^\top \beta'_j + 1_K (\Phi' \odot x_iy_j^\top)1_{H'} \right). \quad (6.1)$$

Similarly, a standard joint PMF model would have the same structure as (6.6), without the covariate term. Variational inference for the joint model proceeds similarly to Algorithm 1, with minor differences in the updates for $\lambda^{(\alpha)}$ and $\mu^{(\alpha)}$. More details are given in Appendix D.

### Table 5

AUC scores for different link prediction algorithms on the two data sets, with $R = 20$.

| Algorithm                                  | User – Destination | User – Source |
|--------------------------------------------|--------------------|---------------|
| Probabilistic matrix factorisation         | 0.93886            | 0.61006       |
| Logistic matrix factorisation              | 0.98079            | 0.95357       |
| Random dot product graph – tSVD            | 0.95050            | 0.69184       |
| Random dot product graph – tKatz           | 0.95392            | 0.71754       |
| Non-negative matrix factorisation          | 0.93985            | 0.61675       |
| Degree-based model                         | 0.95433            | 0.72505       |

This table compares the AUC scores of different link prediction algorithms on the two data sets, with $R = 20$. The algorithms include Probabilistic matrix factorisation, Logistic matrix factorisation, Random dot product graph – tSVD, Random dot product graph – tKatz, Non-negative matrix factorisation, and Degree-based model.
The results are presented in Table 6. The AUC scores were obtained fitting the joint model and then assessing the predictive performance on User – Source and User – Destination separately. Comparing the results with the predictions in Table 2 for the two individual models, joint PMF produces similar results to the individual models. This suggests that users have a similar behaviour across the two graphs, since adding the constraint of identical user features does not significantly decrease the predictive performance.

### Table 6

|                  | User – Destination | User – Source |
|------------------|--------------------|---------------|
| **PMF**          | **EPMF**           | **PMF**       | **EPMF**      |
| **All links**    | 0.98206            | 0.98290       | 0.86061       | 0.95585       |
| **New links**    | 0.94563            | 0.94565       | 0.89414       | 0.94637       |

6.7. Seasonal modelling

To investigate dynamic modelling, binary adjacency matrices $A_1, \ldots, A_{82}$ are calculated for each day across the train and test periods. The seasonal PMF model with the inclusion of covariates (SEPMF) (5) is then compared against EPMF; for EPMF, the adjacency matrices are assumed to be independent realisations randomly generated from a fixed set of latent features. Due to a “9 day-80 hour” work schedule operated at LANL, whereby employees can elect to take vacation every other Friday, the seasonal period is assumed to be comprised of four segments: weekdays (Monday - Thursday), weekends (Saturday and Sunday), and two separate segments for alternating Friday’s. For each model, binary classification is performed using the model predictive scores calculated across the entire period. For the positive class, scores are calculated for all user-host pairs $(i, j)$ such that $A_{ijt} = 1$ for at least one $t$ in the test set; for the negative class, a random sample of $(i, j)$ pairs such that $A_{ijt} = 0$ for all $t$ in the test set are obtained, with sample size equal to three times the total number of observed links.

Table 7 presents the resulting AUC scores. For both networks, the seasonal model does not globally outperform the extended PMF model for all links. However, improvements are obtained for prediction of the new links. One explanation for the weaker overall performance could be the reduced training sample size implied for the seasonal model: EPMF in a dynamic setting assumes that the all daily graphs have been sampled from the same process, whereas if the seasonal model is used then the daily graphs are only informative for the corresponding seasonal segments. In addition, as briefly mentioned in Section 1, elements of the data exhibit strong polling patterns, often due to computers automatically authenticating on users’ behalves (Turcotte, Kent and Hash, 2018); some of the links that exhibit polling will not exhibit seasonal patterns, as the human behaviour has not been separated from the automated behaviour.

On the other hand, improvements in the estimation of new links, despite the reduced training sample size, demonstrates that it can be beneficial to understand the temporal dynamics of the network for these cases. Considering the context of the application, it might be perfectly normal for a user to authenticate to a computer during the week; however,
Table 7
AUC scores for prediction of all and new links using seasonal PMF.

| User – Destination | User – Source |
|--------------------|--------------|
| EPMF              | SEPMF        | EPMF              | SEPMF        |
| All links          | 0.96550      | 0.96205           | 0.93559      | 0.92829      |
| New links          | 0.87107      | 0.89337           | 0.85009      | 0.85748      |

that same authentication would be extremely unusual on the weekends when the user is not present at work. Without the seasonal model this behavioural difference in would be missed.

7. Conclusion and discussion

Extensions of the standard Poisson matrix factorisation model have been proposed, motivated by applications to computer network data, in particular the LANL enterprise computer network. The extensions are threefold: handling binary matrices, including covariates for users and hosts in the PMF framework, and accounting for seasonal effects. The counts \( N_{ijt} \) have been treated as censored, and it has been assumed that only the binary indicator \( A_{ijt} = 1_{N_{ijt}}(N_{ijt}) \) is observed. Starting from the hierarchical Poisson matrix factorisation model of Gopalan, Hofman and Blei (2015), which only includes the latent features \( \alpha_i \) and \( \beta_j \), covariates have been included through the matrix of coefficients \( \Phi \). Seasonal adjustments for the coefficients are obtained through the variables \( \gamma_{it} \) and \( \delta_{jt} \). A variational inference algorithm is proposed, suitably adapted for the Bernoulli-Poisson link. This article mainly considered categorical covariates, but the methodology could be extended to include other forms of covariates, with minimal modifications to the inferential algorithms.

Despite the focus on bipartite graphs here, the proposed methodologies could be readily adapted to undirected and general directed graphs. For an undirected graph, the PMF model with Ber-Po link would assume:

\[
A_{ij} = 1_{N_{ij}}(N_{ij}), \quad N_{ij} \sim \text{Poisson}(\alpha_i^T \alpha_j), \quad i < j, \quad A_{ij} = A_{ji}.
\] (7.1)

For directed graphs on the same node set, it could be assumed that each node has the same behaviour as source and destination of the connection, implying equation (7) for undirected graphs applies, removing the constraint \( A_{ij} = A_{ji} \). Alternatively, each node could be given two latent features: \( \alpha_i \) for its behaviour as source and \( \beta_i \) for its behaviour as destination. This is a special case of the bipartite graph model, where \( U \equiv V \), hence (4) applies.

The results show improvements over alternative models for link prediction purposes on the real computer network data. Including covariates provides significant uplift in predictive performance and allows for prediction for new nodes arriving into the network. The seasonal model provides time-varying anomaly scores and offers marginal improvements for predicting new links, which are of primary interest in cyber-security applications.

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Appendix A: Full conditional distributions in the extended PMF model

First note that, conditional on $N_{ij}$, $Z_{ij} = (Z_{ij1}, \ldots, Z_{ij(R+KH)})$ has a multinomial distribution,

$$Z_{ij} \mid N_{ij}, \alpha_i, \beta_j, \Phi \sim \text{Mult}(N_{ij}, \pi_{ij}),$$

where $\pi_{ij}$ is the probability vector proportional to

$$(\alpha_{i1} \beta_{j1}, \ldots, \alpha_{iR} \beta_{jR}, \phi_{11} x_{i1} y_{j1}, \ldots, \phi_{KH} x_{iK} y_{jH}).$$

Therefore, setting $\psi_{ij} = \alpha_i^\top \beta_j + 1_K^\top (\Phi \odot x_i y_j^\top) 1_H,$

$$p(N_{ij}, Z_{ij} \mid \alpha_i, \beta_j, \Phi, A) = \begin{cases} \text{Pois}_+ (\psi_{ij}) \text{Mult} (N_{ij}, \pi_{ij}) & A_{ij} > 0, \\ \delta_0 (N_{ij}) \delta_0 (Z_{ij}) & A_{ij} = 0, \end{cases} \quad (A.1)$$

where $\text{Pois}_+ (\cdot)$ denotes the zero-truncated Poisson distribution. The user and host latent features complete conditionals are gamma, where

$$\alpha_{ir} \mid \beta_j, \zeta^{(\alpha)}_i, Z \sim \Gamma \left( a^{(\alpha)} + \sum_{j=1}^{|V|} Z_{ijr}, \zeta^{(\alpha)}_i + \sum_{j=1}^{|V|} \beta_j \right),$$

$$\beta_{jr} \mid \alpha_i, \zeta^{(\beta)}_j, Z \sim \Gamma \left( a^{(\beta)} + \sum_{i=1}^{|U|} Z_{ijr}, \zeta^{(\beta)}_j + \sum_{i=1}^{|U|} \alpha_i \right),$$

and

$$\zeta^{(\alpha)}_i \mid \alpha_i \sim \Gamma \left( b^{(\alpha)} + Ra^{(\alpha)} + \sum_{r=1}^R \alpha_{ir} \right),$$

$$\zeta^{(\beta)}_j \mid \beta_j \sim \Gamma \left( b^{(\beta)} + Ra^{(\beta)} + \sum_{r=1}^R \beta_{jr} \right). \quad (A.2)$$

Similarly,

$$\phi_{kh} \mid \zeta^{(\phi)}, Z \sim \Gamma \left( a^{(\phi)} + \sum_{i=1}^{|U|} \sum_{j=1}^{|V|} Z_{ijl}, \zeta^{(\phi)} + \sum_{i=1}^{|U|} x_{ik} \sum_{j=1}^{|V|} y_{jh} \right),$$

$$\zeta^{(\phi)} \mid \Phi \sim \Gamma \left( b^{(\phi)} + KH a^{(\phi)}, c^{(\phi)} + \sum_{k=1}^K \sum_{h=1}^H \phi_{kh} \right),$$

where $l$ is the index corresponding to the covariate pair $(k, h)$. 
Appendix B: Variational inference in the extended PMF model

As all of the factors in the variational approximation given in (4.2) take the same distributional form of the complete conditionals,

\[
q(N_{ij}, Z_{ij} | \theta_{ij}, \chi_{ij}) = \begin{cases} \text{Pois}(\theta_{ij}) \text{Mult}(N_{ij}, \chi_{ij}) & A_{ij} > 0, \\ \delta_0(N_{ij}) \delta_0(Z_{ij}) & A_{ij} = 0. \end{cases} \tag{B.1}
\]

Let \( \psi_{ij} \) denote the rate \( \sum_{r=1}^{R} \alpha_r \beta_j r + \sum_{k=1}^{K} \sum_{h=1}^{H} \phi_{kh} x_{ik} y_{jh} \) of the Poisson distribution for \( N_{ij} \), and \( \psi_{ijl}, l = 1, \ldots, R + KH \), represent the individual elements in the sum. To get the update equations for \( \theta \) and \( \chi \), following (4.2), for \( A_{ij} > 0 \),

\[
\mathbb{E}^q_{-N_{ij}, Z_{ij}} \{ \log p(N_{ij}, Z_{ij} | \alpha_i, \beta_j, \Phi) \} = \sum_l \left\{ Z_{ijl} \mathbb{E}^q_{-N_{ij}, Z_{ij}} (\log \psi_{ijl}) - \log(Z_{ijl}) \right\} + k, \tag{B.2}
\]

where \( k \) is a constant with respect to \( N_{ij} \) and \( Z_{ij} \). Hence:

\[
q^*(N_{ij}, Z_{ij}) \propto \prod_{l=1}^{R+KH} \exp \left\{ \mathbb{E}^q_{-N_{ij}, Z_{ij}} (\log \psi_{ijl}) \right\}^{Z_{ijl}} / Z_{ijl},
\]

with domain of \( Z_{ij} \) constrained to have \( \sum_l Z_{ijl} > 0 \). Multiplying and dividing the expression by \( N_{ij}! \) and \( \left[ \sum_l \exp\{\mathbb{E}^q_{-N_{ij}, Z_{ij}} (\log \psi_{ijl})\} \right]^{N_{ij}} \) gives a distribution which has the same form of (B). Therefore the rate \( \theta_{ij} \) of the zero truncated Poisson is updated using \( \sum l \exp\{\mathbb{E}^q_{-N_{ij}, Z_{ij}} (\log \psi_{ijl})\} \), see step 5 in Algorithm 1 for the resulting final expression. The update for the vector of probabilities \( \chi_{ij} \) is given by a slight extension of the standard result for variational inference in the PMF model (Gopalan, Hofman and Blei, 2015) to include the covariate terms, see step 6 of Algorithm 1. The remaining updates are essentially analogous to standard PMF (Gopalan, Hofman and Blei, 2015).

Appendix C: Inference in the seasonal model

The inferential procedure for the seasonal model follows the same guidelines used for the non-seasonal model. Given the unobserved count \( N_{ijt} \), latent variables \( Z_{ijtl} \) are added, representing the contribution of the component \( l \) to the total count \( N_{ijt} \): \( N_{ijt} = \sum_l Z_{ijtl} \). The full conditional for \( N_{ijt} \) and \( Z_{ijt} \) follows (A), except the rate for the Poisson and probability vectors for the multinomial will now depend on the seasonal parameters \( \gamma_{itr}, \delta_{jtr} \), and \( \omega_{kht} \). Letting \( p \) denote a seasonal segment in \( \{1, \ldots, P\} \) the full conditionals for the rate parameters are:

\[
\alpha_{ir} | Z, \beta, \gamma, \delta_i, \zeta_{i}^{(\alpha)} \sim \Gamma \left( a^{(\alpha)} + \sum_{j=1}^{\left| V \right|} \sum_{t=1}^{T} Z_{ijtr}, \zeta_{i}^{(\alpha)} + \sum_{\gamma_{itr}} \frac{\sum_{j=1}^{\left| V \right|} \sum_{t:t=p}^{T} \beta_{jr} \delta_{jtr}}{\left| V \right|} \right),
\]

\[
\gamma_{ipt} | Z, \beta, \delta, \zeta_{p}^{(\gamma)} \sim \Gamma \left( a^{(\gamma)} + \sum_{j=1}^{\left| V \right|} \sum_{t:t=p}^{T} Z_{ijtr}, \zeta_{p}^{(\gamma)} + \alpha_{ir} \sum_{\gamma_{itr}} \delta_{jtr} \right),
\]

\[
\phi_{kh} | Z, \zeta^{(\phi)} \sim \Gamma \left( a^{(\phi)} + \sum_{i=1}^{\left| U \right|} \sum_{j=1}^{\left| V \right|} \sum_{t=1}^{T} Z_{ijtl}, \zeta^{(\phi)} + T \hat{x}_{k} \hat{y}_{h} \right),
\]
where $\tilde{x}_k = \sum_{i=1}^{[U]} x_{ik}$ and $\tilde{y}_h = \sum_{j=1}^{[V]} y_{jh}$. Similar results are available for $\beta_{jr}$ and $\delta_{jpr}$. Also:

$$q_{\beta}^{(\gamma)} \sim \Gamma \left( b^{(\gamma)} + |U| R a^{(\gamma)} , c^{(\gamma)} + \sum_{i=1}^{[U]} \sum_{r=1}^{R} \gamma_{ipr} \right),$$

and similarly for $\phi^{(\delta)}$. For $q_{\alpha}^{(\alpha)}$ and $q_{\zeta}^{(\beta)}$, the conditional distribution is equivalent to (A). The mean-field variational family is again used implying a factorisation similar to (4.2), so that

$$q(\alpha, \beta, A, \Phi, \gamma, \delta, \zeta, N, Z) = \prod_{i,j,t} q(N_{ijt} | \theta_{ijt}, \chi_{ijt}) \times \prod_{i,r} q(\alpha_{ir} | \lambda_{ir}^{(\alpha)}, \mu_{ir}^{(\alpha)})$$

and similarly for $q(\beta, \Phi)$. The updates for $\lambda_{ir}^{(\alpha)}$ and similar results can be obtained for the host-specific parameters. Again the variational parameters are updated using CAVI and a similar algorithm is obtained to that detailed in Algorithm 1, where steps 7, 8, 9 and 10 are modified to include the time dependent parameters. It follows that for the user-specific parameters the update equations take the form:

$$\lambda_{ir}^{(\alpha)} = a^{(\alpha)} + \sum_{j=1}^{[V]} \sum_{t=1}^{T} \frac{A_{ijt} \theta_{ijt} \chi_{ijtr}}{1 - e^{-\theta_{ijtr}}} \cdot \mu_{ir}^{(\alpha)} = \frac{\nu_{i}^{(\alpha)}}{\xi_{i}^{(\alpha)}} + \sum_{t=1}^{T} \frac{\lambda_{jtr}^{(\gamma)} \lambda_{jlr}^{(\beta)}}{\mu_{ir}^{(\alpha)} \mu_{jr}^{(\beta)}}$$

and similar results can be obtained for the host-specific parameters $\lambda_{jr}^{(\beta)}, \lambda_{jpr}^{(\delta)}$ and $\lambda_{jpr}^{(\delta)}$. The updates for $\nu_{i}^{(\alpha)}, \xi_{i}^{(\alpha)}, \nu_{j}^{(\beta)}$ and $\xi_{j}^{(\beta)}$ are identical to steps 7 and 8 in Algorithm 1. For the covariates

$$\lambda_{kh}^{(\phi)} = a^{(\phi)} + \sum_{i=1}^{[U]} \sum_{j=1}^{[V]} \sum_{t=1}^{T} \frac{A_{ijt} \theta_{ijt} \chi_{ijtr}}{1 - e^{-\theta_{ijtr}}} \cdot \mu_{kh}^{(\phi)} = \frac{\nu_{i}^{(\phi)}}{\xi_{i}^{(\phi)}} + \tilde{x}_k \tilde{y}_h T.$$

The updates for $\nu^{(\phi)}$ and $\xi^{(\phi)}$ are the same as step 9 in Algorithm 1. Finally, for the time dependent hyperparameters:

$$\nu_{p}^{(\gamma)} = b^{(\gamma)} + |U| R a^{(\gamma)} , \xi_{p}^{(\gamma)} = c^{(\gamma)} + \sum_{i=1}^{[U]} \sum_{r=1}^{R} \lambda_{ipr}^{(\gamma)}$$
and similarly for $\nu_p^{(\delta)}$ and $\xi_p^{(\delta)}$.

The updates for $\theta_{ijt}$ and $\chi_{ijt}$ are similar to Appendix B. An expansion similar to (B) can be applied to the expectation $E_{\theta, N_{ijt}, Z_{ijt}} \log p(N_{ijt}, Z_{ijt} | \alpha_i, \beta_j, \gamma_{it}, \delta_{jt}, \Phi)$, and the update equations for $\theta_{ijt}$ and $\chi_{ijt}$ can be derived similarly to Appendix B:

$$
\theta_{ijt} = \frac{1}{R} \sum_{r=1}^{R} \exp \left\{ \Psi(\lambda_i^{(\alpha)}) - \log(\mu_i^{(\alpha)}) + \Psi(\lambda_j^{(\beta)}) - \log(\mu_j^{(\beta)}) + \Psi(\lambda_{it}^{(\gamma)}) - \log(\mu_{it}^{(\gamma)}) + \Psi(\lambda_{jt}^{(\delta)}) - \log(\mu_{jt}^{(\delta)}) \right\} \\
+ \sum_{k=1}^{K} \sum_{h=1}^{H} x_{ik} y_{jh} \exp \left\{ \Psi(\lambda_k^{(\phi)}) - \log(\mu_k^{(\phi)}) \right\},
$$

$$
\chi_{ijtl} \propto \left\{ \begin{array}{ll}
\exp \left\{ \Psi(\lambda_i^{(\alpha)}) - \log(\mu_i^{(\alpha)}) + \Psi(\lambda_j^{(\beta)}) - \log(\mu_j^{(\beta)}) + \Psi(\lambda_{it}^{(\gamma)}) - \log(\mu_{it}^{(\gamma)}) + \Psi(\lambda_{jt}^{(\delta)}) - \log(\mu_{jt}^{(\delta)}) \right\} & l \leq R, \\
x_{ik} y_{jh} \exp \left\{ \Psi(\lambda_k^{(\phi)}) - \log(\mu_k^{(\phi)}) \right\} & l > R.
\end{array} \right.
$$

Appendix D: Inference in the joint model

Variational inference for the joint PMF model presented in Section 6.6 proceeds similarly to Algorithm 1. The conditional posterior distributions are essentially the same as PMF and EPMF. The only exception is the conditional posterior distribution of $\alpha_{ir}$:

$$
\alpha_{ir} | Z, Z', \beta', \lambda_i^{(\alpha)}, \xi_i^{(\alpha)} \sim \Gamma \left( a^{(\alpha)} + \sum_{j=1}^{V'} Z_{ijr} + \sum_{j=1}^{V'} Z'_{ijr}, \xi_i^{(\alpha)} + \sum_{j=1}^{V'} \beta_{jr} + \sum_{j=1}^{V'} \beta'_{jr} \right).
$$

For variational inference, a factorisation similar to (4.2) is assumed, further multiplied by the approximation for the posteriors of the additional components of the model: mainly $q(\beta_{jr}' | \lambda_{jr}^{(\delta)} \cdot \mu_{jr}^{(\delta)})$, $q(\phi_{kh} | \lambda_{kh}^{(\phi)} \cdot \phi_{kh}^{(\phi)})$. Therefore variational inference is also essentially unchanged, except the CAVI update for the parameters of the variational approximation for the components $\alpha_{ir}$, which become:

$$
\lambda_i^{(\alpha)} = a^{(\alpha)} + \sum_{j=1}^{V'} \frac{A_{ij} \theta_{ij} \chi_{ijr}}{1 - e^{-\theta_{ijr}}} + \sum_{j=1}^{V'} \frac{A'_{ij} \theta_{ij}' \chi_{ijr}'}{1 - e^{-\theta_{ijr}}},
\mu_i^{(\alpha)} = \frac{\nu_i^{(\alpha)}}{\xi_i^{(\alpha)}} + \sum_{j=1}^{V'} \frac{\lambda_{jr}^{(\beta)}}{\mu_{jr}^{(\beta)}} + \sum_{j=1}^{V'} \frac{\lambda_{jr}^{(\beta) \prime}}{\mu_{jr}^{(\beta) \prime}}.
$$

Updates for the approximations of the additional components $N_{ij}^{(\alpha)}, Z_{ijr}', \beta_{jr}'$ and $\phi_{kh}'$ follow from the updates for the variational parameters $\theta_{ijr}, \chi_{ijr}, \lambda_{jr}^{(\beta)}, \mu_{jr}^{(\beta)}, \lambda_{kh}^{(\phi)}$ and $\mu_{kh}^{(\phi)}$ in Algorithm 1.