A Stein Goodness-of-fit Test for Exponential Random Graph Models

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Abstract

We propose and analyse a novel nonparametric goodness-of-fit testing procedure for exchangeable exponential random graph models (ERGMs) when a single network realisation is observed. The test determines how likely it is that the observation is generated from a target unnormalised ERGM density. Our test statistics are derived from a kernel Stein discrepancy, a divergence constructed via Stein’s method using functions in a reproducing kernel Hilbert space, combined with a discrete Stein operator for ERGMs. The test is a Monte Carlo test based on simulated networks from the target ERGM. We show theoretical properties for the testing procedure for a class of ERGMs. Simulation studies and real network applications are presented.

1 INTRODUCTION

Complex data from many application areas are often represented as networks, and probabilistic network models help to understand the expected behaviour of such networks. In social science, exponential random graph models (ERGMs) have been successfully employed for this task, see for example Wasserman and Faust [1994]. ERGMs can be viewed as exponential family models or energy-based models, and as typical for such models, statistical inference for ERGMs suffers from intractable normalisation constants. Monte Carlo methods for parameter estimations in ERGMs alleviate this issue [Snijders, 2008], and model diagnoses via maximum likelihood (MLE) and maximum pseudo-likelihood are developed [Morris et al., 2008]. Statistical properties with particular attention to the normalisation constant are studied in Chatterjee and Diaconis [2013]. For analysing distributions with intractable normalisation constants, Stein’s method [Barbour and Chen, 2005; Chen et al., 2010] provides a promising approach [Chwialkowski et al., 2016; Liu and Wang, 2016; Bresler and Nagaraj, 2019]. In Reinert and Ross [2019], Stein’s method is developed for ERGMs but not yet applied to goodness-of-fit tests. Goodness-of-fit tests for random graph models address the problem of whether the proposed model generates the observed network(s), and play a key role in understanding and interpreting network structures in real-world applications. A main issue is that replicates are usually not available; the data are represented as only one network. Standard goodness-of-fit tests for ERGMs to date rely on Monte Carlo tests for particular summary statistics such as vertices degrees [Ouadah et al., 2020], motifs or subgraph counts [Bhattacharyya and Bickel, 2015; Ospina-Forero et al., 2019; Chen and Onnela, 2019], or spectral properties [Shore and Lubin, 2015]. The goodness-of-fit tests for ERGM in Hunter et al. [2008] or Schweinberger [2012] also assess the model assumptions via graphical assessments. Lospinoso and Snijders [2019] combines such statistics into a Mahalanobis-type distance which is assessed via Monte Carlo tests. The consistency of type 1 error and the power of the test have not yet been systematically investigated.

Nonparametric goodness-of-fit tests based on Stein operators [Gorham and Mackey, 2015; Ley et al., 2017] and functions in a reproducing kernel Hilbert space (RKHS) [Berlinet and Thomas, 2004] for data with replicates build on a kernel Stein discrepancy (KSD) that utilises the strength of a Stein operator to treat unnormalised models and optimises over test functions in a rich enough RKHS to best distinguish the data from the model distributions. Such schemes are consistent and have high test power in various scenarios, including multivariate distributions [Chwialkowski et al., 2016; Liu et al., 2016], discrete distributions [Yang et al., 2018], point processes [Yang et al., 2019], directional distributions [Xu and Matsuda, 2020], and...
censored data [Fernandez et al., 2020]. These scenarios are typically based on i.i.d. samples from the distributions. In addition, the properties of kernel mean embeddings [Berlinet and Thomas, 2004; Muan- det et al., 2017] enable the extraction of distributional features to perform model comparison and model criticism [Jitkrittum et al., 2017b, 2018; Kanagawa et al., 2019; Jitkrittum et al., 2020].

Here we propose a novel goodness-of-fit testing procedure for ERGMs combining a Stein operator for ERGMs and functions in an RKHS. The class of ERGMs treated here are undirected networks which, when the number of vertices tends to infinity, can be approximated by a suitably chosen Bernoulli random graph, with edge probability parameter that generally does not equal the MLE. The test is based on only one observed network and estimates the Stein operator through re-sampling edge indicators. This test compares the test statistics from one observed network to the simulated distribution of the statistics under the null model. As the Stein operator characterises the target distribution for this class of ERGMs, under a member of this class serving as null hypothesis we derive theoretical results for the test statistic. We also provide a theoretical justification of the proposed re-sampling procedure.

To assess the performance of the test, we use simulated data as well as three real-world applications: Lazega’s lawyer network [Lazega, 2001], a teenager friendship network [Steglich et al., 2006], and a larger network of legislation co-sponsorship [Fowler, 2006a,b]. We find that on synthetic data, our test is more reliable and has higher power than its competitor tests. For the lawyer network [Lazega, 2001], a teenager friendship network [Steglich et al., 2006], and a larger network of legislation co-sponsorship [Fowler, 2006a,b].

2 BACKGROUND

2.1 Exponential Random Graph Models

Exponential random graph models (ERGM) are frequently used as parametric models for social network analysis [Wasserman and Faust, 1994; Holland and Leinhardt, 1981; Frank and Strauss, 1986]; they include Bernoulli random graphs as well as stochastic blockmodels as special cases. Here we restrict attention to undirected, unweighted simple graphs on n vertices, without self-loops or multiple edges. To define such an ERGM, we introduce the following notations.

Let \( g_{lab}^t \) be a set of vertex-labeled graphs on n vertices and, for \( N = n(n-1)/2 \), encode \( x \in g_{lab}^t \) by an ordered collection of \( \{0,1\} \) valued variables \( x = (x_{ij})_{1 \leq i < j \leq n} \in \{0,1\}^N \) where \( x_{ij} = 1 \) if and only if there is an edge between \( i \) and \( j \). For a graph \( H \) on at most \( n \) vertices, let \( V(H) \) denote the vertex set, and for \( x \in \{0,1\}^N \), denote by \( t(H,x) \) the number of edge-preserving injections from \( V(H) \) to \( V(x) \): an injection \( \sigma \) preserves edges if for all edges \( uv \) of \( H \) with \( \sigma(u) < \sigma(w) \), \( x_{\sigma(u)\sigma(w)} = 1 \). For \( v_H = |V(H)| \geq 3 \) set

\[
t_H(x) = \frac{t(H,x)}{n(n-1)\cdots(n-v_H+3)}.
\]

If \( H = H_1 \) is a single edge, then \( t_H(x) \) is twice the number of edges of \( x \). In the exponent this scaling of counts matches [Bhamidi et al., 2011, Definition 1] and [Chatterjee and Diaconis, 2013, Sections 3 and 4]. An ERGM for the collection \( x \in \{0,1\}^N \) can be defined as follows, see [Reinert and Ross, 2019].

**Definition 1.** Fix \( n \in \mathbb{N} \) and \( k \in \mathbb{N} \). Let \( H_1 \) be a single edge and for \( l = 2, \ldots, k \) let \( H_l \) be a connected graph on at most \( n \) vertices; set \( t_l(x) = t_l(H_l,x) \). For \( \beta = (\beta_1, \ldots, \beta_k)^\top \in \mathbb{R}^k \) and \( t(x) = (t_1(x), \ldots, t_k(x))^\top \in \mathbb{R}^k \), \( X \in g_{lab}^t \) follows the exponential random graph model \( X \sim \text{ERGM}(\beta,t) \) if for \( \forall x \in g_{lab}^t \),

\[
F(X = x) = \frac{1}{\kappa_n(\beta)} \exp \left( \sum_{l=1}^k \beta_l t_l(x) \right).
\]

Here \( \kappa_n(\beta) \) is the normalisation constant.

The vector \( \beta \in \mathbb{R}^k \) is the parameter vector and the statistics \( t(x) = (t_1(x),\ldots,t_k(x))^\top \in \mathbb{R}^k \) are sufficient statistics. Moreover, exchangeability holds; letting
A suitable class of functions $\mathcal{F}$ is such that if $\mathbb{E}_p[\mathcal{T}_q f] = 0$ for all functions $f \in \mathcal{F}$, then $p = q$ follows. It is convenient to take $\mathcal{F} = B_1(\mathcal{H})$, the unit ball of a large enough RKHS $\mathcal{H}$. In particular, the kernel Stein discrepancies (KSD) between two densities $p$ and $q$ based on $\mathcal{T}_q$ is defined as

$$\text{KSD}(p\|q, \mathcal{H}) = \sup_{f \in B_1(\mathcal{H})} \mathbb{E}_p[\mathcal{T}_q f].$$

Under mild regularity conditions, $\text{KSD}(p\|q, \mathcal{H}) \geq 0$ and $\text{KSD}(p\|q, \mathcal{H}) = 0$ if and only if $p = q$ [Chwialkowski et al., 2016], making KSD a proper discrepancy measure between probability densities.

The KSD in Eq.(2) can be used for testing the model goodness-of-fit as follows. One can show that $\text{KSD}^2(p\|q, \mathcal{H}) = \mathbb{E}_{x \sim p}[h_q(x, \tilde{x})]$, where $x$ and $\tilde{x}$ are independent random variables with density $p$ and $h_q(x, \tilde{x})$ is given in explicit form which does not involve $p$:

$$h_q(x, \tilde{x}) = \sum_{i=1}^d \left( \frac{\partial \log q(x)}{\partial x^i} k(x, \cdot) + \frac{\partial k(x, \cdot)}{\partial x^i} \right) + \frac{\partial \log \tilde{x}}{\partial \xi} k(\tilde{x}, \cdot) + \frac{\partial k(\tilde{x}, \cdot)}{\partial \xi} \right).$$

Suppose we have a set of samples $\{x_1, \ldots, x_n\}$ from an unknown density $p$ on $\mathbb{R}^d$ and the goodness-of-fit test aims to check whether $p = q$. Then $\text{KSD}^2(p\|q, \mathcal{H})$ can be empirically estimated by independent samples from $p$ using a U-statistics or V-statistics. The critical value is determined by bootstrap based on weighted chisquare approximations for U-statistics or V-statistics.

For goodness-of-fit test of discrete distributions, Yang et al. [2018] proposed a kernel discrete Stein discrepancy (KSD). Essentially, the differential operator in Eq.(1) is replaced by an appropriately defined difference operator. KSD is a useful method for assessing goodness-of-fit of ERGMs (as discrete random objects) when a large set of networks are observed [Yang et al., 2018, Figure 1(d)], but is not applicable when only one single network is observed. More details can be found in the Supplementary Material F.

2.3 The ERGM Stein Operator

Instead of using the Stein operator from Yang et al. [2018] we employ the Stein operator from Reinert and Ross [2019]. With $N = n(n-1)/2$ let $e_s \in \{0,1\}^N$ be a vector with 1 in coordinate $s$ and 0 in all others: $x^{(s,1)} = x + (1 - x_s)e_s$ has the $s$-entry replaced of $x$ by the value 1, and $x^{(s,0)} = x - x_se_s$ has the $s$-entry of $x$ replaced by the value 0; moreover, $x_{-s}$ is the set of edge indicators with entry $s$ removed. Then a (Glauber dynamics) Markov process on $\{0,1\}^N$ is introduced with transition probabilities

$$\mathbb{P}(x \rightarrow x^{(s,1)}) = \frac{1}{N} - \mathbb{P}(x \rightarrow x^{(s,0)}) = \frac{1}{N} q_x(x^{(s,1)}|x)$$
where \(q_X(x^{(s,1)|x_{-s}}) = \mathbb{P}(X_s = 1|X_{-s} = x_{-s})\). For the ERGM(\(\beta, t\)) from Definition 1,
\[
q(x^{(s,1)|x_{-s}}) := \exp \left( \sum_{k=1}^{k} \beta_k t_k(x^{(s,1)}) \right) \times \left( \exp \left( \sum_{k=1}^{k} \beta_k t_k(x^{(s,1)}) \right) + \exp \left( \sum_{k=1}^{k} \beta_k t_k(x^{(s,0)}) \right) \right)^{-1}
\]
and similarly the probability of the new edge being absent exchanges 1 and 0 in this formula to give \(q(x^{(s,0)|x_{-s}})\). For \(h : \{0,1\}^N \rightarrow \mathbb{R}\) let
\[
\Delta_s h(x) = h(x^{(s,1)}) - h(x^{(s,0)}).
\]
The generator \(T_{\beta,t}\) of this Markov process is the desired Stein operator and its expression simplifies to
\[
T_{\beta,t}f(x) = \frac{1}{N} \sum_{s \in [N]} T_s^{(s)}f(x) \quad (4)
\]
with
\[
T_s^{(s)}f(x) = q(x^{(s,1)|x_{-s}})\Delta_s f(x) + \left( f(x^{(s,0)}) - f(x) \right).
\]
When the ERGM is such that the Markov process is irreducible, then its stationary distribution is unique, and if \(\mathbb{E}[T_{\beta,t}f] = 0\) for all smooth test functions \(f\), then \(p\) is the distribution of ERGM(\(\beta, t\)). Thus, the Stein operator characterises ERGM(\(\beta, t\)). Moreover, for each \(s \in [N]\),
\[
\mathbb{E}_q T_s^{(s)}f = 0. \quad (6)
\]
To see this, write
\[
\mathbb{E}_q T_s^{(s)}f = \sum_{x} q(x_{-s}) \left( q(x^{(s,1)|x_{-s}})T_s^{(s)}f(x^{(s,1)}) + q(x^{(s,0)|x_{-s}})T_s^{(s)}f(x^{(s,0)}) \right).
\]
Substituting \(x^{(s,1)}\) and \(x^{(s,0)}\) in (5) gives
\[
q(x^{(s,1)|x_{-s}})T_s^{(s)}f(x^{(s,1)}) + q(x^{(s,0)|x_{-s}})T_s^{(s)}f(x^{(s,0)}) = q(x^{(s,1)|x_{-s}})q(x^{(s,0)|x_{-s}})f(x^{(s,0)}) - f(x^{(s,1)})
\]
and Eq.(6) follows.

Next, we introduce our kernel Stein statistic for testing the goodness-of-fit of an ERGM based on a single observed network as well as an estimator for it which is based on re-sampling of edge indicators.

### 3 Kernel Stein Statistics from RE-SAMPLING

#### Kernel Stein Statistics

Based on the Stein operator representation Eq.(4), we develop the kernel Stein statistics (KSS)\(^1\) for ERGMs. Similar to KSD in Eq.(2), we use the functions in a unit ball of an RKHS \(\mathcal{H}\) as test functions.

The Stein operator in Eq.(4) can be written as expectation over edge variables \(S\) with uniform probability \(\mathbb{P}(S = s) = \frac{1}{N}, \forall s \in [N] := \{1, \ldots, N\}\), independently of \(x\), namely
\[
T_q f(x) = \sum_{s \in [N]} \mathbb{P}(S = s) T_s^{(s)}f(x) =: \mathbb{E}_S[T_q^{(S)}f(x)].
\]
Note that the expectation is taken over \(S\), with the network \(x\) fixed except for the coordinate \(S\).

After algebraic manipulations, Eq.(5) has the form
\[
T_q^{(s)}f(x) = q(x^{(s,1)|x_{-s}})f(x^{(s,1)}) + q(x^{(s,0)|x_{-s}})f(x^{(s,0)}) - f(x) = \mathbb{E}_{[0,1]}[f(X_s,x_{-s})|x_{-s}] - f(x).
\]
Here \(\mathbb{E}_{[0,1]}\) refers to the expectation taken only over the value which \(X_s\) takes on. Hence,
\[
T_q f(x) = \mathbb{E}_S \left[ \mathbb{E}_{[0,1]}[f(X_s, x_{-s})|x_{-s}] \right] - f(x). \quad (8)
\]

For a fixed network \(x\), we seek a function \(f \in \mathcal{H}\), s.t. \([f]_\mathcal{H} \leq 1\), that best distinguishes the difference in Eq.(8) when \(X\) does not have distribution \(q\); this rationale is similar as for Eq.(2). We define the graph kernel Stein statistics (gKSS) as
\[
gKSS(q;x)x = \sup_{\|f\|_\mathcal{H} \leq 1} \left| \mathbb{E}_S[T_q^{(S)}f(x)] \right|. \quad (9)
\]
It is often more convenient to consider \(gKSS^2(q;x)\). Let the RKHS \(\mathcal{H}\) have kernel \(K\) and inner product \((\cdot, \cdot)_\mathcal{H}\). By the reproducing property of RKHS functions, as for Eq.(3), algebraic manipulation allows the supremum to be computed in closed form:
\[
gKSS^2(q;x) = \frac{1}{N^2} \sum_{s,s' \in [N]} h_x(s,s') \quad (10)
\]
where \(h_x(s,s') = \langle T_q^{(s)}K(x, \cdot), T_q^{(s')}K(\cdot, x) \rangle_\mathcal{H}\).

#### Stein Operator from Edge Re-sampling

When the distribution of \(X\) is known, the expectation in Eq.(8) can be computed for networks with a small

\(^1\)We avoid calling it a discrepancy since our expectation is not taken over all ERGM samples as described in Yang et al. [2018], but instead based on a single network.
Apart from using simple kernels beginning with goodness-of-fit test with the supremum in Eq. (12) is achieved by the Markov process which gives rise to the Stein operator. Let $B$ be the fixed number of edges to be re-sampled. Our re-sampled Stein operator is

$$\tilde{T}_q^B f(x) = \frac{1}{B} \sum_{b \in [B]} T_q^{(s_b)} f(x)$$

(11)

where $b \in B$ and $s_b$ are edge samples from $\{1, \ldots, N\}$, chosen uniformly with replacement, independent of each other and of $x$. The expectation of $T_q^B f(x)$ with respect to the re-sampling is

$$E_B[\tilde{T}_q^B f(x)] = E_S[T_q^{(S)} f(x)] = T_q f(x).$$

We introduce the corresponding re-sampling gKSS:

$$\hat{gKSS}(q;x) = \sup_{\|f\|_H \leq 1} \left| \frac{1}{B} \sum_{b \in [B]} T_q^{(s_b)} f(x) \right|.$$  

(12)

The supremum in Eq. (12) is achieved by $f^*(\cdot) = \frac{1}{B} \sum_b T_q^{(s_b)} k(x, \cdot).$ Similar algebraic manipulations as for Eq. (10) yield

$$\hat{gKSS}^2(q;x) = \frac{1}{B^2} \sum_{b,b' \in [B]} h_x(s_b, s_b').$$

(13)

4 GOODNESS-OF-FIT TEST with KERNEL STEIN STATISTICS

4.1 Goodness-of-fit Testing Procedures

We now describe the proposed procedure to assess the goodness-of-fit of an ERGM for a single network observation. The ERGM can be readily simulated from an unnormalised density via MCMC, see for example Morris et al. [2008]. Suppose that $q$ is the distribution of ERGM($\beta, t$) and $x$ is the observed network for which we want to assess the fit to $q$. We simulate independent networks $z_1, \ldots, z_m \sim q$ and compare the observed $gKSS(q;x)$ with the set of $gKSS(q;z_i), i = 1, \ldots, m$ using a Monte Carlo test. As gKSS assesses the deviation from the null distribution, the test is one-sided; we reject the null model when the observed gKSS is large. The detailed test procedure is given in Algorithm 1.

### Algorithm 1 Kernel Stein Test for ERGM

**Input:**
- Observed network $x$;
- Null model $q$;
- RKHS Kernel $K$;
- Re-sample size $B$;
- Confidence level $\alpha$;
- Number of simulated networks $m$;

**Objective:**
- Test $H_0 : x \sim q$ versus $H_1 : x \not\sim q$.

**Test procedure:**
1: Sample $\{s_1, \ldots, s_B\}$ with replacement uniformly from $[N]$.
2: Compute $\tau = \hat{gKSS}^2(q;x)$ in Eq. (13).
3: Simulate $z_1, \ldots, z_m \sim q$.
4: Compute $\tau_i = \hat{gKSS}^2(q;z_i)$ in Eq. (13) again with re-sampling, choosing new samples $\{s_{1,i}, \ldots, s_{B,i}\}$ uniformly from $[N]$ with replacement.
5: Estimate the empirical $(1 - \alpha)$-quantile $\gamma_{1-\alpha}$ of $\tau_1, \ldots, \tau_m$.

**Output:**
- Reject $H_0$ if $\tau > \gamma_{1-\alpha}$; otherwise do not reject.

4.2 Kernel Choices

**Graph kernels** Apart from using simple kernels between adjacency vectors in $\{0,1\}^N$, we apply graph kernels that take into account graph topology via various measures. Various aspects of graph kernels have been studied [Borgwardt and Kriegel, 2005; Vishwanathan et al., 2010; Shervashidze et al., 2011; Sugiyama and Borgwardt, 2015]. We provide a brief review of some graph kernels in the Supplementary Material B. In our implementation in R, we utilise the `ergm` package related to Morris et al. [2008] for simulating ERGMs and the `graphkernels` package associated with Sugiyama et al. [2018] for computing relevant graph kernels.

**Vector-valued RKHS** As the operator in Eq. (8) has embedded a notion of conditional probability, we may tailor the RKHS accordingly. To incorporate the notion of $x_s$ conditioning on $x_{-s}$, we consider a separate treatment of $x_s$ and $x_{-s}$ and introduce a vector-valued reproducing kernel Hilbert Space (vvRKHS). Similar constructions are studied in Jitkrittum et al. [2020] when testing goodness-of-fit for conditional densities. In the Supplementary Material C, we provide a review on the vvRKHS we use as graph kernels; further details can be found in Caponnetto et al. [2008], Carmeli et al. [2010], or Sriperumbudur et al. [2011].

4.3 Theoretical Properties of gKSS

Let $X \sim q$ and $Y \sim \tilde{q}$, where $\tilde{q}$ is the distribution of an appropriately chosen ER graph. Our theoretical approximation argument has three steps: The first step, Theorem 1, is to approximate $gKSS(q, X)$ by...
gKSS(\bar{q}, Y), with an explicit bound on the approximation error, as the number of vertices \( n \to \infty \). Secondly, Theorem 2 provides a normal approximation for gKSS(\bar{q}, Y)^2 of the approximating Bernoulli random graph as \( n \to \infty \), again with an explicit bound, so that approximate confidence bounds for the test under the null hypothesis can be obtained. Finally, a normal approximation for gKSS(q, X)^2 to a normal distribution with approximate mean gKSS(q, X), as \( B \to \infty \) with \( |B/N| \) fixed, is given in Proposition 2, again with an explicit error bound. These three results combined provide explicit control of the type 1 error.

In Chatterjee and Diaconis [2013] and Reinert and Ross [2019] it is shown that under some conditions on the parameters, an ERGM(\beta, t) is close to an approximately chosen Bernoulli random graph, as follows. For \( a \in [0, 1] \), define the following functions [Bhamidi et al., 2011; Eldan and Gross, 2018], with the notation in Definition 1 for ERGM(\beta, t):

\[
\Phi(a) := \sum_{l=1}^{k} \beta_{l} a^{l-1}, \quad \varphi(a) := \frac{1 + \tanh(\Phi(a))}{2}
\]

where \( e_{l} \) is the number of edges in \( H_{l} \). For a polynomial \( f(x) = \sum_{l=0}^{k} c_{l} x^{l} \), set \( |f(x)| := \sum_{l=1}^{k} |c_{l}| e_{l} x^{l} \). Moreover, \( ||f|| \) denotes the supremum norm. The class of ERGM(\beta, t) in this section are assumed to satisfy the following standard technical assumption.

**Assumption 1.** (1) \( \frac{1}{2} |\Phi'(a)|^2 (1 < 1 \). (2) \( \exists a^{*} \in [0, 1] \) that solves the equation \( \varphi(a^{*}) = a^{*} \).

The value \( a^{*} \) will be the edge probability in the approximating Bernoulli random graph, \( \text{ER}(a^{*}) \). Then the following result holds.

**Proposition 1.** [Theorem 1.7 and Corollary 1.10 [Reinert and Ross, 2019]] Let ERGM(\beta, t) satisfy Assumption 1. Let \( X \sim \text{ERGM}(\beta) \) and \( Y \sim \text{ER}(a^{*}) \). Then for \( h : \{0,1\}^{N} \to \mathbb{R} \),

\[
|\mathbb{E}(h(X)) - \mathbb{E}(h(Y))| \leq ||\Delta h||_{N} \frac{C_{a^{*}}(\beta, t, h)}{\sqrt{n}} \sum_{l=2}^{k} \beta_{l}.
\]

Here \( C_{a^{*}}(\beta, t, h) \) is an explicit constant.

Proposition 1 shows, that for large \( n \), the ERGM can be approximated well by an appropriate ER graph for test functions \( h \) which are properly scaled. In particular, if \( H \) is a connected graph and \( h(x) = t(H, x)n^{-|V(H)|} \), then there is an explicit constant \( C = C(\beta, t, H) \) such that

\[
|\mathbb{E}(h(X)) - \mathbb{E}(h(Y))| \leq C/\sqrt{n}.
\]

This result translates into an approximation for the gKSS, as follows.

**Theorem 1.** Let \( q(x) = \text{ERGM}(\beta, t) \) satisfy Assumption 1 and let \( \tilde{q} \) denote the distribution of \( \text{ER}(a^{*}) \).

For \( f \in \mathcal{H} \) equipped with kernel \( K \), let \( f_{\epsilon}^{*} = \frac{1}{(T_{\epsilon} - T_{\epsilon})K(x, \cdot)} \). Then there is an explicit constant \( C = C(\beta, t, K) \) such that for all \( \epsilon > 0 \),

\[
\mathbb{P}(|gKSS(q, X) - gKSS(\tilde{q}, Y)| > \epsilon) \leq \left( \left( ||\Delta gKSS(q, \cdot)||^{2} + ||\Delta gKSS(\tilde{q}, \cdot)|| \right) 4 \frac{n}{C} \right) \frac{C}{\epsilon^{2}}.
\]

As our goodness-of-fit test statistic is based on the square of the gKSS, the asymptotic behaviour of \( gKSS^{2}(\tilde{q}, Y) \) is of interest. To approximate the distribution of \( gKSS^{2} \) under the null hypothesis we make some additional assumptions on kernel \( K \) of RKHS.

**Assumption 2.** Let \( \mathcal{H} \) be the RKHS associated with the kernel \( K : \{0,1\}^{N} \times \{0,1\}^{N} \to \mathbb{R} \) and for \( s \in [N] \) let \( \mathcal{H}_{s} \) be the RKHS associated with the kernel \( l_{s} : \{0,1\} \times \{0,1\} \to \mathbb{R} \). Then

i) \( \mathcal{H} \) is a tensor product RKHS, \( \mathcal{H} = \otimes_{s \in [N]} \mathcal{H}_{s} \);

ii) \( k \) is a product kernel, \( k(x, y) = \otimes_{s \in [N]} l_{s}(x_{s}, y_{s}) \);

iii) \( \langle l_{s}(x_{s}, \cdot), l_{s}(x_{s}, \cdot) \rangle_{\mathcal{H}_{s}} = 1 \);

iv) \( l_{s}(1, \cdot) - l_{s}(0, \cdot) \neq 0 \) for all \( s \in [N] \).

These assumptions are satisfied for example for the suitably standardised Gaussian kernel \( K(x, y) = \exp\left(-\frac{1}{2} \sum_{s \in [N]} (x_{s} - y_{s})^{2} \right) \).

Letting \( || \cdot ||_{1} \) denote \( L_{1} \)-distance, and \( \mathcal{L} \) denote the law of a random variable, in Supplementary Material A, we show the following normal approximation.

**Theorem 2.** Assume that the conditions i) - iv) in Assumption 2 hold. Let \( \mu = \mathbb{E}[gKSS^{2}(\tilde{q}, Y)] \) and \( \sigma^{2} = \text{Var}[gKSS^{2}(\tilde{q}, Y)] \). Set \( W = \frac{1}{2}[gKSS^{2}(\tilde{q}, Y) - \mu) \) and let \( Z \) denote a standard normal variable. Then there is an explicit constant \( C = C(a^{*}, l_{s}, s \in [N]) \) such that

\[
||\mathcal{L}(W) - \mathcal{L}(Z)||_{1} \leq \frac{C}{\sqrt{N}}.
\]

More details on \( \mu \) and \( \sigma^{2} \) are given in the Supplementary Material A. This normal approximation could also be used to assess the asymptotic distribution under an alternative \( x \sim p \) where \( p(x) = \text{ERGM}(\beta', t') \) satisfies Assumption 1 with edge probability \( b' \) and \( b' \neq a^{*} \). Then asymptotically we can compare the corresponding normal random variables with different means.

For the final step, the re-sampling version, let \( k_{s} \) be the number of times that \( s \) is included in the sample \( B \), where \( |B| = B \). Then, from Eq.(13),

\[
gKSS^{2}(\tilde{q}, x) = \frac{1}{B^{2}} \sum_{s, s' \in [N]} k_{s}k_{s'}h_{x}(s, s').
\]
In this expression, the randomness only lies in the counts \( k_s \), where \( s \in [N] \). These counts are exchangeable and \( k = (k_s, s \in [N]) \) follows the multinomial \( (B; N^{-1}, \ldots, N^{-1}) \) distribution. Hence the statistic 
\[
\frac{1}{N^2} \sum_{s,t \in [N]} k_s k_t h_x(s,t)
\]
is a sum of weakly globally dependent random variables, although due to the network \( x \) being fixed, this is not a classical V-statistic. Instead, Stein’s method will be used to prove the following result in the Supplementary Material.

**Proposition 2.** Let 
\[
Y = \frac{1}{B^2} \sum_{s,t \in [N]} (k_s k_t - E(k_s k_t)) h_x(s,t).
\]

Assume that \( h_x \) is bounded such that \( \text{Var}(Y) \) is non-zero. Then if \( Z \) is mean zero normal with variance \( \text{Var}(Y) \), there is an explicitly computable constant \( C > 0 \) such that for all three times continuously differentiable functions \( g \) with bounded derivatives up to order 3,
\[
|E[g(Y)] - E[g(Z)]| \leq \frac{C}{B}.
\]

When the sampling fraction \( F = \frac{B}{N} \) is kept approximately constant as \( N \to \infty \), noting that
\[
\text{gKSS}^2(q; x) = Y + \text{gKSS}^2 + \frac{N-1}{BN^2} \sum_{s \in [N]} h(s,s) - \frac{1}{BN^2} \sum_{s,t \in [N], s \neq t} h(s,t)
\]
the normal approximation for \( \text{gKSS}^2(q; x) \) with approximate mean \( \text{gKSS}^2(q; x) \) follows for \( N \to \infty \).

5 EXPERIMENTS

To assess the performance of the test, we replicate the synthetic benchmark-type settings from [Lusher et al., 2013; Rolls et al., 2015; Yang et al., 2018]. We then apply our tests to three real data networks: Lazega’s lawyer network [Lazega, 2001] and a friendship network [Steglich et al., 2006] which are both studied in [Yin et al., 2019], as well as a co-sponsorship network from [Fowler, 2006a,b].

5.1 Synthetic Experiments

**Model** In the synthetic example, we assess the test performance on relatively simple but useful ERGMs, with three graphs \( H_1 \) in the statistic \( t \), namely edge, 2-star, and triangle; we abbreviate this model as E2ST. Then the unnormalised density has the form
\[
q(x) \propto \exp \left( \beta_1 E_d(x) + \beta_2 S_2(x) + \beta_3 T_r(x) \right), \tag{14}
\]
where \( E_d(x) \) denotes the number of edges in \( x \); \( S_2(x) \) denotes the number of 2-stars in \( x \) and \( T_r(x) \) denotes the number of triangles in \( x \). We choose the null parameter as \( (\beta_1, \beta_2, \beta_3) = (-2, 0, 0, 0.01) \), which satisfies Assumption 1 and gives \( s^* = 0.1176 \). For the alternative distributions, following similar settings in [Yang et al., 2018], we fix the coefficient \( \beta_1 = -2 \) and \( \beta_3 = 0.01 \) of the E2ST model in Eq.(14), and test the null model of \( H_0 : \beta_2 = 0 \) against the alternative \( H_1 : \beta_2 \neq 0 \) with a perturbed \( \beta_2 \) so that the alternative model satisfies Assumption 1 also.

**The Proposed Methods** We apply the proposed goodness-of-fit test procedures and compare with existing approaches. We use the following abbreviations: **gKSS** stands for the proposed test in Algorithm 1; **gKSS_B100** uses Eq.(13) as the test statistic where \( B = 100 \), and **gKSS_n20** denotes testing the problem with \( n = 20 \) vertices. Results shown in Fig. 1 are based on Weisfeiler-Lehman graph kernels [Shervashidze et al., 2011]; results using other kernels are shown in the Supplementary Material Section E. **EdgeKernel** denotes the gKSS with a kernel between binary edges which corresponds to a test based on edge counts. Re-sampling applies, e.g. **EdgeKernel_B100** indicates that 100 edges are re-sampled from the network.

**The Competing Approaches** We list the goodness-of-fit testing methods which serve as comparisons using the following abbreviations. **Degree_full** stands for degree-based tests [Ouadah et al., 2020], where the variance of degree counts on vertices are used as test statistics. The suffix “full” indicates that all vertices are used. The graphical tests for goodness-of-fit from Hunter et al. [2008] simulate the null distribution of a chosen network statistic from the null model as a visual guideline for goodness-of-fit. We quantify this idea by using total variation (TV) distance between distributions of network statistics of choice as test statistics; **mGra** stands for the modified graphical test, where the TV distance is used to compare the distribution of the summary statistics of choice. Full details are provided in the Supplementary Material D. We append **mGra** by the summary statistics used, so that, for example, **mGraDegree** uses the TV distance between degree distributions as test statistics. **Espart** (or es-partners) stands for edgewise shared partner [Hunter et al., 2008]; **MD_Degree** stands for the test based on Mahalanobis distance between chosen summary statistics [Lospinoso and Snijders, 2019]. The suffix after hyphen indicates that the vertex degree is used as network statistics.

**Test Results** The main results are shown in Fig. 1(a). We see that gKSS has higher power than the competitors, while, as expected, larger re-sampling size per-
forms better. A denser networks can be easier to distinguish as higher subgraph counts are available compared to sparser networks. In our experimental set-up, the network size $n = 20$ is relatively small and the null model, with $\beta_1 = -2$, is fairly sparse. We observe that $\text{mGraDegree}$ has slightly higher power than gKSS when $\beta_2 < -0.3$ so that the graph is sparser; it performs poorly when the alternative model is closer to the null, i.e. $|\beta_2|$ small. This may relate to using the TV distance for comparing the degree distribution; the phenomenon does not occur for $\text{MD\_Degree}$. Overall, gKSS is more reliable and has typically higher power compared to these competing methods.

**Increasing Edge Re-sampling Size** B Fig.1(b) shows the test power of large networks up to $n = 1000$ vertices. The results show that the tests achieve maximal power with a relatively small number of re-sampling edges indicators. With the choice of re-sampling size $B$ and good test power with a relatively small number of re-sampled edge indicators, gKSS is applicable to networks with a large number of vertices, beyond the reach of the graphical-based tests [Hunter et al., 2008]. In particular, the proposed tests can be useful in validating model assumptions in practical problems where the networks have a large number of vertices.

**Computational Time** The computational times for each test are shown in Table 1. The gKSS tests are faster than the mGra tests and of similar speed as the less accurate full degree method. The slow mGra tests are based on the computational demanding as well as hard-to-scale estimation associate with the graphical-based method in Hunter et al. [2008]. Its main computational cost stems from simulating the null graphs from ergm to compute the TV distances. Although the $\text{Degree\_full}$ test is supposed to be fast with computational complexity $O(n)$, due to the estimation of the mean and variance of the degree statistics via simulating the null from ergm, its runtime is comparable with gKSS. $\text{B100}$ with complexity $O(B^2)$ for $B = 100$.

<table>
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<tr>
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<tr>
<td>50</td>
<td>44.09</td>
<td>5127.74</td>
<td>5210.40</td>
</tr>
</tbody>
</table>

Table 1: The computational time for each test, in seconds, for 500 trials.

**5.2 Real Data Applications**

Next we apply our test to two benchmark social network data sets which are analysed in Yin et al. [2019]; Lazega’s lawyer network [Lazega, 2001] consists of a network between 36 laywers; the Teenager friendship network [Steglich et al., 2006] is a friendship data set of 50 secondary school students in Glasglow. Moreover, we apply our proposed test to large network, a co-sponsorship network for pieces of legislation in the U.S. Senate from Fowler [2006a,b]. The network data used here are from Schmid and Desmarais [2017] and consists of 2825 vertices and 28813 edges. For all three networks we fit an ER model with the maximum likelihood estimate as edge probability, an E2ST model, and an ER($a^\star$) model using as edge probability $a^\star$ calculated from the E2ST fit, or, for the co-sponsorship
network, calculated from fitting an additional model detailed below. Table 2 summarises the results.

For the Lawyer network, Lazega [2001] suggests an ER model. Our test does not reject this null hypothesis when testing against the best fitted ER graph, with edge probability \( p = 0.055 \), which supports the assumed model. The fitted E2ST model with \( \beta = (-2.8547, -0.0003, 0.6882) \) is rejected at \( \alpha = 0.05 \). This E2ST is close to an ER graph with \( \beta_{E_k} = -2.774 \) and the corresponding ER\((\alpha^*)\) model is not rejected at \( \alpha = 0.05 \).

For the Teenager network, the fitted ER model with \( p = 0.046 \) is rejected at \( \alpha = 0.05 \); for the fitted E2ST model in Eq.(14) with \( \beta = (-2.3029, -0.3445, 2.8240) \) we do not have strong evidence to reject the null at \( \alpha = 0.05 \). The corresponding ER\((\alpha^*)\) model is also not rejected at \( \alpha = 0.05 \). In particular the maximum likelihood estimator does not give the best fitting ER model.

The co-sponsorship network is well fitted by the ER graph with edge probability \( p = 0.0072 \). In contrast, the fitted E2ST with \( \beta = (-6.4126, -0.0240, 2.4684) \), is rejected at \( \alpha = 0.05 \). Additionally we fit the ERGM proposed in Schmid and Desmarais [2017], which includes party homophily [Zhang et al., 2008] and the alternating k-star statistic [Snijders et al., 2006]:

\[
q^*(x) \propto \exp\{\beta_1 E_d(x) + \beta_2 \Gamma(x; P) + \beta_3 S_{alt}(x; \lambda)\}
\]

where \( P \) denotes the party assignment information between the pieces of legislations, and \( \Gamma(x; P) = \sum_{i,j} x_{ij} P_{ij} \) with the k-star count \( S_k(x) \), the alternating k-star statistic is \( S_{alt}(x; \lambda) = \sum_{k=2}^{n-2} (\frac{1}{\lambda})^{k-2} S_k(x) \). We use the model \( q^* \) with parameters fitted in Schmid and Desmarais [2017], \( \beta_1 = -5.884, \beta_2 = 1.440, \beta_3 = 0.124 \), and the parameter in alternating k-stars \( \lambda = 0.4975 \). This model (with p-value=0.022), as well as its corresponding ER\((\alpha^*)\) model are rejected at \( \alpha = 0.05 \).

### 6 CONCLUSIONS AND DIRECTIONS FOR FURTHER WORK

In this paper we provide a novel goodness-of-fit test for exponential random graph models using Stein’s method. A key feature is that the test relies on the observation of only one network. Probabilistic properties of the test statistic are analysed through comparison with Bernoulli random graphs.

Directions for future work include a thorough analysis of the interplay of the graph kernels used in the RKHS and the GKSD. Adaptive methods for tuning graph kernel hyper-parameters would be interesting; see for example Gretton et al. [2012] or Jitkrittum et al. [2017a].

Further, a large contribution to the computational cost of GKSD stems from sampling from the null model; an issue which affects all main methods for assessing goodness-of-fit for exponential random graph models. Developing a goodness-of-fit testing procedure based on a single network observation which does not require simulations from the null model is an exciting future challenge.

Finally, the approach is of independent interest and holds promise for adaptation to other random graph models.

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### References


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<td>0.060</td>
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<td>2825</td>
<td>0.612</td>
<td>0.002</td>
<td>0.036</td>
</tr>
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</table>

Table 2: Rejection rates for real networks. The results marked blue indicate not rejecting and red the null hypothesis at \( \alpha = 0.05 \), using gKSS\(^2\) with \( B = 200 \).
A Stein Goodness-of-fit Test for Exponential Random Graph Models


N. M. Kriege, P.-L. Giscard, and R. Wilson. On valid optimal assignment kernels and applications to


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Supplementary Material

A Proofs and Additional Lemmas

Proof of Theorem 1

For convenience we re-state the theorem here.

**Theorem 1.** Let \( q(x) = \text{ERGM}(\beta, t) \) satisfy Assumption 1 and let \( \bar{q} \) denote the distribution of ER(\( a^* \)). For \( f \in \mathcal{H} \) equipped with kernel \( K \), let \( f_x^* (\cdot) = \frac{\langle (\mathbb{T}_q - \mathbb{T}_{\bar{q}})K(\cdot), \cdot \rangle}{\| (\mathbb{T}_q - \mathbb{T}_{\bar{q}})K(\cdot) \|_H} \). Then there is an explicit constant \( C = C(\beta, t, K) \) such that for all \( \epsilon > 0 \),

\[
P( |g_{\text{KSS}}(q, X) - g_{\text{KSS}}(\bar{q}, Y) | > \epsilon ) \leq \left\{ ||\Delta(g_{\text{KSS}}(q, \cdot))||^2 (1 + ||\Delta g_{\text{KSS}}(q, \cdot)||) + 4 \sup_x ||\Delta f_x^* ||^2 \right\} \left( \frac{n}{2} \right) \frac{C}{\epsilon^2 \sqrt{n}}.
\]

Under the null hypothesis, \( X \sim q \) which is an ERGM satisfying Assumption 1. Let \( Y \sim \bar{q} \), where \( \bar{q} \) is the Bernoulli random graph with edge probability \( a^* \) and \( a^* \) is a solution to the equation in Assumption 1. We use the triangle inequality,

\[
|g_{\text{KSS}}(q, x) - g_{\text{KSS}}(\bar{q}, y)| \leq |g_{\text{KSS}}(q, x) - g_{\text{KSS}}(\bar{q}, x)| + |g_{\text{KSS}}(\bar{q}, y), x) - g_{\text{KSS}}(\bar{q}, y)|.
\]

(15)

This gives rise to two approximation terms. For the first summand in (15), we start with noting that

\[
g_{\text{KSS}}(q, x) = \sup_{f \in \mathcal{H}, ||f|| \leq 1} |\mathbb{T}_q f(x)| = \sup_{f \in \mathcal{H}, ||f|| \leq 1} ||(\mathbb{T}_q - \mathbb{T}_{\bar{q}} + \mathbb{T}_{\bar{q}})f(x)| \leq \sup_{f \in \mathcal{H}, ||f|| \leq 1} ||(\mathbb{T}_q - \mathbb{T}_{\bar{q}})f(x)| + g_{\text{KSS}}(\bar{q}, x)
\]

and this inequality also holds with the roles of \( q \) and \( \bar{q} \) reversed, so that

\[
|g_{\text{KSS}}(q, x) - g_{\text{KSS}}(\bar{q}, x)| \leq \sup_{f \in \mathcal{H}, ||f|| \leq 1} ||(\mathbb{T}_q - \mathbb{T}_{\bar{q}})f(x)| = \sup_{f \in \mathcal{H}, ||f|| \leq 1} ||(f(\cdot), (\mathbb{T}_q - \mathbb{T}_{\bar{q}})k(x, \cdot))_H||
\]

where we used that due to the RKHS property, \( f(x) = \langle f(\cdot), k(x, \cdot) \rangle_H \). Thus we have an explicit form for the optimal \( f_x^* \) in this expression, namely \( f_x^* (\cdot) = (\mathbb{T}_q - \mathbb{T}_{\bar{q}})k(x, \cdot)/(||\mathbb{T}_q - \mathbb{T}_{\bar{q}}||_H, \text{and}
\]

\[
|g_{\text{KSS}}(q, x) - g_{\text{KSS}}(\bar{q}, x)| \leq ||\mathbb{T}_q - \mathbb{T}_{\bar{q}}|| f_x^*(x)|.
\]

Following the steps for the proof of Theorem 1.7 in Reinert and Ross [2019] but working directly with a function \( f \) without using that it is a solution of a Stein equation, it is straightforward to show that for all \( f \in \mathcal{H} \), it holds that for \( Y \sim \bar{q} \),

\[
E(\mathbb{T}_q f(Y) - \mathbb{T}_{\bar{q}} f(Y)) \leq ||\Delta f|| \left( \frac{n}{2} \right) \frac{C(\beta, t)}{\sqrt{n}}
\]

for an explicit constant \( C \) which depends only on the vectors \( \beta \) and \( t \). Moreover inspecting the proof of Lemma 2.4 in Reinert and Ross [2019] the bound is indeed a stronger bound,

\[
\frac{1}{N} \sum_{s \in N} E(\mathbb{T}_q^{(s)} f(Y) - \mathbb{T}_{\bar{q}}^{(s)} f(Y)) \leq ||\Delta f|| \left( \frac{n}{2} \right) \frac{C(\beta, t)}{\sqrt{n}}.
\]

In particular with the crude bound \( ||\mathbb{T}_q^{(s)} - \mathbb{T}_{\bar{q}}^{(s)} f| \leq 2||\Delta f|| \) it follows that

\[
E \left\{ \left( \frac{1}{N} \sum_{s \in N} (\mathbb{T}_q^{(s)} f(Y) - \mathbb{T}_{\bar{q}}^{(s)} f(Y)) \right)^2 \right\} \leq 2||\Delta f||^2 \left( \frac{n}{2} \right) \frac{C(\beta, t)}{\sqrt{n}}.
\]

Thus, using the Chebychev inequality, for all \( \epsilon > 0 \),

\[
P( ||\mathbb{T}_q - \mathbb{T}_{\bar{q}}|| f^*_Y (Y) | > \epsilon ) \leq \frac{1}{\epsilon^2} \text{Var}(||\mathbb{T}_q - \mathbb{T}_{\bar{q}}|| f^*_Y (Y))) \leq 4 \sup_x (||\Delta f_x^* ||^2) \left( \frac{n}{2} \right) \frac{C(\beta, t)}{\epsilon^2 \sqrt{n}}.
\]
Hence
\[ P(|gKSS(q, Y) - gKSS(\hat{q}, Y)| > \epsilon) \leq 4 \sup_{x} (||\Delta f_{x}^{*}\||^{2}) (n/2) C(\beta, t) \frac{e^{2}/\sqrt{n}}. \]

For the second summand in Eq.(15), to bound \( |gKSS(q, X) - gKSS(q, Y)| \) we consider the test function \( h(x) = gKSS(q, x) \) and apply Theorem 1.7 from Reinert and Ross [2019] to give that
\[ |E(gKSS(q, X) - gKSS(q, Y))| \leq ||\Delta gKSS(q, \cdot)|| \frac{n}{(2)^{\frac{C}{\sqrt{n}}}}. \]

Here \( \bar{C} \) is a new constant which depends only on \( \beta \) and \( t \). Similarly we can approximate the square of the expectation using that \( (a - b)^{2} = a^{2} - b^{2} + 2b(b - a) \) and write
\[ E\{(gKSS(q, X) - gKSS(q, Y))^{2}\} = E\{(gKSS(q, X)^{2}\} - E\{(gKSS(q, Y)^{2}\} + 2E\{(gKSS(q, X)gKSS(q, X) - gKSS(q, Y))\}. \]

The first summand can be bounded with Theorem 1.7 from Reinert and Ross [2019] using the test function \( h(x) = gKSS(q, x)^{2} \). For the second summand, we the Cauchy-Schwarz inequality gives
\[ |E\{(gKSS(q, X)(gKSS(q, X) - gKSS(q, Y))\}| \leq \sqrt{E\{(gKSS(q, X)^{2}\}}\frac{1}{2}\sqrt{E\{(gKSS(q, X) - gKSS(q, Y))^{2}\}} \]
As \( |gKSS(q, x)| \leq 1 \) we obtain
\[ E\{(gKSS(q, X) - gKSS(q, Y))^{2}\} \leq E\{(gKSS(q, X)^{2}\} - E\{(gKSS(q, Y)^{2}\} + 2E\{(gKSS(q, X) - gKSS(q, Y)^{2}\} \frac{1}{2}. \]

Solving this quadratic inequality gives
\[ E\{(gKSS(q, X) - gKSS(q, Y))^{2}\} \leq \left( 1 - \sqrt{1 - E\{(gKSS(q, X)^{2}\} - E\{(gKSS(q, Y)^{2}\}}\right)^{2} \]
and \( |E\{(gKSS(q, X)^{2}\} - E\{(gKSS(q, Y)^{2}\} \leq 1 \) we obtain that
\[ E\{(gKSS(q, X) - gKSS(q, Y)^{2}\} \leq \sqrt{E\{(gKSS(q, X)^{2}\} - E\{(gKSS(q, Y)^{2}\}}\]. \]

With Theorem 1.7 from Reinert and Ross [2019] for the test function \( h(x) = gKSS(q, x)^{2} \) we obtain
\[ E\{(gKSS(q, X) - gKSS(q, Y))^{2}\} \leq (||\Delta gKSS(q, \cdot)||^{2})(n/2) \frac{C}{\sqrt{n}}. \]
where \( \bar{C} \) is another constant which depends only on \( \beta \) and \( t \) but not on \( n \). With the Chebychev inequality and the triangle inequality we conclude that there is an explicitly computable constant \( C \) such that for all \( x \)
\[ P(|gKSS(q, X) - gKSS(\hat{q}, Y)| > \epsilon) \leq (\sup_{x}(|\Delta f_{x}^{*}|^{2}) + ||\Delta gKSS(q, \cdot)||^{2})(1 + ||gKSS(q, \cdot)||^{2})(n/2) \frac{C}{e^{2}/\sqrt{n}}. \]
The assertion follows.

For the approximate distribution of \( gKSS(q, Y) \) it is more convenient to consider the square as given in Eq.(10); this is addressed by Theorem 2.

**Proof of Theorem 2**

For convenience we re-state the assumptions and the theorem here.

To approximate the distribution of \( gKSS^{2} \) under the null hypothesis we make the following assumptions (Assumption 2 in the main text) on the kernel \( K \) for the RKHS \( \mathcal{H} \), namely that for \( x, y \in \{0, 1\}^{N} \),

i) \( \mathcal{H} \) is a tensor product RKHS, \( \mathcal{H} = \otimes_{s \in [n]} \mathcal{H}_{s}; \)

ii) \( k \) is a product kernel, \( k(x, y) = \otimes_{s \in [N]} k_{s}(x_{s}, y_{s}); \)

iii) \( \langle l_{s}(x_{s}, \cdot), l_{s}(x_{s}, \cdot) \rangle_{\mathcal{H}_{s}} = 1; \)

iv) \( l_{s}(1, \cdot) - l_{s}(0, \cdot) \neq 0 \) for all \( s \in [N]. \)
Theorem 2. Assume that the conditions i) - iv) in Assumption 2 hold. Let \(\mu = \mathbb{E}[g_{KSS}(\tilde{q}, Y)]\) and \(\sigma^2 = \text{Var}[g_{KSS}(\tilde{q}, Y)]\). Set \(W = \frac{1}{2}(g_{KSS}(\tilde{q}, Y) - \mu)\) and let \(Z\) denote a standard normal variable. Then there is an explicit constant \(C = C(a^*, l_s, s \in [N])\) such that

\[
||\mathcal{L}(W) - \mathcal{L}(Z)||_1 \leq \frac{C}{\sqrt{N}}.
\]

For the Bernoulli random graph distribution \(\tilde{q}\), and \(s \in [N]\),

\[
T_{\tilde{q}}^{(s)} f(x) = a^* f(x^{(s,1)} - f(x)) + (1 - a^*) f(x^{(s,0)} - f(x)).
\]

Thus,

\[
g_{KSS}(\tilde{q}, x) = \frac{1}{N^2} \sum_{s,s' \in [N]} \left\langle T_{\tilde{q}}^{(s)} K(x, \cdot), T_{\tilde{q}}^{(s')} K(x, \cdot) \right\rangle
\]

\[
= \frac{1}{N^2} \sum_{s,s' \in [N]} \left( a^* \left( K(x^{(s,1)}, \cdot) - K(x, \cdot) \right) + (1 - a^*) \left( K(x^{(s,0)}, \cdot) - K(x, \cdot) \right) \right).
\]

Under Assumptions (i), (ii) and (iii) we can write

\[
K(x^{(s,1)}, \cdot) - K(x, \cdot) = (l_s(1, \cdot) - l_s(x_s, \cdot)) \prod_{t \neq s} l_t(x_t, \cdot)
\]

\[
= (1 - x_s)(l_s(1, \cdot) - l_s(0, \cdot)) l_{s'}(x_{s'}, \cdot) \prod_{t \neq s, s'} l_t(x_t, \cdot).
\]

Similarly,

\[
K(x^{(s,0)}, \cdot) - K(x, \cdot) = -x_s(l_s(1, \cdot) - l_s(0, \cdot)) l_{s'}(x_{s'}, \cdot) \prod_{t \neq s, s'} l_t(x_t, \cdot).
\]

Abbreviating \(g(x^{-s,s'}, \cdot) := \prod_{t \neq s, s'} l_t(x_t, \cdot)\) we obtain that

\[
g_{KSS}(\tilde{q}, x) = \frac{1}{N^2} \sum_{s,s' \in [N]} (a^*(1 - x_s) - (1 - a^*)x_s) (a^*(1 - x_{s'}) - (1 - a^*)x_{s'})
\]

\[
\langle (l_s(1, \cdot) - l_s(0, \cdot)) l_{s'}(x_{s'}, \cdot), ((l'_s(1, \cdot) - l'_s(0, \cdot)) l_s(x_s, \cdot)) \rangle (g(x^{-s,s'}, \cdot), g(x^{-s,s'}, \cdot))
\]

\[
= \frac{1}{N^2} \sum_{s,s' \in [N]} (a^* - x_s)(a^* - x_{s'}) \langle (l_s(1, \cdot) - l_s(0, \cdot)) l_{s'}(x_{s'}, \cdot), ((l'_s(1, \cdot) - l'_s(0, \cdot)) l_s(x_s, \cdot)) \rangle
\]

\[
= \frac{1}{N^2} \sum_{s,s' \in [N]} (a^* - x_s)(a^* - x_{s'}) \langle l_s(x_s, \cdot), l_{s'}(x_{s'}, \cdot) \rangle c(s, s')
\]

with

\[c(s, s') = \langle l_s(1, \cdot) - l_s(0, \cdot), l_{s'}(1, \cdot) - l_{s'}(0, \cdot) \rangle \]

not depending on \(x\). Here we used that by assumptions (ii) and (iii), \((g(x^{-s,s'}, \cdot), g(x^{-s,s'}, \cdot)) = 1\). Thus, when replacing \(x\) by \(Y\), a random vector in \(\{0, 1\}^N\) representing a Bernoulli random graph on \(n\) vertices with edge probability \(p\), then \(g_{KSS}(\tilde{q}, Y)\) is an average of locally dependent random variables. Hence, using Stein’s method we obtain a normal approximation with bound, as follows. Let \(I = \{(s, s') : s, s' \in [N]\}\) so that \(|I| = N^2\). For \(\alpha = (s, s') \in I\) set

\[X_\alpha = \frac{1}{N^2} (a^* - Y_s)(a^* - Y_{s'}) \langle l_s(Y_s, \cdot), l_{s'}(Y_{s'}, \cdot) \rangle c(s, s')\]

then

\[g_{KSS}(\tilde{q}, Y) = \sum_{\alpha \in I} X_\alpha\]
and unless $\alpha$ and $\beta$ share at least one vertex, the random variables $X_\alpha$ and $X_\beta$ are independent. Let $\mu_\alpha = E X_\alpha$ and $\sigma^2 = \text{var}(g\text{KSS}(\tilde{q}, Y)))$; these quantities depend on the chosen kernels $l_*$. We use the standardised count

$$W = \sum_{\alpha \in I} \frac{X_\alpha - \mu_\alpha}{\sigma} = \frac{1}{\sigma} g\text{KSS}(\tilde{q}, Y) - \sum_{\alpha \in I} \frac{\mu_\alpha}{\sigma};$$

then $W$ has mean zero, variance 1, and results from Section 4.7 in Chen et al. [2010] apply. In their notation, with $A_{(s,s')} = \{ \beta = (t, t') \in I : \{(s, s') \cap \{t, t'\} \neq \emptyset, \text{condition (LD1) is satisfied. Applying Theorem 4.13, p.134, from Chen et al. [2010] yields that, with } || \cdot ||_1 \text{ denoting } L_1\text{-distance, } L \text{ denoting the law of a random variable, and } Z \text{ denoting a standard normal variable,}$

$$||L(W) - L(Z)||_1 \leq \sqrt{\frac{\pi}{2}} \sum_{\alpha \in I} (\xi_\alpha \eta_\alpha - E(\xi_\alpha \eta_\alpha)) + \sum_{\alpha \in I} E|\xi_\alpha \eta_\alpha^2| \leq \sqrt{\frac{2}{\pi}} \sqrt{\text{var}(\sum_{\alpha \in I} \xi_\alpha \eta_\alpha)} + \sum_{\alpha \in I} E|\xi_\alpha \eta_\alpha^2|.$$  

(16)

with $\xi_\alpha = (X_\alpha - \mu_\alpha)/\sigma$ and $\eta_\alpha = \sum_{\beta \in A_\alpha} X_\beta$.

To obtain the dependence of the bound on $N$ we assess its magnitude. First note that $|A_\alpha| \leq 2N$. Using that by the assumption (iii), $||l_s|| = 1$ for $s \in [N]$ and that $|a^* - Y_s| \leq 1$ we can use the crude bounds $|c(s, s')| \leq 4$, so that $|X_\alpha| \leq \frac{4}{\sqrt{2}}$ and $\mu_\alpha \leq \frac{4}{\sqrt{2}}$. In particular, $|\xi_\alpha| \leq \frac{8}{N\sigma}$ and $|\eta_\alpha| \leq \frac{16}{N\sigma}$. Thus,

$$\sum_{\alpha \in I} E|\xi_\alpha \eta_\alpha^2| \leq N^2 \times \frac{8}{N^2 \sigma} \times \frac{256}{N^2 \sigma^2} = \frac{2048}{N^2 \sigma^3}.$$ 

To evaluate the variance $\sigma^2$,

$$\sigma^2 = \sum_{\alpha \in I} \text{var}X_\alpha + \sum_{\alpha \in I} \sum_{\beta \in A_\alpha} \text{Cov}(X_\alpha, X_\beta).$$

We evaluate these terms in turn. First, if $\alpha = (s, s)$ then

$$\text{var}X_\alpha \leq \frac{c(s, s)^2}{N^4} a^*(1 - a^*)$$

and if $\alpha = (s, s')$ with $s \neq s'$ then as $\langle l_s(x, \cdot), l_{s'}(y, \cdot) \rangle \leq 1$ from the assumption (iii) and the Cauchy-Schwarz inequality,

$$\text{var}X_\alpha \leq E[X_\alpha^2] \leq \frac{c(s, s)^2}{N^4} [a^*(1 - a^*)]^2.$$

Thus,

$$\sum_{\alpha \in I} \text{var}X_\alpha \leq \frac{c(s, s)^2}{N^4} a^*(1 - a^*).$$

Moreover, if $\alpha = (s, s)$ and $\beta = (s, t) \in A_\alpha$ then

$$|\text{Cov}(X_\alpha, X_\beta)| = \left| \frac{c(s, s)c(s, t)}{N^4} \text{E}\{ (a^* - Y_s)^3(a^* - Y_t)(l_s(Y_s, \cdot), l_t(Y_t, \cdot)) \} - \mu_\alpha \mu_\beta \right| \leq 2 \frac{|c(s, s)c(s, t)|}{N^4}$$

and there are order $N^2$ such terms $(\alpha, \beta)$ in the variance. The main contributions to the variance stem from $\text{Cov}(X_\alpha, X_\beta)$ for $\beta \in I_\alpha$ and for $\alpha = (s, s')$ with $s \neq s'$. Assumption (iv) guarantees that $c(s, s') = 0$. Then for $\beta = (s, t)$, with $t \neq s$,

$$\text{Cov}(X_\alpha, X_\beta) = \frac{1}{N^4} c(\alpha)c(\beta)E(a^* - Y_s)^2(a^* - Y_t)(l_s(Y_s, \cdot), l_t(Y_t, \cdot)) \langle l_s(Y_s, \cdot), l_t(Y_t, \cdot) \rangle$$

$$- 1 \frac{1}{N^4} (a^*)^4(1 - a^*)^4 c(s, s') c(s, t)$$

and expanding the expectation gives a contribution of the order $N^{-4}$. The overall contribution of such covariance terms, of which there are order $N^3$, to the variance is hence of order $N^{-1}$, and therefore $\sigma^2$ is of order $N^{-1}$ and $\sigma$ is of order $\sqrt{N}$. 


Similarly,
\[
\text{Var} \left( \sum_{\alpha \in I} \xi_\alpha \eta_\alpha \right) = \text{Var} \left( \sum_{\alpha \in I, \beta \in A_\alpha} \xi_\alpha \xi_\beta \right) = \sum_{\alpha \in I} \sum_{\beta \in A_\alpha} \sum_{\gamma \in I} \sum_{\delta \in A_\gamma} \text{Cov}(\xi_\alpha \xi_\beta, \xi_\gamma \xi_\delta)
\]
is dominated by the covariances between \(\xi_\alpha \xi_\beta\) and \(\xi_\gamma \xi_\delta\) such that \(\alpha\) and \(\beta\) involve three distinct indices \(s, s', t,\) and \(\gamma\) and \(\delta\) involve three distinct indices \(r, r', u,\) and these two sets of three indices have non-zero intersection. These summands give a contribution of order \(N^3/\sigma^4 N^8\), which is of order \(N^{-1}\), to the variance \(\text{Var}(\sum_{\alpha \in I} \xi_\alpha \eta_\alpha)\). A crude bound is obtained as \(\text{Var}(\sum_{\alpha \in I} \xi_\alpha \eta_\alpha) \leq \frac{512}{\pi^4 N^6}\). These estimates give that the bound in Eq. (16) is of the order \(N^{-\frac{1}{2}}\).

All moment expressions can be bounded explicitly and thus the constant \(C\) can be computed explicitly. The conclusion follows.

**Proof of Proposition 2**

For convenience we re-state the result here again.

**Proposition 2.** Let
\[
Y = \frac{1}{B^2} \sum_{s,t \in [N]} (k_s k_t - \mathbb{E}(k_s k_t)) h_x(s,t).
\]
Assume that \(h_x\) is bounded such that \(\text{Var}(Y)\) is non-zero. Then if \(Z\) is mean zero normal with variance \(\text{Var}(Y)\), there is an explicitly computable constant \(C > 0\) such that for all three times continuously differentiable functions \(g\) with bounded derivatives up to order 3,
\[
|\mathbb{E}[g(Y)] - \mathbb{E}[g(Z)]| \leq \frac{C}{B}.
\]

For normal approximation in the presence of weak dependence, Charles Stein [Stein, 1986] introduced the method of exchangeable pairs: construct a sum \(W'\) such that \((W, W')\) form an exchangeable pair, and such that \(\mathbb{E}^W(W' - W)\) is (at least approximately) linear in \(W\). This linearity condition arises naturally when thinking of correlated bivariate normals. As a multivariate generalisation, Reinert and Röllin [2009] considered the general setting that
\[
\mathbb{E}^W(W' - W) = -\Lambda W + R
\]
for a matrix \(\Lambda\) and a vector \(R\) with small \(\mathbb{E}|R|\) is treated. In a followup paper [Meckes, 2009] the results by Chatterjee and Meckes [2008] and Reinert and Röllin [2009] are combined using slightly different smoothness conditions on test functions as compared to Reinert and Röllin [2009]. In Reinert and Röllin [2009] it was found that a statistic of interest can often be embedded into a larger vector of statistics such that (17) holds with \(R = 0\); this embedding does not directly correspond to Hoeffding projections, although it is related to the latter. In Reinert and Röllin [2010] this embedding is applied to complete non-degenerate U-statistics. Among other examples. In this example the limiting covariance matrix is not of full rank; yet the bounds on the normal approximation are of the expected order.

The general setup is as follows. Denote by \(W = (W_1, W_2, \ldots, W_d)^t\) random vectors in \(\mathbb{R}^d\), where \(W_i\) are \(\mathbb{R}\)-values random variables for \(i = 1, \ldots, d\). We denote by \(\Sigma\) symmetric, non-negative definite matrices, and hence by \(\Sigma^{1/2}\) the unique symmetric square root of \(\Sigma\). Denote by \(\text{Id}\) the identity matrix, where we omit the dimension \(d\). Let \(Z\) denote a random variable having standard \(d\)-dimensional multivariate normal distribution. We abbreviate the transpose of the inverse of a matrix \(\Lambda\) as \(\Lambda^{-t} := (\Lambda^{-1})^t\).

For derivatives of smooth functions \(h : \mathbb{R}^d \to \mathbb{R}\), we use the notation \(\nabla\) for the gradient operator. Denote by \(|\cdot|\) the supremum norm for both functions and matrices. If the corresponding derivatives exist for some function \(g : \mathbb{R}^d \to \mathbb{R}\), we abbreviate \(|g_1| := \sup |\frac{\partial}{\partial x_i} g|\), \(|g_2| := \sup_{i,j} |\frac{\partial^2}{\partial x_i \partial x_j} g|\), and so on.

The following result is shown in Reinert and Röllin [2009].

**Theorem A.1** (c.f. Theorem 2.1 Reinert and Röllin [2009]). Assume that \((W, W')\) is an exchangeable pair of \(\mathbb{R}^d\)-valued random variables such that
\[
\mathbb{E}W = 0, \quad \mathbb{E}WW^t = \Sigma,
\]
with $\sum \in \mathbb{R}^{d \times d}$ symmetric and positive definite. Suppose further that (17) is satisfied for an invertible matrix $\Lambda$ and a $\sigma(W)$-measurable random variable $R$. Then, if $Z$ has $d$-dimensional standard normal distribution, we have for every three times differentiable function $g$

\[ |\mathbb{E}g(W) - \mathbb{E}g(\Sigma^{1/2}Z)| \leq \frac{|g|_2}{4} I + \frac{|g|_2}{12} II + \left( |g|_1 + \frac{1}{2}d\|\Sigma\|^{1/2}|g|_2 \right) III, \]

where, with $\lambda^{(i)} = \sum_{m=1}^{d} |(\Lambda^{-1})_{m,i}|$,

\[
I = \sum_{i,j=1}^{d} \lambda^{(i)} \sqrt{\text{Var}_W(W_i' - W_i)(W_j' - W_j)},
\]

\[
II = \sum_{i,j,k=1}^{d} \lambda^{(i)} \mathbb{E}|(W_i' - W_i)(W_j' - W_j)(W_k' - W_k)|,
\]

\[
III = \sum_{i} \lambda^{(i)} \sqrt{\mathbb{E}R_i^2}.
\]

Here we use the approach for statistics of the form $Y = \frac{1}{B^2} \sum_{s,t \in [N]} (k_s k_t - \mathbb{E}(k_s k_t)) h(s,t)$. The subscript $x$ is suppressed in $h_x$ to simplify notation. To apply Theorem A.1 we employ two additional statistics; including $Y$ as $W_1$,

\[
W_1 = \frac{1}{B^2} \sum_{s,t \in [N]} (k_s k_t - \mathbb{E}(k_s k_t)) h(s,t)
\]

\[
W_2 = \frac{1}{B^2} \sum_{s,t \in [N]} (k_s - \mathbb{E}(k_s)) h(s,t)
\]

\[
W_3 = \frac{1}{B^2} \sum_{s \in [N]} (k_s - \mathbb{E}(k_s)) h(s,s).
\]

Given $k = (k_1, \ldots, k_N)$ we construct an exchangeable pair $(k, k')$ by choosing an index $I \in [N]$ such that $\mathbb{P}(I = i) = \frac{k_i}{\|k\|^2}$ and if $I = i$ we set $k_i' = k_i - 1$ (we take a ball out of bin $i$ in the multinomial construction). Then we pick $J \in [N]$ uniformly and if $J = j$ we set $k_j' = k_j + 1$ - we add the ball to bin $j$ which we took away from bin $i$. All other $k_l'$s are left unchanged; $k_l' = k_l$ if $l \neq I, J$. Note that $I = J$ is possible in which case there is no change. Based on this exchangeable pair we set

\[
W_1' = \frac{1}{B^2} \sum_{s,t \in [N]} (k'_s k'_t - \mathbb{E}(k'_s k'_t)) h(s,t)
\]

\[
W_2' = \frac{1}{B^2} \sum_{s,t \in [N]} (k'_s - \mathbb{E}(k'_s)) h(s,t)
\]

\[
W_3' = \frac{1}{B^2} \sum_{s \in [N]} (k'_s - \mathbb{E}(k'_s)) h(s,s).
\]

With $W = (W_1, W_2, W_3)$ and $W' = (W_1', W_2', W_3')$ we have obtained an exchangeable pair $(W, W')$. Moreover $W$ has mean zero and finite covariance matrix. First we calculate $\mathbb{E}^W (W' - W)$ componentwise, starting with the easiest case to illustrate the argument. For this calculation we use that

\[
k'_I - k_I = -1
\]

\[
k'_J - k_J = 1
\]

\[
k'_s k'_t - k_s k_t = (k'_s - k_s)(k'_t - k_t) + k_s(k'_t - k_t) + k_t(k'_s - k_s).
\]
Then, conditioning on $I$ and $J$,
\[
\mathbb{E}^W(W_3' - W_3) = \frac{1}{B^2} \sum_{s \in [N]} \mathbb{E}^W(k'_s - k_s)h(s, s)
\]
\[
= \frac{1}{B^2} \frac{1}{BN} \sum_{s \in [N]} \sum_{i \in [N]} \sum_{j \in [N]} k_i \sum_{j \in [N]} (-1(s = i)h(i, i) + 1(s = j)h(j, j))
\]
\[
= -\frac{1}{B^2} \frac{1}{B} \sum_{i \in [N]} k_i h(i, i) + \frac{1}{N} \frac{1}{B^2} \sum_{j \in [N]} h(j, j)
\]
\[
= -\frac{1}{B^2} \frac{1}{B} \sum_{i \in [N]} (k_i - \mathbb{E}(k_i))h(i, i)
\]
\[
= -\frac{1}{B} W_3.
\]
Similar arguments yield $\mathbb{E}^W(W_2' - W_2) = -\frac{1}{B} W_2$. Finally,
\[
\mathbb{E}^W(W_1' - W_1) = \frac{1}{B^2} \sum_{s,t \in [N]} \mathbb{E}^W(k'_s k'_t - k_s k_t)h(s, t)
\]
\[
= \frac{1}{B^2} \sum_{s,t \in [N]} \mathbb{E}^W[(k'_s - k_s)(k'_t - k_t) + k_s(k'_t - k_t) + k_t(k'_s - k_s)]h(s, t)
\]
\[
= \frac{1}{B^2} \sum_{s,t \in [N]} \mathbb{E}^W[(k'_s - k_s)(k'_t - k_t)]h(s, t) + 2 \sum_{s,t \in [N]} \mathbb{E}^W[k_i(k'_i - k_i)]h(s, t).
\]
Here we used that $h(s, t) = h(t, s)$ in the last step. We tackle the conditional expectations separately. Again using $h(s, t) = h(t, s)$,
\[
\sum_{s,t \in [N]} \mathbb{E}^W[(k'_s - k_s)(k'_t - k_t)]h(s, t)
\]
\[
= \frac{1}{BN} \sum_{s,t \in [N]} \sum_{i \in [N]} \sum_{j \in [N]} k_i \sum_{j \in [N]} (1(s = I, t = J) + 1(s = J, t = I))(k'_s - k_s)(k'_t - k_t)h(s, t)
\]
\[
= -\frac{2}{BN} \sum_{i \in [N]} \sum_{j \in [N]} 1(i \neq j)h(i, j)
\]
\[
= -\frac{2}{BN} \sum_{i \in [N]} \sum_{j \in [N]} k_i h(i, j) + \frac{2}{BN} \sum_{i \in [N]} k_i h(i, i)
\]
\[
= -\frac{2}{BN} W_2 + \frac{2}{BN} W_3.
\]
Here the centering terms from $W_2$ and $W_3$ add up to 0 because the conditional expectation has mean zero, and are thus not included in the calculation.

Moreover,
\[
\sum_{s,t \in [N]} \mathbb{E}^W[k_i(k'_i - k_i)]h(s, t)
\]
\[
= \frac{1}{BN} \sum_{s,t \in [N]} \sum_{i \in [N]} \sum_{j \in [N]} k_i \sum_{j \in [N]} (-1(s = i)k_i h(i, t) + 1(s = j)k_i h(j, t))
\]
\[
= -\frac{1}{B} \sum_{i \in [N]} \sum_{j \in [N]} k_i k_i h(i, t) + \frac{1}{N} \sum_{i \in [N]} \sum_{j \in [N]} k_i h(j, t)
\]
\[
= -\frac{1}{B} W_1 + \frac{1}{N} W_2.
\]
The largest variance contribution is from

Due to the exchangeable pair construction many sums simplify and the largest contribution to the variance is

Instead of conditioning on $W$ we condition on $W$. This conditioning would only increase the conditional variance.

Hence (17) is satisfied with $R = 0$ and

Hence

\[ \Lambda = \frac{1}{B} \begin{bmatrix} -2 & 2 \frac{(B-1)}{N} & \frac{2}{N} \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \]

giving

\[ \lambda^{(1)} = \frac{B}{2}; \; \lambda^{(2)} = B \frac{N - B + 1}{N}; \; \lambda^{(3)} = B \frac{N + 1}{N}. \]

With $B = FN$ we can bound

\[ \lambda^{(i)} \leq \max(F,1/2)B; \quad i = 1, 2, 3. \]

To complete the argument we need to bound $I$ and $II$ from Theorem A.1.

To bound the conditional variance term $I$ from Theorem A.1,

\[ I = \sum_{i,j=1}^{3} \lambda^{(i)} \sqrt{\text{Var} \, \mathbb{E}^W(W'_i - W_i)(W'_j - W_j)} \leq \max(F,1/2)B \sum_{i,j=1}^{3} \sqrt{\text{Var} \, \mathbb{E}^W(W'_i - W_i)(W'_j - W_j)}. \]

Instead of conditioning on $W$ we condition on $k$. This conditioning would only increase the conditional variance. The largest variance contribution is from

\[ \mathbb{E}^k(W'_i - W_i)^2 \]

\[ = \frac{1}{B^4} \sum_{u,v} \sum_{u,v} \mathbb{E}^k[(k'_u k'_v - k_u k_v)(k'_u k'_v - k_u k_v)h(s,t)h(u,v)] \]

\[ = \frac{1}{B^4} \sum_{i,j} \sum_{u,v} \mathbb{E}^k[k_i ((k'_u - k_u)(k'_v - k_v) + 2k_u(k'_v - k_v)) \times \]

\[ (k'_u - k_u)(k'_v - k_v) + 2k_u(k'_v - k_v))h(s,t)h(u,v)] \]

\[ = \frac{1}{B^4} \sum_{i,j} \sum_{u,v} \mathbb{E}^k[k_i(k'_u - k_u)(k'_v - k_v)(k'_u - k_v)h(s,t)h(u,v)] \]

Due to the exchangeable pair construction many sums simplify and the largest contribution to the variance is
the last term;

\[
\begin{align*}
&4 \frac{1}{B^4} \frac{1}{BN} \sum_{i \in \mathbb{N}} \sum_{j \in \mathbb{N}} \sum_{s,t \in \mathbb{N}} \sum_{u,v \in \mathbb{N}} \mathbb{E}^k [k_i k_s k_u (k'_i - k_t)(k'_u - k_v) h(s, t) h(u, v)] \\
&= 4 \frac{1}{B^3 N} \sum_{i \in \mathbb{N}} \sum_{j \in \mathbb{N}} \sum_{s,t \in \mathbb{N}} \sum_{u,v \in \mathbb{N}} \mathbb{E}^k [k_i k_s k_u (k'_i - k_t)(k'_u - k_v) h(s, t) h(u, v)] (1 = i) + 1 (t = j) \\
&= -4 \frac{1}{B^3 N} \sum_{i \in \mathbb{N}} \sum_{j \in \mathbb{N}} \sum_{s,t \in \mathbb{N}} \sum_{u,v \in \mathbb{N}} \mathbb{E}^k [k_i k_s k_u (k'_i - k_u) h(s, i) h(u, v)] (1 = i) + 1 (v = j) \\
&\quad + 4 \frac{1}{B^3 N} \sum_{i \in \mathbb{N}} \sum_{j \in \mathbb{N}} \sum_{s, t \in \mathbb{N}} \sum_{u,v \in \mathbb{N}} \mathbb{E}^k [k_i k_s k_u (k'_i - k_v) h(s, j) h(u, v)] (1 = i) + 1 (v = j) \\
&= 4 \frac{1}{B^3 N} \sum_{i \in \mathbb{N}} \sum_{j \in \mathbb{N}} \sum_{s \in \mathbb{N}} \sum_{u,v \in \mathbb{N}} k_i k_s k_u h(s, i) h(u, j) - 4 \frac{1}{B^3 N} \sum_{i \in \mathbb{N}} \sum_{j \in \mathbb{N}} \sum_{s \in \mathbb{N}} \sum_{u,v \in \mathbb{N}} k_i k_s k_u h(s, j) h(u, i) \\
&\quad + 4 \frac{1}{B^3 N} B \sum_{j \in \mathbb{N}} \sum_{s \in \mathbb{N}} \sum_{u,v \in \mathbb{N}} k_i k_s k_u h(s, j) h(u, j).
\end{align*}
\]

These terms have a variance contribution of order \(\frac{1}{B^4 N^2} B^6 N^8\) as long as \(h(i, j)\) is bounded. The mixed variances in \(I\) can be bounded using the Cauchy-Schwarz inequality. Overall the contribution to the term \(I\) of Theorem A.1 is thus of order \(B\sqrt{\frac{1}{B^2}} = \frac{1}{B}\).

For the term \(II\) of Theorem A.1,

\[
\sum_{a,b,c=1}^3 \chi^{(a)} \mathbb{E} \left| (W_a - W_b)(W_b - W_b)(W_c - W_c) \right| \leq \max(F, 1/2) B \sum_{a,b,c=1}^3 \mathbb{E} \left| (W_a - W_b)(W_b - W_b)(W_c - W_c) \right|.
\]

The largest contribution to this term is

\[
\begin{align*}
\mathbb{E} \left| (W_1 - W_1)^3 \right| \\
\leq \frac{1}{B} \frac{1}{B^3 N} \sum_{s,t \in \mathbb{N}} \sum_{u,v \in \mathbb{N}} \sum_{x,y \in \mathbb{N}} \mathbb{E} \left| (k'_s k'_t - k_s k_t)(k'_u k'_v - k_u k_v)(k'_x k'_y - k_x k_y) \right|
\leq \frac{1}{B} \frac{1}{B^3 N} \sum_{i \in \mathbb{N}} \sum_{j \in \mathbb{N}} \sum_{s,t \in \mathbb{N}} \sum_{u,v \in \mathbb{N}} \sum_{x,y \in \mathbb{N}} \mathbb{E} \left| k_i ((k'_s - k_s)(k'_t - k_t) + 2 k_s (k'_t - k_t)) \right.
\left. (k'_u - k_u)(k'_v - k_v) + 2 k_u (k'_v - k_v))) \right| (k'_x - k_x)(k'_y - k_y) + 2 k_x (k'_y - k_y)) \right| \\
\leq \frac{8}{B^2} \frac{1}{B^3 N} \sum_{i \in \mathbb{N}} \sum_{j \in \mathbb{N}} \sum_{s,t \in \mathbb{N}} \sum_{u,v \in \mathbb{N}} \sum_{x,y \in \mathbb{N}} \mathbb{E} \left| k_i ((k'_s - k_s)(k'_t - k_t) + 2 k_s (k'_t - k_t)) \right.
\left. (k'_u - k_u)(k'_v - k_v) + 2 k_u (k'_v - k_v))) \right| (k'_x - k_x)(k'_y - k_y) + 2 k_x (k'_y - k_y)) \right|.
\end{align*}
\]

With \(\|h\| = \max_{i,j} |h(i,j)|\) the leading term in this expression is

\[
\frac{8}{B^2} \frac{1}{B^3 N} \sum_{i \in \mathbb{N}} \sum_{j \in \mathbb{N}} \sum_{s,t \in \mathbb{N}} \sum_{u,v \in \mathbb{N}} \sum_{x,y \in \mathbb{N}} \mathbb{E} \left| k_i k_s k_u (k'_i - k_t) k_u(k'_u - k_v) (k'_y - k_y) \right|.
\]

Now, not all of \(t, v, y\) can be distinct for a non-zero contribution to this term; we can bound it by

\[
\frac{16}{B^2} \frac{1}{B^3 N} \sum_{i,j,t,u,v,x} \mathbb{E} k_i k_s k_u k_x (1(t = i) + 1(t = j))(1(v = i) + 1(v = j)) \leq \frac{64}{\|h\|^3 B^3}.
\]

Here we used that \(\sum_i k_i = B\). All other cross-expectations can be bounded using the Cauchy-Schwarz inequality. Hence we conclude that the term \(II\) in Theorem A.1 is of order \(B^{-2}\). All higher moments can be bounded explicitly and hence \(C\) can be bounded explicitly. The conclusion follows.
B Graph Kernels

For a vertex-labeled graph \( x = \{x_{ij}\} \) \( 1 \leq i, j \leq n \in \mathcal{G}^{lab} \), with label range \{1, \ldots, c\} = [c], denote the vertex set by \( V \), the edge set by \( E \), and the label set by \( \Sigma \). Consider an vertex-edge mapping \( \psi : V \cup E \rightarrow [c] \). In this paper we use the following graph kernels.

**Vertex-Edge Histogram Gaussian Kernels** The **vertex-edge label histogram** \( h = (h^{11}, h^{211}, \ldots, h^{ccc}) \) = \( h(\psi, x) \) has as components \( h^{l_1l_2l_3} = |\{v \in V, (v, u) \in E \mid \psi(v, u) = l_1, \psi(u) = l_2, \psi(v) = l_3\}| \), for \( l_1, l_2, l_3 \in [c] \); it is a combination of vertex label counts and edge label counts. Let \( h(x), h(x') = \sum_{l_1,l_2,l_3} \sigma^{l_1,l_2,l_3} h(x)^{l_1,l_2,l_3} h(x')^{l_1,l_2,l_3} \). Following Sugiyama and Borgwardt [2015], we define the vertex-edge histogram Gaussian (VEG) kernel between two graphs \( x, x' \) as

\[
K_{VEG}(x, x'; \sigma) = \exp \left\{ -\frac{\| h(x) - h(x') \|^2}{2\sigma^2} \right\}.
\]

The VEG kernel is a special case of histogram-based kernels for assessing graph similarity using feature maps, which are introduced in Kriege et al. [2016]. Adding a Gaussian RBF as in Sugiyama and Borgwardt [2015], yielding the VEG kernel, significantly improved problems such as classification accuracy, see [Kriege et al., 2020]. In our implementation, as in Sugiyama et al. [2018], \( \psi \) is induced by the vertex index. If the vertices are indexed by \( i \in [n] \) then the label of vertex \( v_i \) is \( \psi(v_i) = i \); for edges, \( \psi(u, v) = 1 \) if \( (u, v) \in E \) is an edge and 0 otherwise.

**Geometric Random Walk Graph Kernels** A \( k \)-step random walk graph kernel [Sugiyama and Borgwardt, 2015] is built as follows. Take \( A_\otimes \) as the adjacency matrix of the direct (tensor) product \( G_\otimes = (V_\otimes, E_\otimes, \psi_\otimes) \) [Gärtner et al., 2003] between \( x \) and \( x' \) such that vertex labels match and edge labels match:

\[
\begin{align*}
V_\otimes &= \{(v, v') \in V \times V' \mid \psi(v) = \psi'(v')\}, \\
E_\otimes &= \{((v, u), (v', u')) \mid E \times E' \mid \psi(v, u) = \psi(v', u')\},
\end{align*}
\]

and use the corresponding label mapping \( \psi_\otimes(v, v') = \psi(v) = \psi'(v') \); \( \psi_\otimes((v, v'), (u, u')) = \psi(v, u) = \psi'(v', u') \).

With input parameters \( (\lambda_0, \ldots, \lambda_k) \), the \( k \)-step random walk kernel between two graphs \( x, x' \) is defined as

\[
K^k_\otimes(x, x') = \left[ \sum_{i,j=1}^{\mid V_\otimes \mid} \sum_{t=0}^{k} \lambda_t A_\otimes^t \right]_{i,j}.
\]

A geometric random walk kernel between two graphs \( x, x' \) takes the \( \lambda \)-weighted infinite sum from the \( k \) step random walk kernels:

\[
K_{GRW}(x, x') = \sum_{i,j=1}^{\mid V_\otimes \mid} \left[ (I - \lambda A_\otimes)^{-1} \right]_{i,j}.
\]

In our implementation we choose, \( \lambda_l = \lambda, \forall l = 1, \ldots, k \) and \( \lambda = \frac{1}{2} \).

**Shortest Path Graph Kernels** Shortest Path Graph Kernels, introduced by Borgwardt and Kriege [2005], are based on a transformation of the graph \( x \), the Floyd transformation. The Floyd transformation \( F \) turns the original graph into the so-called shortest-path graph \( y = F(x) \); the graph \( y \) is a complete graph with vertex set \( V \) with each edge labelled by the shortest distance in \( x \) between the vertices on either end of the edge. For two networks \( x \) and \( x' \) the 1-step random walk kernel \( K^1_\otimes \) between the shortest-path graphs \( y = F(x) \) and \( y' = F(x') \) gives the shortest-path (SP) kernel between \( x \) and \( x' \):

\[
K_{SP}(x, x') = K^1_\otimes(y, y').
\]

Lemma 3 in Borgwardt and Kriege [2005] showed that this kernel is positive definite.

**Weisfeiler-Lehman Graph Kernels** Weisfeiler-Lehman Graph Kernels have been proposed by Shervashidze et al. [2011]; these kernels are based on the Weisfeiler-Lehman test for graph isomorphisms and involve counting matching subtrees between two given graphs. Theorem 3 in Shervashidze et al. [2011] showed the positive definiteness of these kernels. In our implementation, we adapted an efficient implementation from the graphkernel package [Sugiyama et al., 2018].
C Vector-Valued RKHS

The general set-up for vector-valued RKHS for finite networks is as follows. Let \( N = \binom{s}{2} \) denote the index set of vertex pairs in a graph \( x \in \{0, 1\}^N \). For \( s \in [N] \) let \( x^{-s} \in \{0, 1\}^{N-1} : X^{-s} \) denote the collection of edge indicators except the one for \( s \) and let \( x_s \in \{0, 1\} : X^s \) denote the edge indicator for \( s \). When the underlying graph is random, we use similar notation \( X^{-s}, X^s \) to denote the corresponding random variables. For \( s \in [N] \), let \( l_s : \mathcal{X}^s \times \mathcal{X}^s \rightarrow \mathbb{R} \) be reproducing kernels, with associated RKHS \( \mathcal{H}_{l_s} \). Let \( \varphi_s : x_s \in \mathcal{X}^s \mapsto l_s(\cdot, x^s) \in \mathcal{H}_{l_s} \) denote the corresponding feature maps of \( (l_s)_{s\in [N]} \).

The RKHS kernels \( l_s \), or those used in Chwialkowski et al. [2016] or Liu et al. [2016], have scalar outputs, while the RKHS kernel \( \ell_{-s} \) has an output in \( \mathcal{L}(\mathcal{H}_{l_s}) \), the Banach space of bounded operators from \( \mathcal{H}_{l_s} \) to \( \mathcal{H}_{l_s} \); we refer to the space \( \mathcal{H}_{l_s} \) for \( \ell_{-s} \) as a vector-valued RKHS (vvRKHS). All the kernels used here are assumed to be positive definite and bounded. As composition preserves positive definiteness, we then consider the kernel: \( K : (\mathcal{X}^s \otimes \mathcal{X}^{-s}) \times (\mathcal{X}^s \otimes \mathcal{X}^{-s}) \rightarrow \mathbb{R} \), with associate RKHS \( \mathcal{H}_K \).

In our experiments we assume that the \( l_s \) corresponds to the same RKHS function: \( l_s \equiv l, \forall s \in [N] \). We further assume the vvRKHS \( \mathcal{H}_l \) has the form

\[
\ell(x^{-s}, (x')^{-s'}) = k(x^{-s}, (x')^{-s'}) I_{\mathcal{H}_l \times \mathcal{H}_l},
\]

where \( I_{\mathcal{H}_l \times \mathcal{H}_l} \) is the identity map from \( \mathcal{H}_l \) to \( \mathcal{H}_l \) and \( k \) is the graph kernel of choice. The RKHS defined via composition reads

\[
K((x^s, x^{-s}), ((x')^{s'}, (x')^{-s'})) = k(x^{-s}, (x')^{-s'}) l((x^s, (x')^{s'}).)
\]

For a single observed network \( x \), as \( \mathcal{H}_l \), \( \mathcal{H}_l \) are the same for all \( s \), it holds that for \( s, s' \in [N] \):

\[
K((x^s, x^{-s}), (x'^{s'}, x'^{-s'})) = l(x^s, x'^{s'}).)
\]

In our implementation we use the kernels \( k(x^{-s}, \cdot) = k(x^{(s,1)}, \cdot) + k(x^{(s,0)}, \cdot) \) from Section B, defined not on the whole graph \( x \) but on the set \( x^{-s} \).

D Additional Details on Distance-based Test Statistics

D.1 Modified Graphical Tests with Total-Variation Distance

Here we give the details of the modified graphical tests based on Total-Variation (TV) distance, \texttt{mGra}, presented in Section 5. To assess the goodness-of-fit to a specific ERGM, Hunter et al. [2008] proposed to compare network statistics from the observed network to those of simulated networks from the null model via box plots and Monte-Carlo \( p \)-values. These network statistics are

- the degree distribution, with \( d_k \) the number of vertices which have degree \( k \);
- the number of edge-wise shared partners, which is the number of pairs of vertices which are neighbours and which have exactly \( k \) common neighbours;
- the number of dyad-wise shared partners, which is the number of pairs of vertices which have exactly \( k \) common neighbours (but are not necessarily themselves neighbours);
- the triad census, with 4 possible triads where triads are configurations on 3 vertices; the configurations are 0 edges, 1 edge, 2 edges and 3 edges;
- the statistics which are included in the ERGM as in Definition 1.

Fig. 2 shows an example of a graphical test based on the E2ST model Eq.(14) with the 2-star coefficient \( \beta_2 \) perturbed. By comparing whether the observed statistics (the bold line) deviates from the simulated null, one can visually assess whether the null hypothesis should be rejected. For instance, in Fig. 2(a) where the network is generated from the null distribution, the observed network statistics are all within the range in which 95 percent of the simulated observations fall.
(b) A small perturbation of the null model

(c) A moderate perturbation of the null model

(d) A larger perturbation of the null model

Figure 2: Graphical Tests with different beta parameters

When the difference between the null distribution and the distribution which generates the data is small, the graphical method may not easily distinguish the two models depending on the network statistics of choice. As shown in Fig. 2(b), with a network from a model with small perturbation from the null distribution, we see this effect. However, when the difference between data simulated under the null distribution and the data is substantial enough, we can see, e.g. from Fig. 2(c), that the minimum geodesic distance and the triad census from the observed network clearly differ from the simulated null, and the null hypothesis can be rejected. The box plots are also used to carry out Monte Carlo tests for each possible observation (for example a specific triad count) by giving a p-value for this specific test.

While every observed value can be used for a Monte Carlo test, Hunter et al. [2008] does not provide a systematic procedure to reach an overall conclusion about rejection. For instance, it is not clear whether the null is to be rejected when Fig. 2(d) is observed. To surpass such issue, we further develop the testing procedure by using the TV distance between distributions for the observed and simulated distributions of the summary statistics from Hunter et al. [2008]. Denote by $S$ the random variable of a network statistic of choice and by $S$ the space for $S$. Using the vertex degree of a simple undirected network on $n$ vertices as an example, $S$ is a discrete random variable taking values from $0$ to $n - 1$. Further denote by $S_{z'}$, the network statistic of an observation $z'$ from the null model $q$ and by $S_x$ the network statistics from the observed $x$. Then with $\mathcal{R}$ denoting the set of possible values of $S$,

$$d_{TV}(S_{z'}; S_x) = \sup_{A \subset \mathcal{R}} |E[h_A(S_{z'}) - h_A(S_x)]| = \frac{1}{2} \sum_{s \in S} |P(S_{z'} = s) - P(S_x = s)|$$

where $h_A(s) = 1$ if $s \in A$ and $0$ otherwise. Our test statistic measures the distance between the
distribution of a network statistic $S$ in the observed network $x$ and under the null model $q$ as follows:

$$D_{TV}(q, x; S) = \mathbb{E}_{z' \sim q}[d_{TV}(S_{x'}; S_x)].$$

To estimate $\mathbb{E}_q$, we simulate $m'$ networks from the null model $q$, i.e. $z'_1, \ldots, z'_{m'} \sim q$ and use as empirical estimate for $D_{TV}(q, x; S)$

$$\hat{D}_{TV}(q, x; S) = \frac{1}{m'} \sum_{j=1}^{m'} [d_{TV}(S_{z'_j}; S_x)].$$

To assess how the test statistics is distributed under the null hypothesis, i.e. $x \sim q$, we simulate $z \sim q$ from the null distribution. Similar to a Monte-Carlo test, we simulate independent network samples $z_1, \ldots, z_m \sim q$ and compute $\hat{D}_{TV}(q, z_i; S)$, for $i \in [m]$. Then we reject the null if $\hat{D}_{TV}(q, x; S)$ exceeds the $(1 - \alpha)$-quantile level in the simulated observations $\{\hat{D}_{TV}(q, z_1; S), \ldots, \hat{D}_{TV}(q, z_m; S)\}$ under the null distribution.

### D.2 Test Statistics with Mahalanobis Distance

Lospinoso and Snijders [2019] proposed using a Mahalanobis distance instead of the total variation distance. Suppose that a vector $S(x)$ of network summaries is observed and that the null distribution is parametrised by $\theta$. Denote $\mu(\theta) = \mathbb{E}_\theta(X)$ as the expectation and $\Sigma(\theta) = \text{Cov}_\theta(X)$ as the covariance matrix under $\theta$. The Mahalanobis distance

$$D_M(x, \theta; S) = (S(x) - \mu(\theta))^\top \Sigma(\theta)^{-1}(S(x) - \mu(\theta))$$

can then be used as test statistic. In practice, $\mu(\theta)$ and $\Sigma(\theta)$ are estimated using independent simulations $x_k, k = 1, \ldots, m$, from the distribution specified by $\theta$:

$$\hat{\mu} = \frac{1}{m} \sum_{k=1}^{m} S(x_k); \quad \hat{\Sigma} = \frac{1}{m} \sum_{k=1}^{m} (S(x_k) - \hat{\mu})(S(x_k) - \hat{\mu})^\top;$$

$$\hat{D}_M(x) = (S(x) - \hat{\mu})^\top \hat{\Sigma}^{-1}(S(x) - \hat{\mu}).$$

The $p$-value of the test is estimated by the plug-in estimator

$$\hat{p} = \frac{1}{m} \sum_{k=1}^{m} \mathbb{I}\{\hat{D}_M(x_k) > \hat{D}_M(x)\}.$$

In the main text this approach is abbreviated $\text{MD}$ and applied to the degree distribution for ERGMs.

### E Additional Experiment Results

**Test performances with graph kernels** Fig.3(a) shows the results for testing the E2ST model Eq.(14) with the 2-star coefficient $\beta_2$ perturbed using the different kernels described in Section B. Using the abbreviations from Section B, the relevant choices of kernel parameters are $\sigma = 1$ for the VEG kernel, level= 5 for the WL kernel, and $\lambda = \frac{1}{2}$ in the GRW kernel. Similar to the WL kernel used in the main text, the other choices of graph kernels achieve fairly good test power with the gKSS statistic. In our additional experimental results on the rejection rate, the re-sample size is $B = 100$ for all kernel choices. From Fig.3(a) we see that the test power is slightly higher with a small perturbed coefficient when the SP kernel and the VEG kernel are employed, while for larger perturbed coefficient (resulting in sparser graphs) the WL kernel better distinguishes the observation from the null. For large negative $\beta_2$ the GRW kernel has the poorest rejection rate. These differences in performance are no surprise as different choices of kernel emphasise different aspect of graph topology.

**Computational time** In Fig.3(b), we give more results for the computational time for one test, with 1,000 simulated networks. These results complement the reported results of Table 1 in the main text. As the number of vertices in the network increases, there is an increase in the computational complexity. However, as the main computation costs come from simulating the ERGM, we see from the plot that the slope is not substantial compared to the difference in testing procedures.
A Stein Goodness-of-ﬁt Test for Exponential Random Graph Models

−0.8 −0.6 −0.4 −0.2 0.0 0.2
0.0 0.2 0.4 0.6 0.8 1.0

Perturbation of Coefficients
Rejection Rate gKSS_B100_WL
gKSS_B100_GRW
gKSS_B100_VEG
gKSS_B100_SP

(a) \( n = 20, \alpha = 0.05 \), with \( \beta_2 \) in Eq.(14) perturbed

(b) log computational time for one test, in seconds, with \( m = 1000 \) simulated networks

Figure 3: Additional experiment results

F Comparison with the Kernel Discrete Stein Discrepancy on Testing Goodness-of-ﬁt

F.1 Discrete Stein Operator

In this section, we compare our approach with the discrete Stein operator introduced in Yang et al. [2018]. First we need some deﬁnitions.

Deﬁnition 2. [Deﬁnition 1 [Yang et al., 2018]](Cyclic permutation). For a set \( N \) of ﬁnite cardinality, a cyclic permutation \( \gamma : N \rightarrow N \) is a bijective function such that for some ordering \( x[1], x[2], \ldots, x[|X|] \) of the elements in \( N \), \( \gamma(x[i]) = x[(i+1) \mod |X|], \forall i = 1, 2, \ldots, |X| \).

Deﬁnition 3. [Deﬁnition 2 [Yang et al., 2018]] Given a cyclic permutation \( \gamma \) on \( N \), for any d-dimensional vector \( x = (x_1, \ldots, x_d)^\top \in N^d \), write \( \gamma_i x := (x_1, \ldots, x_{i-1}, \gamma(x_i), x_{i+1}, \ldots, x_d)^\top \). For any function \( f : N^d \rightarrow \mathbb{R} \), denote the (partial) difference operator as

\[
\Delta_{x_i} f(x) := f(x) - f(\gamma_i x), \quad i = 1, \ldots, d
\]

and introduce the difference operator:

\[
\Delta_f(x) := (\Delta_{x_1} f(x), \ldots, \Delta_{x_d} f(x))^\top.
\]

Here we use the notation \( \Delta_f \) to distinguish it from the notation in the main text, where we used \( \Delta_s h(x) = h(x(s,1)) - h(x(s,0)) \) and \( ||\Delta h|| = \sup_{x \in \mathbb{N}} |\Delta_s h(x)| \).

For discrete distributions \( q \), Yang et al. [2018] proposed the following discrete Stein operator, which is based on the difference operator \( \Delta_f \), constructed from a cyclic permutation:

\[
T_q^D f(x) = f(x) \frac{\Delta_f q(x)}{q(x)} - \Delta_f^* f(x),
\]

where \( \Delta_f^* \) denotes the adjoint operator of \( \Delta_f \).

In particular, for \( q \) the distribution of an ERGM, with \( N = \{0, 1\}^N \), the discrete Stein operator proposed [Yang et al., 2018] can be written in the form of \( T_q^D f(x) = \sum_s T_q^{D,s} f(x) \) where

\[
T_q^{D,s} f(x) = (-1)^{1_{x = x(s,0)}} \frac{f(x(s,1)) q(x(s,0)) - f(x(s,0)) q(x(s,1))}{q(x)}.
\]
Recall the ERGM Stein operator of the form $\mathcal{T}_q f(x) = \frac{1}{N} \sum_{s \in [N]} \mathcal{T}_q^{(s)} f(x)$ and Eq.(5),

$$\mathcal{T}_q^{(s)} f(x) = q(x^{(s,1)} | x) \Delta_s f(x) + \left( f(x^{(s,0)}) - f(x) \right)$$

$$= \frac{q(x^{(s,1)})}{q(x^{(s,1)}) + q(x^{(s,0)})} \left( f(x^{(s,1)}) - f(x^{(s,0)}) \right) + \left( f(x^{(s,0)}) - f(x) \right)$$

$$= \frac{1}{q(x^{(s,1)}) + q(x^{(s,0)})} \left( f(x^{(s,1)}) - f(x^{(s,0)}) \right).$$

We illustrate the difference between the ERGM Stein operator and the discrete Stein operator for a Bernoulli random graph with $P(s = 1) = q, \forall s$. Due to the independence, we have $q(x^{(s,1)} | x) = q$ and $q(x^{(s,0)} | x) = 1 - q$. With Eq.(5), our Stein operator becomes

$$\mathcal{T}_q f(x) = \frac{1}{N} \sum_s (q - x_s) \left( f(x^{(s,1)}) - f(x^{(s,0)}) \right). \tag{21}$$

The K SDS in this case can be written as:

$$\mathcal{T}_q^D f(x) = \frac{1}{q(x)} \sum_s (-1)^{1-x_s} \left( (1 - q) f(x^{(s,1)}) - q f(x^{(s,0)}) \right)$$

with $q(x) = \sum_s x^s (1 - q)^{N - \sum_s x^s}$. Thus, for different values, Eq.(21) is a weighted sum of the terms $\left( f(x^{s,1}) - f(x^{s,0}) \right)$, while KSDS is a weighted sum of the terms $(1 - q)f(x^{s,1}) - qf(x^{s,0})$ and requires the calculation of the binomial probability $q(x)$.

The operators in Eq.(20) and Eq.(5) clearly differ in their scaling as well as in their repercussions for resampling. While the operator in Eq.(5) emerges from Glauber dynamics and hence has a natural resampling interpretation, no such interpretation is available for the operator in Eq.(20). Explicitly, the discrete Stein operator $\mathcal{T}_q^D$ has $q(x)$ in the denominator, indicating the fixed $x$ realisation; however, the Stein ERGM operator $\mathcal{T}_q$ has $q(x^{s,1})$ in the denominator which stems from the conditioning in Glauber dynamics. Consequently, the corresponding Stein discrepancy (called KDS) differs from Eq.(2) in the main text, and, although usually only one network is available, the goodness-of-fit test in Yang et al. [2018] requires independent and identically distributed network observations.

A second key difference is that the test in Yang et al. [2018] requires the support of the unknown network distribution to be identical to the support of the ERGM which is described by $q$. In practice this condition is difficult if not impossible to verify. In contrast, $gKSS$ does not make any such assumption.

### F.2 Comparison Between Graph Testing

#### Testing with multiple graph observations

The relevant kernel discrete Stein discrepancy (KSD) from the discrete Stein operator [Yang et al., 2018] is defined via taking the supreme over appropriate unit ball RKHS test functions, similar as in Eq.(2)

$$\text{KSD}_q(q||p; \mathcal{H}) = \sup_{\|f\|_\mathcal{H} \leq 1} \mathbb{E}_p[\mathcal{T}_q^D f(x)]. \tag{22}$$

Yang et al. [2018] built a goodness-of-fit testing procedure based on the KSD for ERGM for multiple graph observations. Let $x_1, \ldots, x_m \sim p$, be $m$ independent identically distributed graph observations. The KSD is empirically estimated from the observed samples; and as the number of observed samples $m \to \infty$, in probability,

$$\frac{1}{m} \sum_i [\mathcal{T}_q^D f(x_i)] \to \mathbb{E}_p[\mathcal{T}_q^D f(x)].$$

The rejection threshold is determined via a wild-bootstrap procedure [Chwialkowski et al., 2014].

While the $gKSS$ type of statistics based on the ERGM Stein operator in Eq.(4), $\mathcal{T}_q f(x) = \frac{1}{N} \sum_{s \in [N]} \mathcal{T}_q^{(s)} f(x)$, focuses on a single graph observation, this ERGM Stein operator could similarly be used to assess goodness-of-fit
A Stein Goodness-of-fit Test for Exponential Random Graph Models

When multiple graph observations are available. In particular, \( \mathbb{E}_q[T_q f(x)] = 0 \). Hence, we introduce the graph kernel Stein discrepancy (gKSD) as

\[
g\text{KSD}(q \parallel p; \mathcal{H}) = \sup_{\|f\|_{\mathcal{H}} \leq 1} \mathbb{E}_p[T_q f(x)] = \sup_{\|f\|_{\mathcal{H}} \leq 1} \mathbb{E}_p \left[ \frac{1}{N} \sum_s T_q^{(s)} f(x) \right].
\]

Here the sum is taken over all \( N \) pairs of vertices and the expectation is taken with respect to the ERGM \( q \). When there are \( m \) independent observations \( x_1, \ldots, x_m \sim p \) available then we can empirically estimate \( g\text{KSD}(q \parallel p; \mathcal{H}) \) by

\[
\frac{1}{m} \sum_i \left[ \frac{1}{N} \sum_s T_q^{(s)} f(x_i) \right],
\]

which is weakly consistent by the law of large numbers. Then we use this statistic to build a goodness-of-fit test for multiple graph observations, determining the threshold via the same wild-bootstrap procedure as for the KDSD.

To compare the KDSD and the gKSD tests we consider the goodness-of-fit test setting as studied in Yang et al. [2018], using the E2ST model as presented in Eq.(14). We set the null parameters \( \beta \) to \( (\beta_1, \beta_2, \beta_3) = (-2, 0, 0.01) \) and carry out a test at significance level \( \alpha = 0.05 \) using 100 repeats. For the alternative, we perturb the coefficient for 2-stars, \( \beta_2 \), and report the rejection rate in Table 3. Note that \( \beta_2 = 0.00 \) recovers the null distribution. In this experiment, with a small number of graph observations, \( m = 30 \), gKSD captures the difference between the null model and the alternative model better, resulting in a higher test power, compared to KDSD. Both gKSD and KDSD have higher power for \( \beta_2 > 0 \) than for \( \beta_2 < 0 \) of the same magnitude. This finding is plausible as increasing \( \beta_2 \) leads to denser networks.

<table>
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<th>( \beta_2 )</th>
<th>-0.1</th>
<th>-0.08</th>
<th>-0.06</th>
<th>-0.04</th>
<th>-0.02</th>
<th>0.00</th>
<th>0.02</th>
<th>0.04</th>
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<td>0.28</td>
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<tr>
<td>KDSD</td>
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<td>0.06</td>
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<td>0.03</td>
<td>0.06</td>
<td>0.12</td>
<td>0.16</td>
</tr>
</tbody>
</table>

Table 3: Rejection rate for the E2ST model \( (\beta_1, \beta_2, \beta_3) = (-2, 0, 0.01) \) with perturbation of the 2-star coefficient \( \beta_2 \): W.L. Kernel of level 3; sample size \( m = 30 \); graph size \( n = 20 \); test significance level \( \alpha = 0.05 \).

**Testing with a single graph observation** The ERGM Stein operator satisfies the mean zero property Eq.(6) when flipping each edge \( s \) given the rest of the graph \( x_{-s} \). This is a key ingredient that KDSD does not satisfy; KDSD relies on a cyclic permutation as in Definition 2 to construct the partial difference operator in Definition 3, which depends on the order sequence of the cyclic permutation. As such, the mean zero property of their Stein operator is based on sign flips in each state of the discrete variable, instead of flipping the edge probability. Thus, the discrete Stein operator \( T_q^D \) could not easily be adapted to construct a subsampled Stein statistic such as gKSS to perform goodness-of-fit testing with a single graph observation.

**Testing with a few graph observations** An interesting setting which is related to that of a single graph observation, is that a few graphs are observed, with the number of graphs assumed to be finite and not tending infinity with network size. With the proposed gKSD goodness-of-fit test for a single graph observation, a possible approach and a potential future research direction is applying multiple tests of goodness-of-fit, one for each observed network, with a Bonferroni correction [Bonferroni, 1936] to correct for multiple testing.