Estimating Temporal Exponential Random Graph Models by Bootstrapped Pseudolikelihood

R package vignette for **xergm** 1.0

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This package vignette is designed as a hands-on tutorial for estimating temporal exponential random graph models (TERGMs) (Desmarais and Cranmer 2010, 2012b; Hanneke et al. 2010) and assessing goodness of fit and predictive performance (Cranmer and Desmarais 2011; Leifeld and Cranmer 2014) using the **xergm** package (Leifeld et al. 2014) for the statistical computing environment **R** (**R** Core Team 2014).

The **xergm** package is compatible with the syntax of **statnet** (Handcock et al. 2008; Goodreau et al. 2008; Morris et al. 2008) and uses some of its functions, particularly from the **ergm** package (Hunter et al. 2008) and the **network** package (Butts 2008).

A basic familiarity with ERGMs and their estimation, as in **ergm**, and network data management, as in **statnet**, is assumed and thus not treated extensively in this tutorial.

Throughout the examples provided below, a dataset collected by Andrea Knecht on the dynamics of adolescent friendship networks in a Dutch school class is used as an illustration (Knecht 2006, 2008; Knecht et al. 2010; Steglich and Knecht 2009). This dataset is delivered with the **xergm** package and is the classic textbook example for estimating stochastic actor-oriented models (SAOM) using **SIENA** and **RSiena** (Ripley et al. 2011; Snijders et al. 2010).

1 TERGMs without cross-temporal dependencies

1.1 Preparatory steps

Several **R** packages should be loaded for running the examples presented below: the **texreg** package (Leifeld 2013) will be used for displaying estimation results; the **statnet**

suite of network analysis packages provides basic functions for handling network data (Handcock et al. 2008), and the **xergm** package (Leifeld et al. 2014).

```
R> require("statnet")
R> require("texreg")
R> require("xergm")
```

After loading the packages, we attach the Knecht dataset to the workspace. The dataset contains four waves of a friendship network (stored as matrices in a list object called friendship) and several nodal and dyadic covariates (see help(knecht) for details). Of particular interest are the sex of the pupils (stored in a data frame called demographics) and a network called primary, which contains dyadic information on which pupils co-attended the same primary school.

```
R> data("knecht")
```

1.2 Exploring the dataset

To get a first impression of the networks, we plot them using methods from the **statnet** suite of packages. The resulting networks are shown in Figure 1.

We would like to explain edge formation at these four time steps, first by assuming independence between the time steps (this section) and in subsequent examples by modeling network evolution as a process with cross-temporal dependencies (sections 2 and 3).

For the sake of simplicity, we replicate a basic model described in Snijders et al. (2010). In this model, the topology (i.e., the geometric shape) of the networks is determined by the following quantities (with the corresponding model terms of the ergm package given in brackets—see help("ergm-terms") for details):

- a baseline probability of establishing edges (edges),
- the indegree and outdegree of the nodes in the network (computed using the degree function and modeled using nodeocov and nodeicov terms),
- the sex of ego, the sex of alter, and sex match of ego and alter (nodeofactor, nodeifactor, and nodematch, respectively),
- primary school co-attendance (edgecov),

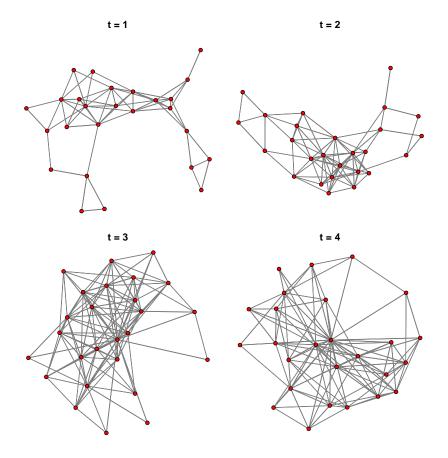


Figure 1: The four networks in the Knecht dataset.

- the tendency of edges to be reciprocated (mutual),
- and the number of cyclic triples, transitive triples, and transitive ties (ctriple, ttriple, and transitiveties, respectively).

1.3 Preprocessing the networks and covariates

Before we can estimate a model containing these terms, the data must be preprocessed. Preprocessing can take several different forms and is often necessary to ensure that the data matrices containing variable information are conformable at any given temporal wave and/or across temporal waves. Data matrices may not be conformable because of missing values, node entry, or node exit (known as composition change).

At each time step, all covariates and the dependent network should be composed of the same set of nodes. Because the btergm estimation function in the **xergm** package cannot handle any missing values, something must be done to address such values. One has several options. Perhapse most common is to replace NA values with the modal value (usually 0—this approach is also taken by **RSiena**). This makes sense in situations where one can assume that all present edges will be observed, though we may not have a

specific recording of 0 for absent edges. Note, however, that the erronious introduction of 0s where edges actually exist is a form of measurement error that will result in biased statistical models. A second option is to remove nodes with incomplete edge profiles from the dataset. This strategy, at best, is inefficient because removing a node—perhaps because of a single missing value in one of its edges—requires removing all incoming and outgoing ties from that node. In other words, the network nature of the data means that an entire row and column of the data matrix will be removed any time we remove a node. This compounds the inefficiency of the casewise deletion process compared to that same inefficiency in a normal, rectangular, data frame. At worst, casewise deletion of nodes with missing edges results in bias. Bias will occur from this proceedure any time the occurrence of missing edges is not completely random (e.g., if the occurrence of missing values is related to any attributes of the edge or node, observed or unobserved, bias will be the result). Lastly, missing edge values may be imputed with one of several techniques from a new and budding literature (Handcock and Gile 2010; Koskinen et al. 2013; Robins et al. 2004). With this cautionary note, the **xergm** package provides the **handleMissings** function to aid the user in removing or imputing missing data iteratively.

Moreover, when cross-temporal dependencies are modeled (such as delayed reciprocity, delayed triadic closure, a lagged dependent network, or edge stability over time), consecutive time steps should feature the same set of nodes. This is not necessarily the case because new nodes may join the network, there may be panel attrition, or respondents may be absent during some waves of data collection. The xergm package provides a function called adjust to adjust the dimensions of a matrix to the dimensions of another matrix by matching row and column labels and removing rows and columns from matrix A which are absent in matrix B as well as adding new NA-filled rows and columns to matrix A where matrix B has additional nodes.

A third function, preprocess, serves to automatize both the handling of missing data and the adjustment of matrix dimensions in a single call—it serves as an interface to both functions. Before we can use the preprocess function, we must ensure that the dependent networks and covariates have node labels because the networks are matched on the labels. The preprocess function requires consecutive networks to be saved as a list of matrices. The friendship networks are already provided as a list of matrices, but the nodes are not labeled. Hence we have to make sure first that the matrices have row and column names.

```
R> for (i in 1:length(friendship)) {
          rownames(friendship[[i]]) <- 1:nrow(friendship[[i]])
          colnames(friendship[[i]]) <- 1:ncol(friendship[[i]])
          }
R> rownames(primary) <- rownames(friendship[[1]])
R> colnames(primary) <- colnames(friendship[[1]])</pre>
```

In the friendship matrices, missing data are marked as NA values, and the incoming and outgoing edges of absent nodes (so-called structural zeroes) are marked by entries of 10. In the next step, the preprocess function takes the friendship networks, replaces missing entries by the modal value (here: 0), iteratively removes nodes that have rows or columns with structural zeroes, and adjusts the friendship matrices at each time step to the dimensions of the primary school network and the nodal sex covariate.

```
R> dep <- preprocess(friendship, primary, demographics$sex,
+ lag = FALSE, covariate = FALSE, na = NA,
+ na.method = "fillmode", structzero = 10,
+ structzero.method = "remove")</pre>
```

This command must be repeated for all covariates that have composition changes or missing data or structural zeroes. In this example, none of the covariates has missing data or composition change.

The first argument of the preprocess function is the list of matrices to be adjusted, followed by several other objects (matrices, vectors or lists) to which the dimensions of the first object shall be adjusted. If lag = TRUE is set, the object will be adjusted across time steps. If the object to be adjusted is a covariate, covariate = TRUE should be set. The combination of these arguments allows flexible preprocessing of the network matrices. For example, lag = TRUE and covariate = FALSE adjusts the dimensions of the second friendship matrix to the first primary matrix, the third to the second, and the fourth friendship matrix to the third primary matrix. If lag = TRUE and covariate = TRUE are specified, this will adjust the first friendship matrix to the second matrix and so on, effectively generating a lagged dependent network for use as an edge covariate to explain current network activity by previous network activity. Whenever the lag = TRUE argument is set, one of the time steps is effectively lost due to the temporal conditioning.

It should be noted that at least three time steps are required by the estimation function to compute meaningful measures of uncertainty when a model with cross-temporal effects is estimated. When no temporal conditioning is needed, two time steps are sufficient for the estimation.

The new object, dep, should still have four time steps because lag = FALSE. Moreover, Node 21 dropped out of the panel after the second time step, hence the dimensions of the dep object should be different from the dimensions of the friendship object. We can verify this by calling:

```
R> length(dep)
R> sapply(friendship, dim)
R> sapply(dep, dim)
R> rownames(dep[[3]])
```

Next, the dimensions of the constant covariates have to be adjusted. We would like to have three consecutive matrices per covariate, and these matrices should have the same dimensions as the dependent network at time steps two, three, and four:

```
R> primary.cov <- preprocess(primary, dep, demographics$sex,
+ lag = FALSE, covariate = TRUE)
R> sex.cov <- preprocess(demographics$sex, primary.cov, friendship,
+ lag = FALSE, covariate = TRUE)</pre>
```

The next step consists of converting the friendship matrices to **network** objects, computing the square root of the outdegree and indegree centralities for each node at every time step, and adding these centralities as well as the sex attribute as vertex attributes to the networks.

1.4 Estimation

With these modifications, we are now able to estimate our first TERGM. As in cross-sectional ERGM estimation, nodal covariates are usually provided as vertex attributes of the dependent network, and dyadic covariates are provided as separate matrices or networks. In a temporal setting, dyadic covariates can be either constant or time-varying. Constant covariates can be provided as network or matrix objects. Time-varying covariates can be provided as lists of networks or matrices. In the Knecht example, primary is a constant covariate.

The TERGM is estimated with the btergm function, which implements the bootstrapping proceedure outlined in Desmarais and Cranmer (2010) and Desmarais and Cranmer (2012b) and stands for "bootstrapped TERGM." The first argument of the btergm function is a formula like in the ergm function, but accepting lists of networks or matrices instead of a single network or matrix as the dependent variable. In all other regards, the syntax of btergm and the syntax of ergm are identical. The second argument, R, is the number of bootstrapping replications used for estimation. The more, the better (but also slower). Options for parallel processing on multicore CPUs or HPC servers are available (see help("btergm")). As a rule of thumb, at least 100 replications are necessary for testing purposes, while something on the order of 1,000 replications should be used for publication purposes.

```
+ nodeifactor("sex") + nodematch("sex") + edgecov(primary.cov),
+ R = 100)
```

A TERGM without cross-temporal dependencies is essentially a pooled ERGM. The model and the coefficients therefore describe a single data-generating process that applies to all four time steps independently. The resulting btergm object model1 can be displayed as follows.

```
R> summary(model1, level = 0.95)
```

Summary of model fit

```
Formula: dep ~ edges + mutual + ttriple + transitiveties + ctriple + nodeicov("idegsqrt") + nodeicov("odegsqrt") + nodeocov("odegsqrt") + nodeofactor("sex") + nodeifactor("sex") + nodematch("sex") + edgecov(primary.cov)
```

Bootstrapping sample size: 100

Estimates and 95% confidence intervals:

	Estimate	2.5%	97.5%
edges	-9.17591	-10.4516	-8.6876
mutual	2.96172	2.4657	3.7487
ttriple	0.21316	0.1274	0.3343
transitiveties	0.36794	0.2223	0.4270
ctriple	-0.67677	-0.9357	-0.5076
nodeicov.idegsqrt	1.17509	0.9975	1.4825
nodeicov.odegsqrt	-0.28432	-0.5840	-0.1844
nodeocov.odegsqrt	1.19846	1.1637	1.4470
nodeofactor.sex.2	0.60720	0.4228	0.8283
nodeifactor.sex.2	0.22578	0.0732	0.3629
nodematch.sex	1.76805	1.5660	2.1493
<pre>edgecov.primary.cov[[i]]</pre>	1.05123	0.7605	1.3889

By default, a 95% confidence interval is reported around the estimates. This can be changed by modifying the level argument. The primary term, for example, has an estimate of 1.05, which means that going to primary school together increases the odds of being friends later on by $100 \cdot (\exp(1.05) - 1) \approx 186\%$ on average conditional on the rest of the network. The effect is significant because 0 is outside the confidence interval of [0.76; 1.39]. See, for example, Desmarais and Cranmer (2012a) for further details on interpretation of ERGMs and TERGMs.

1.5 Goodness-of-fit assessment

To assess the goodness of fit, statnet-style boxplots of simulated networks versus the observed network(s) or measures of classification performance can be employed. For either of these options, the gof function has to be called.

```
R > gof1 \leftarrow gof(model1, nsim = 25)
```

The nsim = 25 argument causes the gof function to simulate a total of 100 networks (25 from each of the four time steps). Naturally, when estimating models for publication, more simulations are preferable. Here, however, exposition is accomplished with fewer simulations and less computing time. The resulting gof1 object can be printed to the console in order to obtain comparison tables of the edge-wise shared partner, dyad-wise shared partner, geodesic distance, indegree, outdegree, instar and outstar distributions of the simulated versus the observed networks. Just like in the ergm package, this comparison can be done visually by using the plot.btergmgof method (for the result, see Figure 2). Interpretation of these plots is straightforward; the model is said to fit better the closer the medians of the boxplots (based on the simulated networks) come to the line that plots the actual value of these statistics in the observed network.

```
R> gof1
R> plot(gof1)
```

The model fit looks acceptable. The theme of the next section will be an alternative model which takes into account cross-temporal dependencies.

2 Network evolution with temporal effects

It makes sense to conceive of consecutive measurements of a friendship network, and indeed many longitudinally observed networks, as a process over time rather than independent phenomena. We therefore want the ability to control for friendship choices at each previous time step as well as edge stability ("inertia", or "memory"). Controlling for the history of the network is straightforward; a lagged outcome network may be included and functions as an autoregressive term does in regression analysis. The meaning of a "memory" term can be somewhat vague, and different types of memory terms may be preferred depending on the density of the network and the substantive interest of the analyst. For networks of medium density, a change statistic on a network that sums $(x_{ij}^{t-1} - x_{ij}^t)$ over the dyad ij would be 1 if $x_{ij}^{t-1} = 1$ and -1 if $x_{ij}^{t-1} = 0$. This would be a memory term in which 1s and 0s have the same effect. Alternatively, one can include separate indicators for edge innovation (the creation of a new edge from t-1 to t) and edge loss (the dissolution of an edge from t-1 to t) in order to recover separate coefficients for these two processes. This may be useful when one or the other (or both) are of specific theoretical interest. Lastly, a memory term that captures absolute stability, one coded 1 any time i and j have the same value at time t-1 and t

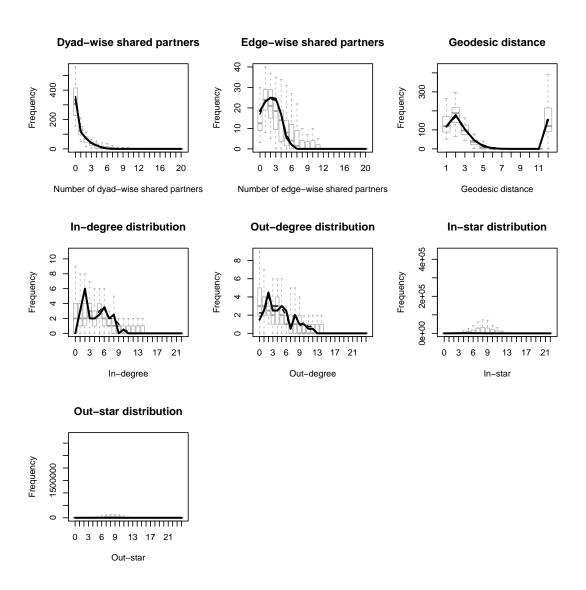


Figure 2: Goodness-of-fit assessment using statnet-style boxplots.

(be that value 1 for a connection or 0 for a non-connection) may be useful for modeling sparse networks, where connection is a fairly rare event. Each of these memory terms capture somewhat different processes, and the choice of appropriate memory terms will usually depend on the application. Different types of temporal dependencies may also be used in conjunction with one another. For example, a stability memory term may be used to capture the temporal stability, and a lagged outcome network will, in addition, capture the extent to which temporally stable relationships tend to be one.

One may also theorize about other cross-temporal dependencies like single-period delayed reciprocity, in which a directed edge formed at t-1 is reciprocated in t. Opportunities for such temporally dependent network statistics are many, and a thorough review of one's options is beyond the scope of the present tutorial.

2.1 Preprocessing the data

As in the last section, the matrices have to be preprocessed. If cross-temporal dynamics are modeled, at least one time step is lost. One usually has to drop the first time step from the list of dependent networks. The reason is that the estimation is conditioned on the covariates at the previous time step each time, and for the first observed network, there is simply no previous time step. Therefore, estimation starts at t=2 and ends at t=4 in the friendship network example, and the covariates start at t=1 and end at t=3.

To achieve this, we first create the list of dependent networks. If lag = TRUE and covariate = FALSE are set, this will remove the first time step from the list of friendship matrices. Moreover, the following code will remove structural zeroes and adjust the dimensions of the matrices to the dimensions at the previous time steps.

```
R> dep <- preprocess(friendship, primary, demographics$sex,
+ lag = TRUE, covariate = FALSE, na = NA,
+ na.method = "fillmode", structzero = 10,
+ structzero.method = "remove")</pre>
```

Next, we create a lagged dependent network for use as a covariate because we can assume that current friendship ties are often the result of previous friendship ties. The following command will remove the last time step from the list of friendship networks and adjust the dimensions of the matrices to the next time step.

```
R> lag <- preprocess(friendship, primary, demographics$sex,
+ lag = TRUE, covariate = TRUE, na = NA,
+ na.method = "fillmode", structzero = 10,
+ structzero.method = "remove")</pre>
```

We can also model dyadic stability using a memory term. A memory term is a matrix which contains cell entries of 1 where the current and previous matrix have the same value (i.e., in both cases, there is a tie, or in both cases, there is no tie) and otherwise 0. We can generate a memory term by specifying lag = TRUE, covariate = TRUE, and additionally memory = TRUE in the preprocess function.

```
R> mem <- preprocess(friendship, primary, demographics$sex,
+ lag = TRUE, covariate = TRUE, memory = TRUE, na = NA,
+ na.method = "fillmode", structzero = 10,
+ structzero.method = "remove")</pre>
```

We can confirm that there are three time steps for all objects and that there are 26, 25, and 25 nodes at these three time steps after the adjustment.

```
R> length(dep)
R> sapply(dep, dim)
R> sapply(lag, dim)
R> sapply(mem, dim)
```

Next, the dimensions of the covariates have to be adjusted. We would like to have three consecutive matrices per covariate, and these matrices should have the same dimensions as the dependent network at time steps two, three, and four:

```
R> primary.cov <- preprocess(primary, dep, demographics$sex,
+ lag = FALSE, covariate = TRUE)
R> sex.cov <- preprocess(demographics$sex, primary.cov, friendship,
+ lag = FALSE, covariate = TRUE)</pre>
```

Another plausible cross-temporal model term would be single-period delayed reciprocity: If there is a tie from v' to v at t-1, does this increase the odds that we see a tie from v to v' at t? In other words, are friendship choices reciprocated over time (possibly in addition to reciprocation that occurs within a time step)? To create such a term, one can simply transpose the friendship matrices and create a lagged covariate using the preprocess function:

Finally, the node attributes sex, indegree and outdegree must be added to the dependent network, as in the previous section.

2.2 Estimation

We are now ready to estimate the second model, this time with temporal dynamics. The syntax is the same as in section 1. The lagged network, the memory term, and delayed reciprocity are added as edge covariates.

As before, we can look at the results using summary(model2). For a direct comparison of the first and the second model, we can employ the screenreg, texreg, and htmlreg functions from the texreg package:

R> screenreg(list(model1, model2))

	==========	===========
	Model 1	Model 2
edges	-9.18 *	
mutual	[-10.45; -8.69] 2.96 *	[-12.94; -8.51] 2.34 *
A4		[1.84; 2.69]
ttriple	0.21 * [0.13; 0.33]	0.09 [-0.01; 0.15]
transitiveties	0.37 * [0.22; 0.43]	0.43 * [0.36; 0.53]
ctriple	-0.68 *	-0.58 *
nodeicov.idegsqrt	[-0.94; -0.51] 1.18 *	[-0.71; -0.48] 1.24 *
v .	[1.00; 1.48]	[1.11; 1.60]
nodeicov.odegsqrt	-0.28 * [-0.58; -0.18]	-0.08 [-0.26; 0.18]
nodeocov.odegsqrt	1.20 * [1.16; 1.45]	1.66 * [1.49; 2.45]
nodeofactor.sex.2	0.61 *	0.62 *
nodeifactor.sex.2	[0.42; 0.83] 0.23 *	[0.51; 0.86] 0.38 *
	[0.07; 0.36]	[0.31; 0.60]
nodematch.sex	1.77 * [1.57; 2.15]	1.48 * [1.37; 1.83]
edgecov.primary.cov[[i]]	1.05 *	0.40 *
edgecov.delrecip[[i]]	[0.76; 1.39]	[0.18; 1.15] 0.69 *
odmonov lam[[i]]		[0.24; 1.59] 1.47 *
edgecov.lag[[i]]		[1.17; 2.48]
edgecov.mem[[i]]		-1.77 * [-2.46; -1.28]

* O outside the confidence interval

The coefficients and confidence intervals can also be explored visually using the plotreg function from the **texreg** package. The resulting forest plot is shown in Figure 3.

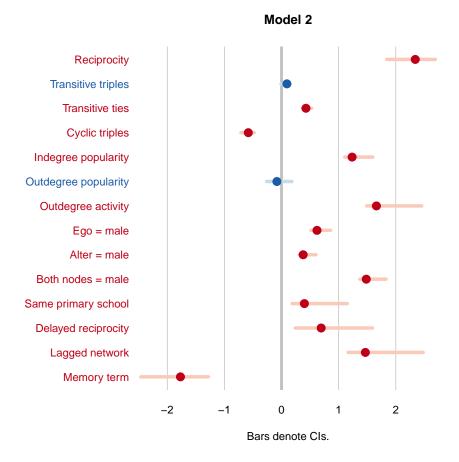


Figure 3: Estimates and confidence intervals of the TERGM with temporal dynamics.

With the inclusion of the three significant temporal effects, transitive triples and one of the outdegree terms are no longer significant.

2.3 Goodness of fit

As in section 1, we assess the goodness of fit as follows.

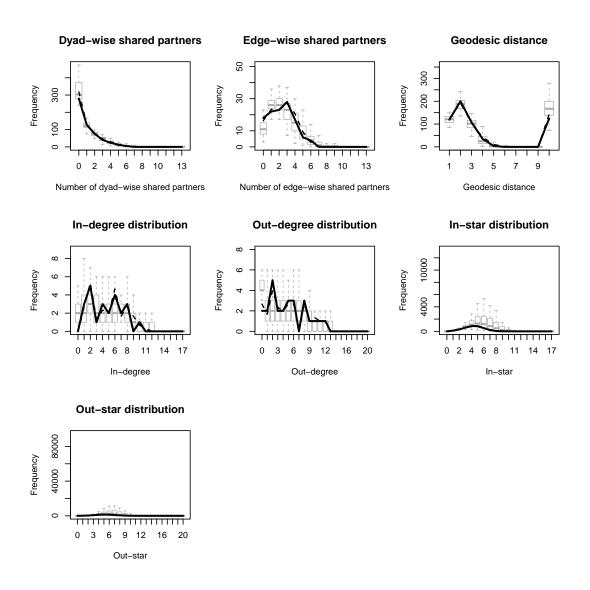


Figure 4: Goodness-of-fit assessment of the second TERGM.

The boxplot diagrams (Figure 4) show a similar goodness of fit as in the first model (shown in Figure 2). We seem to capture the data-generating process reasonably well with both specifications.

3 Out-of-sample prediction with TERGMs

For predicting the network at future time points and to gain more confidence in the robustness of the results, we may consider out-of-sample prediction based on our model specification. As an illustration, we will try to predict the network at t=4 using a model estimated from the three previous networks and based on the covariates at t=3 and t=4.

We can recycle the lists of objects prepared in the previous section. Particularly, the first two out of the three elements of the dep object contain the friendship network at time steps two and three while the first two items of the covariate lists contain time steps one and two because we modeled cross-temporal dynamics (i. e., there is a lag). Within the formula of the btergm estimation function, it is possible to index the lists to work only with the first two items in each list because we want to reserve the last item for comparison with the results. To verify that the coefficients are substantively similar as before, we can print a table with the three models using the screenreg function from the texreg package (Leifeld 2013).

Next, we can employ the gof function to simulate 100 networks from the model and compare them to the observed network at t=4. Remember that the model was estimated based on time steps two to three for the dependent networks and one to two for the lagged covariates (hence we used index [1:2] above). The dependent network at t=4 and the covariates at t=3 can therefore be accessed by using the index [[3]] when we use the gof function.

This function call simulates 100 new networks based on model 3 (i.e., without the last time step) and based on the covariates at t=3 and compares the simulations to the observed network at t=4. The target argument specifies the network to which we are comparing the simulations. The coefficients are taken from the model3 object. We specify an explicit formula where we tell the gof function to simulate from the covariates at t=3.

Now we have four options to assess the predictive performance: we can display boxplot diagrams as above (results not reported here), we can print the output of the $\mathbf{gof3}$ object to the \mathbf{R} console (results not reported here), we can plot a receiver operating characteristics (ROC) curve of the out-of-sample prediction of network ties, and we can plot a precision-recall (PR) curve of the prediction.

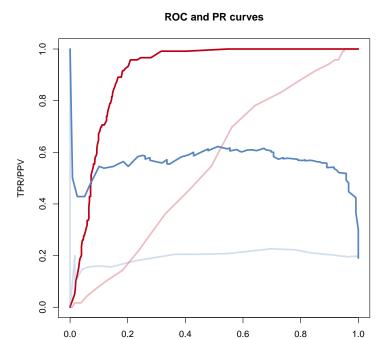


Figure 5: Out-of-sample predictive fit of model 3 versus a null model.

FPR/TPR

The two curves are displayed in Figure 5. The dark red curve shows the ROC curve for model 3 while the light red curve is the ROC curve of a random graph of the same size with the same density (i. e., the same model but only with an edges term). Model 3 clearly has a much better predictive performance than the null model. The dark blue curve shows the PR curve for model 3 while the light blue curve is the PR curve of the null model. PR curves are better suited for sparse networks because absent ties are not taken into account. For the Knecht data, however, this is not an issue. The PR curve also shows that the predictive fit is good.

ROC and PR curves can be used to compare different model specifications, also for within-sample goodness of it. To condense the performance into a single measure, the area under the curve (AUC) can be reported for both curves. AUC values are stored in the btergmgof objects and are printed along with other goodness-of-fit measures when

the object (here: gof3) is called. They can be accessed directly by calling gof3\$auc.roc and gof3\$auc.pr.

4 Other TERGM-related functions

The **xergm** package provides several other TERGM-related functions.

Checking for model degeneracy is possible using the gof function and specifying the argument checkdegeneracy = TRUE (which is the default value). When the resulting btergmgof object is printed, a table indicates which network statistics are problematic. Note that at least 1,000 simulations should be created for the degeneracy check (argument nsim = 1000).

The gof function thus serves to assess degeneracy, goodness of fit (via statnet-like boxplot diagrams), and (out-of-sample or within-sample) predictive performance using ROC and PR curves. For easy comparison of different types of models, there are gof methods for btergm, ergm, and sienaAlgorithm objects (the latter produced by RSiena) (Leifeld and Cranmer 2014).

The simulate.btergm method serves to create new networks given a btergm model and a set of covariates. The confint.btergm method can be used to recompute confidence intervals at arbitrary confidence levels. The same result can be achieved by using the level argument of the summary.btergm method. The btergm.se function computes standard errors and p values for the estimates. btergm.timesteps extracts the number of distinct time steps from a btergm object. There is also a coef.btergm and a nobs.btergm method for extracting the estimates and the number of observations, respectively. The formula can be extracted from a btergm object (or from an ergm object) using the getformula function.

Finally, the generic interpret function accepts ergm and btergm models and facilitates micro-level interpretation of the effects, as suggested by Desmarais and Cranmer (2012a).

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