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# A Structural Model for the Coevolution of Networks and Behavior\*

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## Abstract

This paper introduces a structural model for the coevolution of networks and behavior. We characterize the equilibrium of the underlying game and adopt the Bayesian Double Metropolis-Hastings algorithm to estimate the model. We fur-

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\*This paper has grown out of ideas in a manuscript circulated under the title “Network Formation with Local Complements and Global Substitutes: The Case of R&D Networks”, which is now split into two papers. In this paper, we propose a general econometric model for the coevolution of networks and behavior incorporating both network formation externalities and unobserved heterogeneity. In the second paper, we focus on the equilibrium characterization, estimation and policy implications of dynamic R&D network models. We thank the Co-Editor Bryan Graham and three anonymous referees for valuable comments and suggestions. We also thank Vincent Boucher, Lung-fei Lee, Angelo Mele, Olivier Parent, Eleonora Patacchini, and the seminar participants at the Barcelona GSE summer forum on “Networks: Information, Contracts, and Communities”, the 2019 Asia Meeting of the Econometric Society, the 2019 China Meeting of the Econometric Society, the 29th Annual Meeting of the Midwest Econometrics Group, and XIII World Conference of the Spatial Econometrics Association for helpful discussions. We further thank Christian Helmers for data sharing and Sebastian Ottinger for the excellent research assistance.

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ther extend the model to incorporate unobserved heterogeneity and show that ignoring unobserved heterogeneity can lead to biased estimates in simulation experiments. We apply the model to study R&D investment and collaboration decisions in the chemical and pharmaceutical industry and find a positive knowledge spillover effect. Our model also provides a tractable framework for a long-run key player analysis.

Key words: network interactions, strategic network formation, stochastic best-response dynamics, unobserved heterogeneity, double Metropolis-Hastings algorithm, R&D collaboration networks, key players

JEL: C11, C31, C63, C73, L22

## 1 Introduction

Since the seminal paper by Manski (1993), substantial progress has been made in the econometric analysis of networks following two research strands. The first strand studies the interdependence of individual behavior in a network under the assumption that the network structure is exogenously given. A popular model in this literature is the linear social-interaction model (see, e.g., Bramoullé et al., 2009; Lee et al., 2010; Liu and Lee, 2010; Blume et al., 2015). The second strand focuses on the modeling and estimation of the network formation process, with some recent developments including Christakis et al. (2010), Snijders (2011), Graham (2015, 2017), Leung (2015), Boucher and Mourifié (2017), Mele (2017, 2018), Menzel (2017), Sheng (2017), Chandrasekhar and Jackson (2018), De Paula et al. (2018), Dzemski (2018), and Mele and Zhu (2019). To link these two research strands, we introduce a unified framework to model the coevolution of networks and behavior in this paper.

The microfoundation of our structural model is a network game where agents make decisions on actions and network links to maximize their utilities. The utility function is a generalization of the linear-quadratic utility function in Ballester et al. (2006) by including

direct payoffs from the network structure given by *homophily/heterophily*, *congestion* and *cyclic triangle* effects. An important feature of the utility function is that it incorporates the two-way interdependence between networks and behavior (see Figure 1 for an illustration). We show that, under some mild assumptions, the utility function admits a potential function (Monderer and Shapley, 1996). The potential function aggregates individual incentives to change from the status quo and thus greatly simplifies the equilibrium analysis.

[insert Figure 1 here]

The coevolution of networks and behavior is modeled as stochastic best-response dynamics (Blume, 1993). In each period, a randomly selected agent gets a chance to update his action or meet with another agent to adjust the link between them as the best response to the current actions and links of the rest of the network. We show that this process follows a Markov chain that converges to a unique stationary distribution of networks and actions characterized by a Gibbs measure (i.e., an exponential family distribution that depends on the potential function).

With a snapshot of the network and actions drawn from the stationary distribution, the structural parameters can be estimated based on the maximum likelihood principle. However, as pointed out in Mele (2017), the frequentist maximum likelihood method or Bayesian Metropolis-Hastings (MH) algorithm (Chib and Greenberg, 1995) are computationally infeasible due to the intractable normalizing constant in the Gibbs measure. To bypass the evaluation of the intractable normalizing constant, we adopt the Bayesian Double Metropolis-Hastings (DMH) algorithm (Liang, 2010; Mele, 2017) to sample from the posterior distribution of the structural parameters. Compared with Mele (2017), we face the additional complication as we need to simulate actions as well as networks to generate auxiliary data in the DMH algorithm. We propose a computationally simple MH algorithm for this purpose. Another contribution relative to Mele (2017) is that we incorporate unobserved heterogeneity in the empirical model to capture the potential correlation between

action choices and network formation decisions. In Monte Carlo simulations, we find that ignoring unobserved heterogeneity leads to a biased estimate of the network spillover effect.

To illustrate the empirical relevance of our structural model, we apply it to study the interdependence of R&D investment and collaboration decisions in the chemical and pharmaceutical industry. Using a unique dataset on R&D collaborations matched to firms' balance sheets, we find a positively significant knowledge spillover effect on firms' R&D investment decisions. We also find that an R&D collaboration is more likely to form between firms in the same sub-sector (the *homophily* effect), firms with different productivities (the *heterophily* effect), and firms with a common collaboration partner (the *cyclic triangle* effect). A firm is less likely to form a new link if it has many existing R&D collaborations (the *congestion* effect).

Finally, the proposed structural model has important policy implications as it allows the policy maker to identify the *key player* whose exit would have the largest impact on welfare in the long run. Conventional key player analysis assumes the links between the other agents are not affected by the exit of the key player (Ballester et al., 2006). This assumption makes sense if the key player analysis is considered as a short-run policy analysis, because it takes time for the other agents to adjust their links in response to the exit of the key player. However, in the long run, it is difficult to justify this assumption. Our structural model provides a tractable framework for a long-run key player analysis. In the empirical study, we find that the key player rankings in the short run and in the long run do not coincide with each other. We also find that the key player ranking is correlated with both R&D expenditure and network centrality measures (including degree, betweenness, closeness and eigenvector centralities) of a firm. Therefore, the key player ranking incorporates information on both R&D investment and network centrality of a firm.

Our paper is related to recent papers that study the identification and estimation of social interaction models with endogenous networks (Goldsmith-Pinkham and Imbens, 2013; Hsieh and Lee, 2016; Auerbach, 2019; Battaglini et al., 2019; Johnsson and Moon, 2019; Lee

et al., 2020). The focus of these papers is to consistently estimate social interaction effects controlling for the unobserved heterogeneity in the network formation process. In particular, Auerbach (2019) and Johnsson and Moon (2019) take a fixed-effect approach and allow the unobserved heterogeneity to affect link formation nonparametrically. Since it is difficult to distinguish link externalities from a flexible form of unobserved heterogeneity (Graham, 2015), link externalities are excluded a priori from their network formation models. By contrast, this paper takes a random-effect treatment of the unobserved heterogeneity and develops a parametric framework that incorporates both link externalities and unobserved heterogeneity. Hsieh et al. (2019) propose a two-stage network game, where the network is formed in the first stage and, in the second stage, individuals choose their actions taking the network as given. The equilibrium concept for the first stage of the game relies on a transferable utility assumption that allows agents to make side payments. The transferable utility assumption is reasonable for small networks, but is difficult to justify when the network is large. The closest work to ours is Badev (2018), which proposes a network formation game where agents make decisions on *binary* actions and network links in the absence of unobserved heterogeneity. Our model, on the other hand, considers continuous actions and allows for unobserved heterogeneity.

The rest of the paper is organized as follows. Section 2 introduces the structural model, Section 3 presents the estimation strategy, Section 4 provides an empirical illustration, and Section 5 concludes. The proofs and technical details are collected in the online appendix.

## 2 Structural Model

### 2.1 Preferences

Consider a network  $g \in \mathcal{G}$  consisting of a set of agents  $\mathcal{N} \equiv \{1, \dots, n\}$ , where  $\mathcal{G}$  is the set of all networks with  $n$  nodes. The topology of the network is represented by an  $n \times n$  adjacency matrix  $G = [g_{ij}]$ , where  $g_{ij} = 1$  if agents  $i$  and  $j$  form a link and  $g_{ij} = 0$  otherwise. The

network links are reciprocal, that is,  $g_{ij} = 1$  implies  $g_{ji} = 1$ . As a normalization, we set  $g_{ii} = 0$  for all  $i \in \mathcal{N}$ . Let  $\mathcal{N}_i \equiv \{j \in \mathcal{N} | g_{ij} = 1\}$  denote the set of agent  $i$ 's peers (or, loosely speaking, “friends”).

Agent  $i$ , with his exogenous characteristics given by a (row) vector  $X_i$ , makes decisions on network links  $g_{ij}$  and effort of action  $y_i$  to maximize utility. We assume  $X_i$  can be observed by all the agents. To introduce unobserved heterogeneity in the econometric model, we allow some components of  $X_i$  to be unobservable to the econometrician. Let  $Y = (y_1, \dots, y_n)'$ , and let  $Y_{-i}$  denote the effort levels of all agents but  $i$ . The utility of agent  $i$  follows a linear-quadratic function given by

$$U_i(g, Y, X) = a_i(g, X) + b(X_i)y_i + \lambda \sum_{j \in \mathcal{N}} g_{ij}y_i y_j - \frac{1}{2}y_i^2, \quad (1)$$

where

$$a_i(g, X) = \sum_{j \in \mathcal{N}} g_{ij} \left\{ \delta_0 + h(X_i, X_j, \delta_1) + \delta_2 \sum_{k \in \mathcal{N} \setminus \{i, j\}} g_{ik} + \delta_3 \sum_{k \in \mathcal{N} \setminus \{i, j\}} g_{ik}g_{jk} \right\}. \quad (2)$$

The first term of Equation (1),  $a_i(g, X)$ , measures the *direct* utility from links.<sup>1</sup> In particular,  $\delta_0$  is the fixed cost of maintaining links, and  $h(X_i, X_j, \delta_1)$  captures the (dis)similarity between agents  $i$  and  $j$  in exogenous characteristics, with the coefficient vector  $\delta_1$  representing the *homophily* or *heterophily* effect depending on its sign.  $\sum_{k \in \mathcal{N} \setminus \{i, j\}} g_{ik}$  is the total number of links of agent  $i$  excluding the link  $g_{ij}$ , with the coefficient  $\delta_2$  representing the *congestion* effect.  $\sum_{k \in \mathcal{N} \setminus \{i, j\}} g_{ik}g_{jk}$  is the number of common “friends” between agents  $i$  and  $j$ , with the coefficient  $\delta_3$  representing the *cyclic triangle* effect.<sup>2</sup> We impose the following

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<sup>1</sup>We consider undirected network links to be consistent with the empirical study of R&D networks. If network links are directed,  $a_i(g, X)$  can be specified in a similar manner as Equation (1) in Mele (2017).

<sup>2</sup>It is possible to include additional terms in  $a_i(g, X)$  as long as there exists a correspond-



assumption on  $h(X_i, X_j, \delta_1)$  to guarantee the existence of a potential function.

**Assumption 1.**  $h(X_i, X_j, \delta_1) = h(X_j, X_i, \delta_1)$  for any  $i, j \in \mathcal{N}$ .

The second term of Equation (1),  $b(X_i)y_i$ , measures the *direct* utility from effort, with the marginal utility of effort given by  $b(X_i)$ . The third term,  $\lambda \sum_{j \in \mathcal{N}} g_{ij}y_i y_j$ , is the *social* utility, with the coefficient  $\lambda$  representing the *spillover* effect. Finally, we assume the cost of exerting effort is given by the last term of Equation (1),  $\frac{1}{2}y_i^2$ , which exhibits increasing marginal cost. Maximizing Equation (1) with respect to  $y_i$  gives the best response function for the effort choice

$$y_i = \lambda \sum_{j \in \mathcal{N}} g_{ij}y_j + b(X_i), \quad (3)$$

which coincides with the one in Ballester et al. (2006).

**Remark 1.** In the network formation game considered in Mele (2017), agents only make decisions on links  $g_{ij}$  to maximize the *direct* utility from links. In our model, agents make decisions on links  $g_{ij}$  as well as effort  $y_i$ , taking into account the *direct* utility from links, the *direct* utility from effort, and the *social* utility. In the social interaction models with endogenous networks (see, e.g., Auerbach, 2019; Johnsson and Moon, 2019), links are assumed to be pairwise independent (conditional on observed and unobserved individual attributes). In our model, links are interdependent with externalities given by the *congestion* and *cyclic triangle* effects in  $a_i(g, X)$ . Furthermore, Auerbach (2019) and Johnsson and Moon (2019) assume actions depend on links but not the other way around (conditional on observed and unobserved individual attributes). In our model, the *social* utility component in Equation (1) captures the two-way interdependence between actions and links. Badev (2018) considers a network formation game where agents make decisions on *binary* actions and network links. In our model, the action space is allowed to be continuous and the utility function implies a best response function given by Equation (3) that underlies many well known linking potential function under suitable restrictions.

ear social-interaction models in the literature (see, e.g., Bramoullé et al., 2009; Liu and Lee, 2010; Blume et al., 2015).

## 2.2 Coevolution of Networks and Behavior

Let the realization of the network in period  $t$  be denoted by  $g_t$  with the adjacency matrix  $G_t = [g_{ij,t}]$ , and let the network including all the current links but  $g_{ij,t}$  be denoted by  $g_{-ij,t}$ . Similarly, the effort profile of  $\mathcal{N}$  in period  $t$  is given by the vector  $Y_t = [y_{i,t}]$ , and the effort profile of  $\mathcal{N} \setminus \{i\}$  is written as  $Y_{-i,t}$ . To simplify notation, we drop  $X$  from  $U_i(g, Y, X)$  henceforth.

The coevolution of networks and behavior is specified as stochastic best-response dynamics (Blume, 1993). We assume time is discrete. Each time period is either a link-adjustment period (with probability  $0 < \rho_0 < 1$ ) or an effort-adjustment period (with probability  $1 - \rho_0$ ). In the following, we give details of these two adjustment periods and characterize the stationary distribution of the stochastic process.

**Link Adjustment** In a link-adjustment period, a pair of agents  $i$  and  $j$  is randomly selected from the population with probability  $\rho(g_{t-1}, X_i, X_j)$ . To make the equilibrium analysis feasible, we impose the following assumption on the selection rule characterized by  $\rho(g_{t-1}, X_i, X_j)$ .<sup>3</sup>

**Assumption 2.** (i)  $\rho(g_{t-1}, X_i, X_j) = \rho(g_{t-1}, X_j, X_i)$ ; (ii)  $\rho(g_{t-1}, X_i, X_j)$  does not depend on  $g_{ij,t-1}$ ; and (iii)  $\rho(g_{t-1}, X_i, X_j) > 0$  for all  $(i, j) \in \mathcal{N} \times \mathcal{N}$ .

Conditional on being selected, agents  $i$  and  $j$  update the link  $g_{ij}$  to maximize their utilities taking the rest of the network and effort choices as given. As in Mele (2017), we assume that agents do not take into account the effect of their decisions on the future effort choices and network evolution. To capture the uncertainty (from the perspective of the econometrician)

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<sup>3</sup>See Mele (2017) for more discussion on the selection (or meeting) rule.

in the link adjustment process, we introduce an idiosyncratic shock to the utility and assume that a link is formed if and only if it improves the average utility of agents  $i$  and  $j$  given by  $\bar{U}_{ij}(g, Y) = [U_i(g, Y) + U_j(g, Y)]/2$ . More specifically,  $g_{ij,t} = 1$  if and only if

$$\bar{U}_{ij}(g_{ij,t} = 1, g_{-ij,t-1}, Y_{t-1}) + \epsilon_{ij,t}^{(1)} \geq \bar{U}_{ij}(g_{ij,t} = 0, g_{-ij,t-1}, Y_{t-1}) + \epsilon_{ij,t}^{(0)}, \quad (4)$$

where  $\epsilon_{ij,t}^{(1)}$  and  $\epsilon_{ij,t}^{(0)}$  are independent from each other, i.i.d. across links and time periods, and follow a Gumbel distribution with the distribution function  $F(\epsilon) = \exp[-\exp(-\epsilon/\sigma^2)]$ . The parameter  $\sigma^2$  captures the level of “noise” in link adjustment decisions.<sup>4</sup>

**Effort Adjustment** In an effort-adjustment period, an agent  $i$  is randomly selected from the population with probability  $\rho(X_i)$ . We assume any agent can be selected with positive probability in the following assumption.

**Assumption 3.**  $\rho(X_i) > 0$  for all  $i \in \mathcal{N}$ .

Conditional on being selected, agent  $i$  updates the effort level  $y_{it} \in \mathcal{Y}$  to maximize his utility, where  $\mathcal{Y}$  is the set of all possible effort choices. We allow  $\mathcal{Y}$  to be continuous and assume that, taking the network  $g_{t-1}$  and the effort levels of the other agents  $Y_{-i,t-1}$  as given, the probability that agent  $i$  chooses an effort level in  $\mathcal{Z} \subset \mathcal{Y}$  in period  $t$  is given by

$$\Pr(y_{it} \in \mathcal{Z} | g_t = g_{t-1}, Y_{-i,t} = Y_{-i,t-1}) = \frac{\int_{\mathcal{Z}} \exp[\sigma^{-2}U_i(g_{t-1}, z, Y_{-i,t-1})]dz}{\int_{\mathcal{Y}} \exp[\sigma^{-2}U_i(g_{t-1}, y, Y_{-i,t-1})]dy}. \quad (5)$$

Similar to Equation (4) in the link adjustment period, the probability given in Equation (5) can be justified by an additive random utility model over a nonfinite choice set (McFadden, 1976), where the parameter  $\sigma^2$  captures the level of “noise” in effort adjustment decisions.

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<sup>4</sup>The parameter  $\sigma^2$  can be identified because the coefficient of  $y_i^2$  is normalized to  $-1/2$  in the utility function given by Equation (1).

Equation (5) admits the probability density function

$$p(y_{it}|g_t = g_{t-1}, Y_{-i,t} = Y_{-i,t-1}) = \frac{\exp[\sigma^{-2}U_i(g_{t-1}, y_{it}, Y_{-i,t-1})]}{\int_{\mathcal{Y}} \exp[\sigma^{-2}U_i(g_{t-1}, y, Y_{-i,t-1})]dy}. \quad (6)$$

**Equilibrium** In the stochastic process described above, the coevolution of the network  $g_t$  and effort choices  $Y_t$  follows a Markov chain. In the following proposition, we show that the Markov chain converges to a unique stationary distribution. Let  $\gamma$  denote the vector of all unknown parameters in the potential function defined in Equation (7) and  $\theta = (\gamma', \sigma^2)'$ .

**Proposition 1.** *Let*

$$Q(g, Y) \equiv Q(g, Y, X) = a(g, X) + \sum_{i \in \mathcal{N}} b(X_i)y_i + \frac{\lambda}{2} \sum_{i \in \mathcal{N}} \sum_{j \in \mathcal{N}} g_{ij}y_iy_j - \frac{1}{2} \sum_{i \in \mathcal{N}} y_i^2, \quad (7)$$

where

$$a(g, X) = \frac{1}{2} \sum_{i \in \mathcal{N}} \sum_{j \in \mathcal{N}} g_{ij} \left\{ \delta_0 + h(X_i, X_j, \delta_1) + \delta_2 \sum_{k \in \mathcal{N} \setminus \{i,j\}} g_{ik} + \frac{2}{3} \delta_3 \sum_{k \in \mathcal{N} \setminus \{i,j\}} g_{ik}g_{jk} \right\}.$$

Under Assumptions 1-3, the coevolution process of the network and behavior converges to a unique stationary distribution characterized by the Gibbs measure

$$\pi(g, Y|\theta) = c(\theta)^{-1} \exp[\sigma^{-2}Q(g, Y|\gamma)], \quad (8)$$

where  $c(\theta) = \sum_{g \in \mathcal{G}} \int_{\mathcal{Y}^n} \exp[\sigma^{-2}Q(g, Y|\gamma)]dY$ .

**Remark 2.**  $Q(g, Y)$  defined in Equation (7) is known as the potential function (Monderer and Shapley, 1996). As the change in the utility of an agent (or the average utility of a pair of agents) from adjusting his effort level (or their link) is identical to the corresponding change in the potential function, the potential function keeps track of individual incentives to deviate from the status quo, and thus greatly simplifies the equilibrium characterization of the coevolution process.

**Remark 3.** The Gibbs measure defined in Equation (8) bears a resemblance to that in an exponential random graph model (ERGM) (Pattison and Wasserman, 1996). Nevertheless, there is an important difference. As the ERGM only models the network formation process without taking individual behavior into account, the corresponding Gibbs measure is a distribution of networks. By contrast, our framework jointly models the interdependent link and effort adjustment processes, and the resulting Gibbs measure is a joint distribution of networks and efforts. This poses a novel challenge for the estimation of model parameters.

### 2.3 Key Player Analysis

An advantage of the proposed structural model (compared to a reduced form model) is that it can be used by policy makers to conduct counterfactual studies. In this paper, we focus on a particular counterfactual study called *key player analysis* (Zenou, 2016). The key player analysis measures the importance of a node according to the reduction in the total activity level (Ballester et al., 2006) or social welfare (König et al., 2019), were it to be removed from the network. The key player analysis has important policy implications. Take the inter-firm R&D network as an example. The exit of a firm from the network could be due to either financial reasons, such as the recession experienced by the American automobile manufacturing industry during the global financial downturn of 2007-2008, or legal reasons, such as the recent emission-fraud scandal of Volkswagen in 2015. In the former case, the key player analysis can help the policy maker to know the overall welfare gain of “bailing out” a bankrupting firm, while, in the latter case, the key player analysis can help the policy maker to know the overall welfare cost by inflicting high penalties that might threaten the continued existence of a firm.

Conventional key player analysis assumes that the network is exogenously given and does not adapt to the removal of a node (henceforth referred to as the invariant network

assumption).<sup>5</sup> For a short-run key player analysis, this assumption is reasonable because it takes time for the network to rewire after a node is removed. However, to conduct a long-run key player analysis, it is desirable to relax this assumption and develop a model that allows the remaining network to evolve to a new equilibrium. Our model can be used for this purpose.

In the long run, the key player is the agent whose removal from the network leads to the largest reduction in expected social welfare. More specifically, the reduction in expected social welfare from the removal of agent  $i$  is given by  $\Delta W_i = W(g, Y) - E[W(\tilde{g}_{-i}, \tilde{Y}_{-i})]$ , where  $W(g, Y) = \sum_{i=1}^n U_i(g, Y)$  is the initial welfare level with the observed network  $g$  and effort profile  $Y$ , and  $E[W(\tilde{g}_{-i}, \tilde{Y}_{-i})]$  is the expected welfare level of the network without agent  $i$ . The key player is defined as  $i^* = \arg \max_{i \in \mathcal{N}} \Delta W_i$ .

The expected welfare level  $E[W(\tilde{g}_{-i}, \tilde{Y}_{-i})]$  is evaluated under the Gibbs measure  $\pi(\tilde{g}_{-i}, \tilde{Y}_{-i} | \theta)$  defined in Equation (8), which is difficult to compute numerically. Hence, we take a simulation approach to implement the long-run key player analysis. With the estimated model parameters, we run a simulation of the above-described coevolution process starting from the observed network  $g_{-i}$  and effort profile  $Y_{-i}$  without agent  $i$ , and calculate  $W(\tilde{g}_{-i}, \tilde{Y}_{-i})$  based on the network  $\tilde{g}_{-i}$  and effort profile  $\tilde{Y}_{-i}$  after the process converges. We repeat the simulation many times and use the average value of  $W(\tilde{g}_{-i}, \tilde{Y}_{-i})$  as an approximation for  $E[W(\tilde{g}_{-i}, \tilde{Y}_{-i})]$ .<sup>6</sup>

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<sup>5</sup>The only exception we know is Lee et al. (2020), which adopts the framework in Mele (2017) to model the evolution process of the network after the key player is removed. Compared with our model, the network formation model in Lee et al. (2020) assumes link formation decisions do not depend on individual behavior conditional on observed and unobserved individual attributes.

<sup>6</sup>This analysis can be extended to conduct a key group analysis as in Ballester et al. (2010), where one calculates the expected welfare loss from removing every possible combination of a certain number of agents and finds the group associated with the largest loss. As the

### 3 Estimation

In this section, we discuss how to estimate the structural parameters based on the Gibbs measure defined in Equation (8). We first assume all components in  $X_i$  can be observed by the econometrician in Sections 3.1 and 3.2. Then, to introduce unobserved heterogeneity, we allow some components of  $X_i$  to be unobservable in Section 3.3.

#### 3.1 Computational Problem and the Exchange Algorithm

Given an observation  $(g, Y)$  from the stationary distribution defined in Equation (8), we can estimate the parameter vector  $\theta$  based on the maximum likelihood principle. However, as pointed out in Mele (2017), the frequentist maximum likelihood method is impractical due to the computational difficulty in evaluating the normalizing constant  $c(\theta)$  in Equation (8), and a standard Bayesian method would encounter the same problem because, with the prior distribution  $p(\theta)$ , the posterior distribution  $p(\theta|g, Y) \propto \pi(g, Y|\theta)p(\theta) = c(\theta)^{-1} \exp[\sigma^{-2}Q(g, Y|\gamma)]p(\theta)$  also contains the normalizing constant  $c(\theta)$ . To sample from the posterior using Markov Chain Monte Carlo (MCMC) simulations, a standard MH algorithm (Chib and Greenberg, 1995) updates  $\theta$  to  $\tilde{\theta}$ , a random draw from the proposal distribution  $q_\theta(\tilde{\theta}|\theta)$ , according to the acceptance probability

$$\alpha_{\theta, MH} = \min \left\{ 1, \frac{p(\tilde{\theta}|g, Y)q_\theta(\theta|\tilde{\theta})}{p(\theta|g, Y)q_\theta(\tilde{\theta}|\theta)} \right\} = \min \left\{ 1, \frac{c(\theta) \exp[\tilde{\sigma}^{-2}Q(g, Y|\tilde{\gamma})]p(\tilde{\theta})q_\theta(\theta|\tilde{\theta})}{c(\tilde{\theta}) \exp[\sigma^{-2}Q(g, Y|\gamma)]p(\theta)q_\theta(\tilde{\theta}|\theta)} \right\}.$$

The computational problem still exists as  $c(\theta)$  and  $c(\tilde{\theta})$  in the acceptance probability do not cancel each other.

A way to bypass the evaluation of the intractable normalizing constant  $c(\theta)$  is to use the exchange algorithm (Møller et al., 2006; Murray et al., 2006) as follows.

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analysis is simulation-based and computationally expensive, the key group analysis is only feasible for small networks.

**Algorithm 1** (Exchange Algorithm). *At each iteration:*

**Step 1** Draw  $\tilde{\theta}$  from the proposal distribution  $q_{\theta}(\tilde{\theta}|\theta)$ .

**Step 2** Generate  $(\tilde{g}, \tilde{Y})$  from the distribution  $\pi(\tilde{g}, \tilde{Y}|\tilde{\theta})$  using a perfect sampler.

**Step 3** Accept  $\tilde{\theta}$  according to the acceptance probability

$$\begin{aligned} \alpha_{\theta, EX} &= \min \left\{ 1, \frac{p(\tilde{\theta}|g, Y)q_{\theta}(\theta|\tilde{\theta})\pi(\tilde{g}, \tilde{Y}|\theta)}{p(\theta|g, Y)q_{\theta}(\tilde{\theta}|\theta)\pi(\tilde{g}, \tilde{Y}|\tilde{\theta})} \right\} \\ &= \min \left\{ 1, \frac{\exp[\tilde{\sigma}^{-2}Q(g, Y|\tilde{\gamma})]p(\tilde{\theta})q_{\theta}(\theta|\tilde{\theta}) \exp[\sigma^{-2}Q(\tilde{g}, \tilde{Y}|\gamma)]}{\exp[\sigma^{-2}Q(g, Y|\gamma)]p(\theta)q_{\theta}(\tilde{\theta}|\theta) \exp[\tilde{\sigma}^{-2}Q(\tilde{g}, \tilde{Y}|\tilde{\gamma})]} \right\}. \end{aligned} \quad (9)$$

The main advantage of the exchange algorithm is that the acceptance probability does not contain the normalizing constant  $c(\theta)$  and thus can be evaluated. The following proposition shows that the unique stationary distribution of the above described exchange algorithm is the posterior distribution  $p(\theta|g, Y) \propto \pi(g, Y|\theta)p(\theta)$ .

**Proposition 2.** *The unique stationary distribution of Algorithm 1 is  $p(\theta|g, Y)$ .*

## 3.2 Double Metropolis-Hastings Algorithm

In the second step of the exchange algorithm, we need to generate auxiliary data using a perfect sampler (Propp and Wilson, 1996), which is computationally costly. To overcome this issue, Liang (2010) and Mele (2017) propose a DMH algorithm, which uses a finite run of the MH algorithm initialized at the observed  $(g, Y)$  to generate auxiliary data  $(\tilde{g}, \tilde{Y})$ . More specifically, at each iteration, the DMH algorithm follows the same steps as the exchange algorithm with the second step replaced by:

**Step 2\*** *Generate  $(\tilde{g}, \tilde{Y})$  from the distribution  $\pi(\tilde{g}, \tilde{Y}|\tilde{\theta})$  using a finite run of the MH algorithm initialized at the observed  $(g, Y)$ .*



Compared with Mele (2017), one additional complication is that we need to simulate both networks  $\tilde{g}$  and effort choices  $\tilde{Y}$  in Step 2\* of the DMH algorithm. To generate auxiliary data  $(\tilde{g}, \tilde{Y})$ , one could design a sampler following the process described in Section 2.2. However, the convergence of such a sampler could be slow in practice. To improve convergence and reduce computational burden, we propose the following MH algorithm to generate  $(\tilde{g}, \tilde{Y})$ :

**Algorithm 2** (Auxiliary Data Generation). *Given  $\theta$ , at each iteration:*

**Step 1** Draw  $\tilde{g}$  from the proposal distribution  $q_g(\tilde{g}|g)$ . Let  $\tilde{G}$  denote the adjacency matrix of  $\tilde{g}$ .

**Step 2** Generate  $\tilde{Y} \sim N(\tilde{Y}^*, \Sigma_{\tilde{Y}})$ , where  $\tilde{Y}^* \equiv (I_n - \lambda\tilde{G})^{-1}B(X)$ , with  $B(X) = [b(X_1), \dots, b(X_n)]'$ , is the equilibrium effort vector derived from the best response function (3), and  $\Sigma_{\tilde{Y}} = \sigma^2(I_n - \lambda\tilde{G})^{-1}$ .

**Step 3** Accept  $(\tilde{g}, \tilde{Y})$  according to the acceptance probability

$$\begin{aligned} \alpha_{(g,Y),MH} &= \min \left\{ 1, \frac{\pi(\tilde{g}, \tilde{Y}|\theta)p_Y(Y|g)q_g(g|\tilde{g})}{\pi(g, Y|\theta)p_Y(\tilde{Y}|\tilde{g})q_g(\tilde{g}|g)} \right\} \\ &= \min \left\{ 1, \frac{\exp[\sigma^{-2}Q(\tilde{g}, \tilde{Y}|\gamma)]p_Y(Y|g)q_g(g|\tilde{g})}{\exp[\sigma^{-2}Q(g, Y|\gamma)]p_Y(\tilde{Y}|\tilde{g})q_g(\tilde{g}|g)} \right\}, \end{aligned}$$

where  $p_Y(\tilde{Y}|\tilde{g})$  denotes the density function of  $N(\tilde{Y}^*, \Sigma_{\tilde{Y}})$ .

In the following proposition, we show that the long run stationary distribution of the proposed MH algorithm is the Gibbs measure defined in Equation (8).

**Proposition 3.** *The unique stationary distribution of Algorithm 2 is  $\pi(g, Y|\theta)$ .*

**Remark 4.** If Step 1 of Algorithm 2 adopts a local sampler, where only one randomly selected link is updated at each iteration, the convergence can be slow as shown in Mele (2017). Therefore, we follow Mele's suggestion (see Appendix B of Mele, 2017) to allow for large steps, where multiple links are swapped at the same time, to improve convergence.

**Remark 5.** In Step 2 of Algorithm 2, we generate  $\tilde{Y}$  from a multivariate normal distribution because (i) it is computationally simple to sample from a normal distribution, and (ii) it resembles the effort adjustment process described in Section 2.2. To see the second point, we assume that link adjustment periods arrive much less frequent than effort adjustment periods in the coevolution process. Given the network  $\tilde{g}$ , it follows a standard Gibbs sampler argument that the transition density defined in Equation (6) converges to

$$p_Y(\tilde{Y}|\tilde{g}) = \frac{\exp[\sigma^{-2}Q(\tilde{g}, \tilde{Y})]}{\int_{\mathcal{Y}^n} \exp[\sigma^{-2}Q(\tilde{g}, Y)]dY}. \quad (10)$$

where

$$\begin{aligned} Q(g, Y) &= a(g) + \sum_{i \in \mathcal{N}} b(X_i)y_i + \frac{\lambda}{2} \sum_{i \in \mathcal{N}} \sum_{j \in \mathcal{N}} g_{ij}y_i y_j - \frac{1}{2} \sum_{i \in \mathcal{N}} y_i^2 \\ &= a(g) + B(X)'Y - \frac{1}{2}Y'(I_n - \lambda G)Y. \end{aligned} \quad (11)$$

Inserting Equation (11) into Equation (10), it follows by the Gaussian integral formula (Bronshtein et al., 2015) that

$$\begin{aligned} p_Y(\tilde{Y}|\tilde{g}) &= \frac{\exp[\sigma^{-2}B(X)'\tilde{Y} - \frac{1}{2}\sigma^{-2}\tilde{Y}'(I_n - \lambda\tilde{G})\tilde{Y}]}{\int_{\mathcal{Y}^n} \exp[\sigma^{-2}B(X)'Y - \frac{1}{2}\sigma^{-2}Y'(I_n - \lambda\tilde{G})Y]dY} \\ &= (2\pi)^{-n/2} |\det \Sigma_{\tilde{Y}}|^{-1/2} \exp[-\frac{1}{2}(\tilde{Y} - \tilde{Y}^*)'\Sigma_{\tilde{Y}}^{-1}(\tilde{Y} - \tilde{Y}^*)], \end{aligned}$$

which is the density function of  $N(\tilde{Y}^*, \Sigma_{\tilde{Y}})$ .

**Remark 6.** In Algorithm 2, we often need to evaluate  $(I_n - \lambda\tilde{G})^{-1}$  and  $\det(I_n - \lambda\tilde{G})$ , where  $\tilde{G}$  is the adjacency matrix of the network  $\tilde{g}$  resulting from adding/removing a link to/from the network  $g$ . The computational cost of the inverse and determinant can be high when the network size is large. To alleviate the computational burden, we adopt a matrix perturbation technique detailed in the online appendix, and derive a result that facilitates the computation of  $(I_n - \lambda\tilde{G})^{-1}$  and  $\det(I_n - \lambda\tilde{G})$  when  $(I_n - \lambda G)^{-1}$  and  $\det(I_n - \lambda G)$  are

known.

### 3.3 Unobserved Heterogeneity

The structural model introduced in Section 2 allows some component of exogenous characteristics  $X_i$  to be unobservable to the econometrician. More specifically, let  $X_i = [X_i^O, x_i^U]$ , where  $X_i^O = (x_{i1}^O, \dots, x_{iK}^O)$  is a  $K$ -dimensional vector of exogenous characteristics observable to the econometrician and  $x_i^U \sim i.i.d.(0, \varsigma_x^2)$  is a scalar random variable capturing *unobserved heterogeneity*. Further, let  $Z_{ij}$  be a vector of dyad-specific exogenous characteristics based on  $X_i^O$  and  $X_j^O$ . For example, one could define the  $l$ th element of  $Z_{ij}$  as  $z_{ij,l} = |x_{il}^O - x_{jl}^O|$  if  $x_{il}^O$  is a continuous variable or  $z_{ij,l} = 1(x_{il}^O = x_{jl}^O)$  if  $x_{il}^O$  is a binary indicator variable. In the empirical model, we assume that  $b(X_i)$  in Equation (1) is given by

$$b(X_i) = \beta_0 + X_i^O \beta_1 + \beta_2 x_i^U \quad (12)$$

and  $h(X_i, X_j, \delta_1)$  in Equation (2) is given by

$$h(X_i, X_j, \delta_1) = Z_{ij} \delta_1 + x_i^U + x_j^U. \quad (13)$$

As the unobserved heterogeneity shows up in both the *direct* utility from links and the *direct* utility from effort, it introduces an additional layer of correlation between links and effort.

We regard  $x^U = (x_1^U, \dots, x_n^U)'$  as individual random effects with a density function denoted by  $p(x^U)$ . Instead of sampling  $\theta$  from the marginal posterior distribution

$$p(\theta|g, Y) = \int p(\theta|g, Y, x^U) p(x^U) dx^U,$$

which does not have a closed form expression, we adopt the Bayesian data augmentation approach (Tanner and Wong, 1987; Albert and Chib, 1993) to sample  $\theta$  together with  $x^U$  from the joint posterior distribution  $p(\theta, x^U|g, Y) \propto \pi(g, Y|\theta, x^U) p(\theta) p(x^U)$  in the MCMC

procedure. The details of the MCMC procedure can be found in the online appendix.

### 3.4 Monte Carlo Experiments

We conduct a Monte Carlo simulation with 100 repetitions to examine the performance of the proposed MCMC procedure. In each repetition, we generate a network of size  $n = 100$  and the corresponding effort levels according to the Gibbs measure defined in Equation (8). The detailed data generating process (DGP) runs as follows. First, we generate exogenous individual characteristics  $x_i^O$  and  $x_i^U$  in Equation (12) from log-normal distribution  $\ln x_i^O \sim N(1.5, 0.5)$  and normal distribution  $x_i^U \sim N(0, 1)$ , respectively, with the coefficients  $\beta_1 = 0.5$  and  $\beta_2 = 0.5$ .<sup>7</sup> The dyad variable  $Z_{ij}$  in Equation (13) is generated by  $Z_{ij} = |x_i^O - x_j^O|$  using the variable  $x_i^O$  previously produced. We set the spillover effect  $\lambda = 0.03$ , the fixed linking cost  $\delta_0 = -2.5$ , the homophily effect  $\delta_1 = 0.5$ , the congestion effect  $\delta_2 = -0.25$ , the cyclic triangle effect  $\delta_3 = 0.15$ , and the noise parameter  $\sigma^2 = 0.5$ .<sup>8</sup> Then, we generate the network and effort levels by Algorithm 2 in Section 3.2 with 1,000,000 iterations and treat the realization of the last iteration as the generated sample. On average, the generated network has the average degree equals to 3.306, the density equals to 0.033, and the clustering coefficient equals to 0.028. The average effort level is 2.952.

We perform the MCMC procedure for estimation, with and without controlling for unobserved heterogeneity, for 20,000 iterations. We drop the first 10,000 draws for burn-in and use the rest draws for computing the posterior mean as the estimate of each parameter. The simulation results are reported in Table 1 and the values reported are the mean and standard deviation of the 100 repetitions.

*[insert Table 1 here]*

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<sup>7</sup>We suppress the intercept  $\beta_0$  in Equation (12) in the Monte Carlo experiment.

<sup>8</sup>The parameter values we choose in the Monte Carlo experiment are comparable to the empirical estimates in Section 4.

From the estimation results of Model 1 reported in the left panel of Table 1, we can see that the spillover effect  $\lambda$  is overestimated by 54.3% when unobserved heterogeneity is not controlled for. The estimates of other parameters are also affected: the estimate of  $\beta_1$  is downward biased by 9.7%; the estimates of the fixed linking cost  $\delta_0$  and the homophily effect  $\delta_1$  are downward biased by 14.1% and 38.5%, respectively; the estimates of the congestion effect  $\delta_2$  and the cyclic triangle effect  $\delta_3$  are upward biased by 58.6% and 28.4%, respectively; and the estimate of the noise parameter  $\sigma^2$  is also upward biased by 31.2%. These numbers reveal that neglecting unobserved heterogeneity could cause severe biases in the estimation. On the other hand, the estimation results of Model 2 reported in the right panel of Table 1 show that the proposed MCMC procedure can successfully recover the true model parameters under the correct model specification that takes unobserved heterogeneity into account.

Furthermore, to see how ignoring unobserved heterogeneity affects the direction of estimation bias of the spillover effect parameter  $\lambda$ , we redo the simulation experiment with  $\beta_2 = -0.5$  and other parameters unchanged. The simulation results are reported in Table 2. Comparing Tables 1 and 2, we find that the spillover effect parameter  $\lambda$  is overestimated when  $\beta_2$  is positive and underestimated when  $\beta_2$  is negative. Our intuition for this result is the following. In Equation (13),  $x^U$  captures the unobserved degree heterogeneity (Graham, 2017). That is, an agent with a higher  $x^U$  is likely to form more links. If  $\beta_2 > 0$  in Equation (12), then an agent with a higher tendency to form links is likely to spend more effort. Thus, ignoring  $x^U$  would confound this effect with the spillover effect and lead to an upward bias for the estimated spillover effect. For the same reason, when  $\beta_2 < 0$ , ignoring  $x^U$  would cause a downward bias on the estimated spillover effect.<sup>9</sup>

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*[insert Table 2 here]*

<sup>9</sup>More simulation results on the performance of the proposed MCMC procedure can be found in the online appendix.

## 4 Empirical Illustration

To illustrate the empirical relevance of our model and estimation strategy, we apply it to study R&D investment and collaborations. R&D collaborations have become a widespread phenomenon especially in industries with rapid technological innovations such as the chemical and pharmaceutical industries (Hagedoorn, 2002; Roijakkers and Hagedoorn, 2006). Through such collaborations firms generate knowledge spillovers not only to their collaboration partners but also to other firms that are indirectly connected to them within a complex R&D network (König et al., 2019). The network perspective is thus crucial to understand outcomes in R&D intensive markets where collaborations can be frequently observed (Powell et al., 1996, 2005).

### 4.1 A Simple Model of R&D Collaborations

The microfoundation of our empirical illustration is a Cournot competition model with firms engaging in R&D investment and collaborations to lower production cost. This model has been adopted by d’Aspremont and Jacquemin (1988), Goyal and Moraga-Gonzalez (2001), Petrakis and Tsakas (2018) and König et al. (2019) to study R&D networks. More specifically, consider a set of firms  $\mathcal{N} = \{1, \dots, n\}$  with their characteristics given by  $X_i$ . Firms can reduce their production costs by investing in R&D as well as by benefiting from an R&D collaboration with another firm. The amount of cost reduction depends on the R&D effort  $y_i$  of firm  $i$  and the R&D efforts of firm  $i$ ’s collaboration partners. The marginal *production cost*  $c_i$  of firm  $i$  is given by

$$c_i = -b_1(X_i) - y_i - \lambda \sum_{j=1}^n g_{ij}y_j, \quad (14)$$

where  $b_1(X_i)$  captures firm heterogeneity with regard to productivity and  $g_{ij}$  indicates whether firms  $i$  and  $j$  have an R&D collaboration. The parameter  $\lambda$  captures the *knowledge spillover* effect. We assume that the cost of R&D effort is given by  $\frac{1}{2}y_i^2$ . We further assume it

is costly to maintain R&D collaborations with the *collaboration cost* given by  $-a_i(g)$ . With output  $q_i$ , firm  $i$ 's profit is given by

$$\Pi_i = (p_i - c_i)q_i - \frac{1}{2}y_i^2 + a_i(g), \quad (15)$$

where  $p_i$  is the price of the good produced by firm  $i$ . We assume firms are local monopolies with the inverse demand function  $p_i = b_0 - q_i$ , where  $b_0$  represents the market size. Substitution of the inverse demand function and Equation (14) into Equation (15) yields

$$\Pi_i = [b_0 - q_i + b_1(X_i) + y_i + \lambda \sum_{j=1}^n g_{ij}y_j]q_i - \frac{1}{2}y_i^2 + a_i(g). \quad (16)$$

Profit maximization with respect to  $y_i$  gives  $q_i = y_i$ . Substitution of  $q_i = y_i$  into Equation (16) gives

$$\Pi_i = a_i(g) + b(X_i)y_i + \lambda \sum_{j=1}^n g_{ij}y_iy_j - \frac{1}{2}y_i^2, \quad (17)$$

where  $b(X_i) = b_0 + b_1(X_i)$ . Equation (17) conforms to the general payoff function defined in Equation (1). In the empirical study, we assume that  $a_i(g)$  is given by Equation (2) with  $h(X_i, X_j, \delta_1)$  defined in Equation (13) and that  $b(X_i)$  is given by Equation (12).

## 4.2 Data

In the empirical illustration, we focus on the sector ‘‘Chemicals and Allied Products’’ (with two-digit SIC code 28), as it is one of the most active sectors regarding R&D collaborations. Our data of inter-firm R&D collaborations stems from two sources which have been widely used in the literature (Schilling, 2009). The first is the Cooperative Agreements and Technology Indicators (CATI) database (Hagedoorn, 2002). The database only records agreements for which a combined innovative activity or an exchange of technology is at least part of the agreement. The second is the Thomson Securities Data Company (SDC) alliance database. SDC collects data from the U.S. Securities and Exchange Commission (and their interna-

tional counterparts) filings, trade publications, wires, and news sources. We include only alliances from SDC which are classified explicitly as R&D collaborations.<sup>10</sup> We then merge the CATI database with the Thomson SDC alliance database. For the matching of firms across datasets we adopt and extend the name matching algorithm developed as part of the NBER patent data project (Trajtenberg et al., 2009).<sup>11</sup> The systematic collection of inter-firm alliances in CATI started in 1987 and ended in 2006. We take 2006 as the base year and assume that an alliance lasts for 5 years (Rosenkopf and Padula, 2008). We construct the R&D collaboration network by coding  $g_{ij}$  as one if an alliance between firms  $i$  and  $j$  exists in 2006, and zero otherwise.

The combined CATI-SDC database only provides the names of the firms in an alliance. To obtain information about their balance sheets and income statements we match the firms' names in the CATI-SDC database with the firms' names in Standard & Poor's Compustat U.S. and Global Fundamentals databases, as well as Bureau van Dijk's Orbis database (Bloom et al., 2013). For the purpose of matching firms across databases, we employ the above mentioned name matching algorithm. Compustat and Orbis databases only contain firms listed on the stock market, so they typically exclude small private firms. However, they should include most R&D intensive firms, as R&D is typically concentrated in publicly listed firms (Bloom et al., 2013).

We use a firm's log-R&D expenditure to measure its R&D effort. Moreover, the firms' productivities are measured by their log-R&D capital stocks (lagged by one year). As in Hall et al. (2000), Bloom et al. (2013) and König et al. (2019), the R&D capital stock is computed using a perpetual inventory method based on the firms' R&D expenditures with

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<sup>10</sup>For a comparison and summary of different alliance databases, including CATI and SDC, see Schilling (2009).

<sup>11</sup>See <https://sites.google.com/site/patentdataproyect>. We would like to thank Enghin Atalay and Ali Hortacsu for sharing their name matching algorithm with us.



a 15% depreciation rate. We drop firm observations with missing values on either R&D expenditure or R&D capital stock which results in a sample of 347 firms and 139 R&D alliances in the SIC-28 sector. The SIC-28 sector has eight sub-sectors coded with 3-digit SIC codes. Among them, the sub-sector “Drugs” (SIC-283) is the largest in our sample with 256 firms and 119 R&D alliances. Descriptive statistics of the sample are shown in Table 3.

[insert Table 3 here]

### 4.3 Estimation Results

Assuming the observed R&D expenditures and collaborations follow the stationary distribution defined in Equation (8), we estimate the model parameters using the MCMC procedure described in Section 3. We run the MCMC algorithm for 35,000 iterations and drop the first 5,000 draws for burn-in and keep every 20th of the remaining draws to conduct the posterior analysis, i.e., compute the posterior mean (as a point estimate) and posterior variance for each parameter. To check the convergence of the MCMC algorithm, we provide the trace plot of draws for the spillover effect parameter  $\lambda$  in Figure 2. The trace plot of MCMC draws for  $\lambda$  and its posterior distribution in the upper and middle panels show that the MCMC draws are stable and have good variations. The autocorrelation function (ACF) plotted in the bottom panel indicates that the correlation among draws decline gradually over iterations. The draws pass the convergence diagnostic test of Geweke (1992) with a p-value of 0.4698.<sup>12</sup>

[insert Figure 2 here]

[insert Table 4 here]

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<sup>12</sup>The convergence diagnostic test tests for an equal mean of the first 10% versus the last 50% of the draws. We also try different proportions (e.g., 30% versus 70%), and obtain similar results for the convergence of the MCMC algorithm.

The estimation results are reported in Table 4. To capture firm heterogeneity in the marginal production cost given by Equation (14), we include a productivity measure defined as a firm’s one-year-lagged log-R&D capital stock and sub-sector dummies (defined at the 3-digit SIC level). As expected, the estimate of  $\beta_1$  shows that higher time-lagged R&D capital stock reduces the marginal production cost.

The estimated spillover effect  $\lambda$  is statistically significant. As the estimated coefficient  $\beta_2$  of unobserved heterogeneity in the marginal production cost is statistically insignificant, the spillover effect is only slightly overestimated when unobserved heterogeneity is ignored. On the other hand, unobserved heterogeneity still plays an important role in the estimation of the collaboration cost given by Equation (2). When unobserved heterogeneity is controlled for, we find that the collaboration cost is lower between firms in the same sub-sector (reflected by  $\delta_{11}$ ; the *homophily* effect), firms with different productivities (reflected by  $\delta_{12}$ ; the *heterophily* effect), and firms with a common collaboration partner (reflected by  $\delta_3$ ; the *cyclic triangle* effect). A firm is less likely to form a new link if it has many existing R&D collaborations (reflected by  $\delta_2$ ; the *congestion* effect).

[insert Figure 3 here]

Finally, we evaluate the model’s goodness-of-fit following Hunter et al. (2008). We generate 1000 networks with the estimates of Model 1 and Model 2 reported in Table 4 respectively. The model’s goodness-of-fit is examined by comparing the 1000 generated networks with the observed network in terms of three network statistics: the degree (the number of links of a firm), the minimum geodesic distance (the number of links in the shortest path between two firms), and the number of edge-wise shared partners (the number of shared partners of two connected firms). The degree is included because it is a fundamental measure of network structure and it often does a reasonably good job of explaining other higher-order network statistics (Faust, 2007; Graham, 2015). The geodesic distance is included because it is relevant to the speed of knowledge diffusion, which is especially important for R&D networks. The geodesic distance is also the basis of some well-known network centrality

measures (Wasserman and Faust, 1994). The number of edge-wise shared partners is included based on the work by Snijders et al. (2006). The three network statistics are related to different aspects of network structure and provide independent criteria for goodness-of-fit.

We plot the distributions of the three network statistics of the observed network (in solid lines) and the corresponding means and 95% confidence intervals of the 1000 generated networks (in dashed lines) for both models in Figure 3. From the figure we can see that Model 2 provides a better fit to the observed network than Model 1. We also calculate the spectral goodness-of-fit (SGOF) proposed by Shore and Lubin (2015) for both models. The SGOF is analogous to the standard  $R^2$  in a linear regression. It measures how well a network model explains the structure of an observed network based on the spectrum of the graph Laplacian. We calculate the SGOF based on the 1000 networks previously generated, and find that Model 2 improves the goodness-of-fit of Model 1 by 51% and this improvement is significant at the 5% level.<sup>13</sup>

#### 4.4 Key Player Analysis

*[insert Table 5 here]*

With the estimates of Model 2 reported in the right panel of Table 4, we can conduct the key player analysis described in Section 2.3. We consider both short-run and long-run key player analyses. For the short-run key player analysis, we assume the network does not rewire after a firm is removed. For the long-run key player analysis, we simulate the coevolution process of R&D investment and collaborations for the remaining  $n - 1$  firms using Algorithm 2 in Section 3.2 after a firm is removed. We run the simulation for  $n^2$  iterations and use the observation of the last iteration to calculate the welfare loss. We then repeat this procedure 200 times and report the average welfare loss of removing that firm. The results for the key player analysis are reported in Table 5. Some main findings are summarized as follows.

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<sup>13</sup>The details on how to calculate the SGOF can be found in the online appendix.

- In general, the welfare loss is lower in the long run, because firms can mitigate the welfare loss by forming new links with other remaining firms.
- The short-run and long-run key player rankings do not always coincide with each other. However, there is a high correlation (0.9277) between short-run and long-run welfare losses. This suggests the key player analysis has some robustness with respect to the invariant network assumption.
- The long-run welfare loss is highly correlated with the log-R&D expenditure, degree centrality, betweenness centrality, closeness centrality, and eigenvector centrality with correlation coefficients 0.7378, 0.8829, 0.8222, 0.7974, and 0.8368 respectively. Therefore, the key player ranking incorporates information on both R&D investment and network centrality of a firm.

## 5 Conclusion

This paper proposes a structural model for the coevolution of networks and behavior. We provide a microfoundation for the model and characterize the equilibrium of the coevolution process. We show the model can be estimated using an MCMC algorithm and investigate the finite sample performance of the estimation procedure in a Monte Carlo simulation experiment. We then apply the model to study R&D investment and collaboration decisions in the chemicals and pharmaceutical industry and find a positive knowledge spillover effect. We also demonstrate how to use the model estimates to conduct a long-run key player analysis.

Due to the generality of the utility function we consider, we believe that our structural framework – from both theoretical and empirical perspectives – can be applied to a variety of related contexts, where externalities can be modelled in the form of an adaptive network. Examples include peer effects in education, crime, risk sharing, scientific coauthorship, etc. (Jackson and Zenou, 2014).

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Table 1: Monte Carlo simulation results (Part I)

	True value	Model 1		Model 2	
$\lambda$	0.0300	0.0463	(0.0117)	0.0280	(0.0049)
$\beta_1$	0.5000	0.4516	(0.0332)	0.5029	(0.0220)
$\beta_2$	0.5000			0.4930	(0.0591)
$\delta_0$	-2.5000	-2.8531	(0.5701)	-2.4361	(0.3476)
$\delta_1$	0.5000	0.3075	(0.0786)	0.5332	(0.0708)
$\delta_2$	-0.2500	-0.1035	(0.0548)	-0.2860	(0.0700)
$\delta_3$	0.1500	0.1927	(0.0929)	0.1423	(0.0417)
$\sigma^2$	0.5000	0.6562	(0.1136)	0.4755	(0.0735)
$\zeta_x^2$	1.0000			1.1684	(0.1410)

*Notes:* Model 1 ignores unobserved heterogeneity and Model 2 controls for unobserved heterogeneity. Standard deviations in parentheses.

Table 2: Monte Carlo simulation results (Part II)

	True value	Model 1		Model 2	
$\lambda$	0.0300	-0.0027	(0.0092)	0.0316	(0.0077)
$\beta_1$	0.5000	0.5531	(0.0197)	0.5009	(0.0187)
$\beta_2$	-0.5000			-0.4675	(0.0441)
$\delta_0$	-2.5000	-2.9573	(0.3369)	-2.4445	(0.3690)
$\delta_1$	0.5000	0.3266	(0.0808)	0.5371	(0.0744)
$\delta_2$	-0.2500	-0.0593	(0.0478)	-0.2951	(0.0748)
$\delta_3$	0.1500	0.2172	(0.1075)	0.1513	(0.0452)
$\sigma^2$	0.5000	0.7023	(0.0715)	0.4663	(0.0904)
$\zeta_x^2$	1.0000			1.1993	(0.1549)

*Notes:* Model 1 ignores unobserved heterogeneity and Model 2 controls for unobserved heterogeneity. Standard deviations in parentheses.

Table 3: Descriptive statistics.

Sector	# of firms	log-R&D expenditure			productivity			# of R&D alliances		
		mean	min	max	mean	min	max	mean	min	max
SIC-28	347	9.6574	3.2109	15.2467	11.1018	5.0706	16.8160	0.8012	0	15
SIC-283	256	9.4861	3.2109	15.2467	10.8352	5.0706	16.8160	0.9297	0	15

*Notes:* R&D expenditure is measured by thousand U.S. dollars in 2006. A firm's productivity is measured by its log-R&D capital stock (lagged by one year).

Table 4: Estimation results.

		Model 1		Model 2	
spillover effect	$(\lambda)$	0.0125	(0.0027)***	0.0113	(0.0021)***
<b>Production Cost</b>					
productivity	$(\beta_1)$	0.8599	(0.0284)***	0.8807	(0.0074)***
unobs. heterogeneity	$(\beta_2)$			0.0275	(0.0219)
sub-sector dummies		Yes		Yes	
<b>Collaboration Cost</b>					
constant	$(\delta_0)$	-4.6716	(0.6963)***	-4.2383	(0.4652)***
same sub-sector	$(\delta_{11})$	0.8086	(0.2420)***	0.6498	(0.1115)***
diff-in-productivity	$(\delta_{12})$	0.0618	(0.0461)	0.1599	(0.0332)***
congestion	$(\delta_2)$	0.0319	(0.0355)	-0.2215	(0.0635)***
cyclic triangle	$(\delta_3)$	0.3151	(0.1386)**	0.1219	(0.0565)**
<b>Noise Parameters</b>					
noise in decisions	$(\sigma^2)$	0.4833	(0.0744)***	0.2674	(0.0481)***
unobs. heterogeneity	$(\zeta_x^2)$			0.7697	(0.0773)***

*Notes:* Model 1 ignores unobserved heterogeneity and Model 2 controls for unobserved heterogeneity. Standard errors in parentheses. \*\*\*, \*\*, and \* indicate that the highest density range does not cover zero at 99%, 95%, and 90% levels.

Table 5: Key player ranking.

	log-R&D expenditure	degree	short run		long run	
			welfare loss	rank	welfare loss	rank
Pfizer Inc.	15.2467	15	-0.5322	1	-0.4224	1
Novartis	14.7913	15	-0.4789	2	-0.3697	2
Amgen Inc	14.6398	13	-0.3837	5	-0.2848	3
Johnson & Johnson Inc	15.1535	7	-0.4254	3	-0.2767	4
Merck & Co Inc	14.6794	10	-0.4178	4	-0.2714	5
Bayer	14.1742	10	-0.3755	7	-0.2522	6
Bristol-Myers Squibb Co	14.2351	6	-0.3775	6	-0.2137	7
Wyeth	14.2487	2	-0.3123	8	-0.1471	8
Takeda Pharmaceutical Co Ltd	13.6225	7	-0.2749	11	-0.1454	9
Abbott Laboratories Inc.	14.5658	3	-0.3119	9	-0.1398	10

*Notes:* In the short run, the remaining network is assumed to be fixed after a firm exits. In the long run, the network evolves to a new equilibrium after a firm exits. R&D expenditure is measured by thousand U.S. dollars in 2006. Welfare loss is measured in percentage.

Figure 1: Interdependence between networks and behavior in R&D networks.

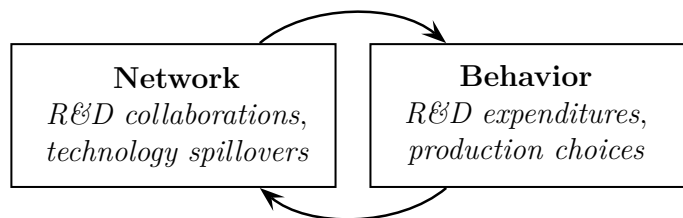




Figure 2: Trace plot for MCMC draws of  $\lambda$ .

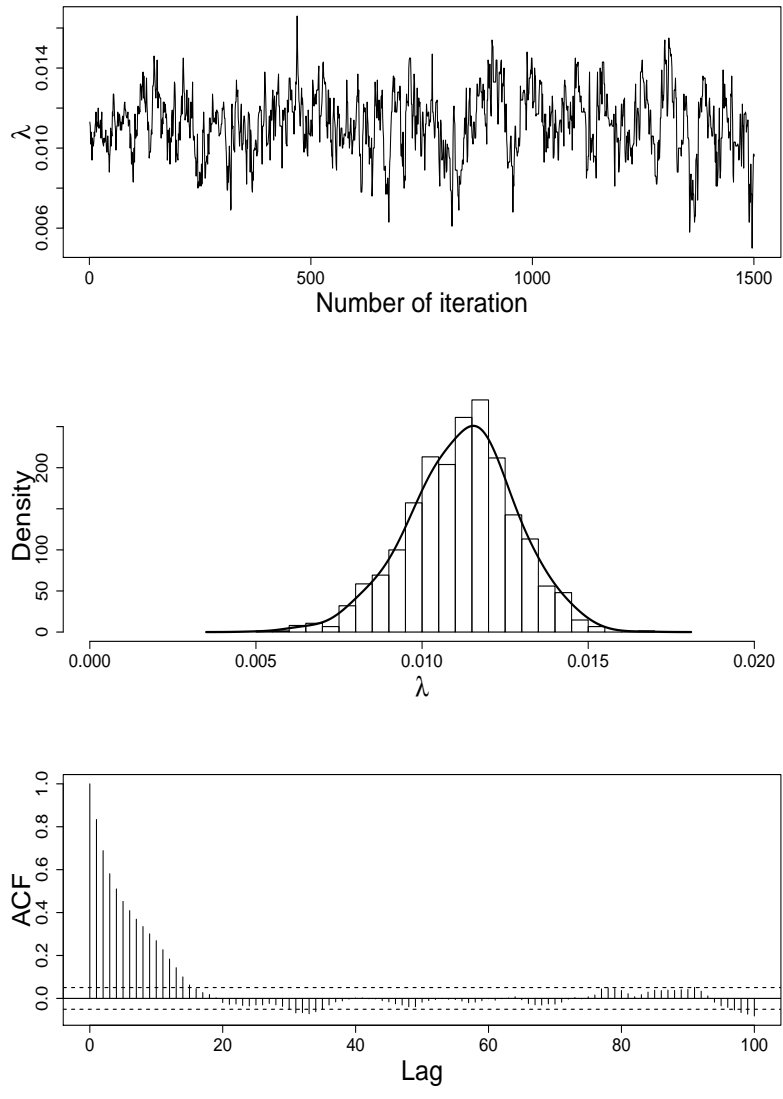
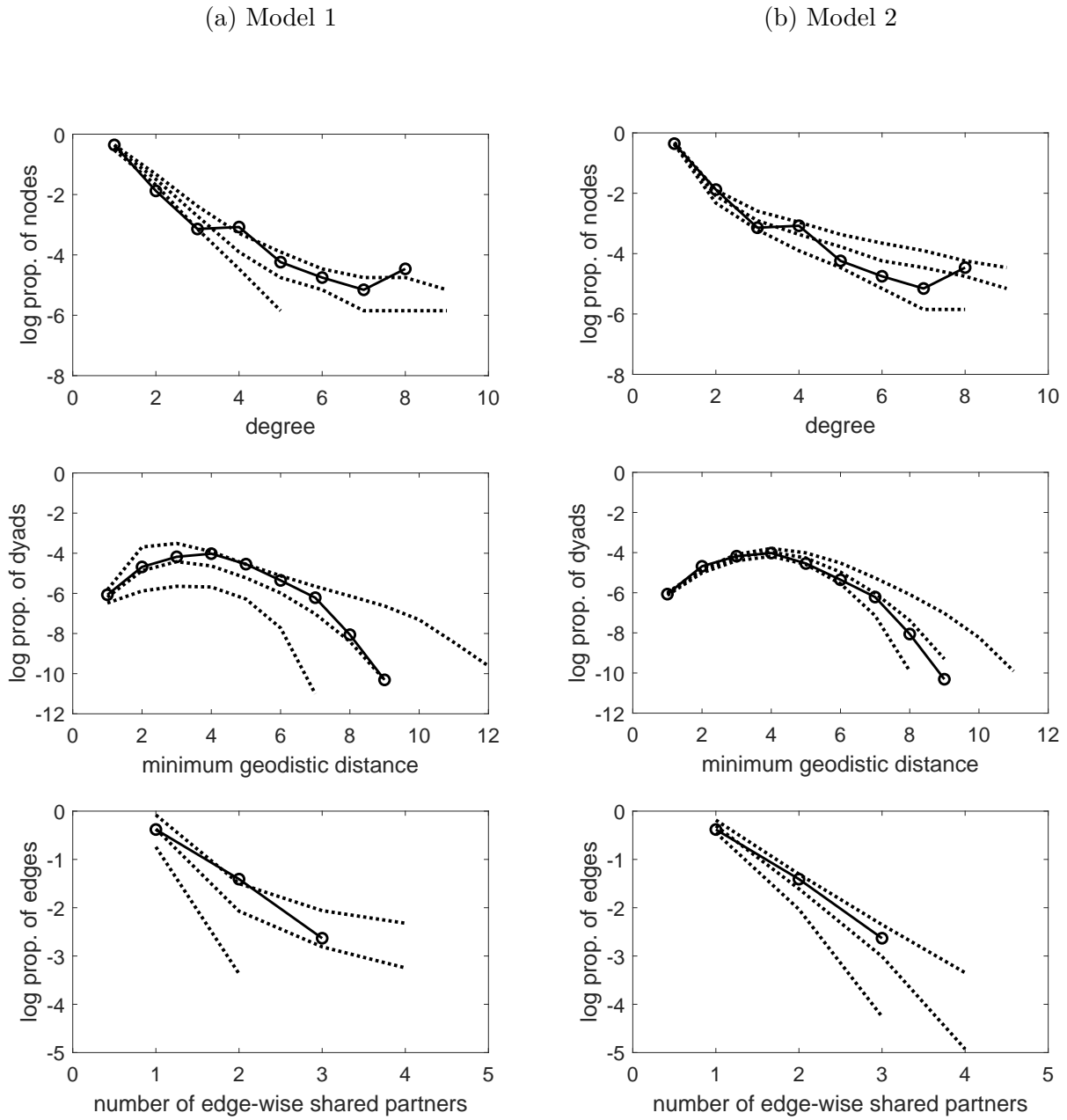


Figure 3: Goodness-of-fit statistics.



*Notes:* Network statistics of the observed network are in solid lines and the corresponding means and 95% confidence intervals of the 1000 generated networks are in dashed lines.

# Online Appendix for “A Structural Model for the Coevolution of Networks and Behavior”

by Chih-Sheng Hsieh, Michael D. König, and Xiaodong Liu

## A Proofs

*Proof of Proposition 1.* The proof consists of two parts. Part (I) proves that  $Q(g, Y, X)$  defined in Equation (7) is the potential function. Part (II) proves the Gibbs measure given in Equation (8) is the unique stationary distribution of the coevolution process.

(I) First, we consider the case where the effort level of agent  $i$  is updated from  $y_0$  to  $y_1$ , while  $g$  and  $Y_{-i}$  remain unchanged. In this case,

$$\begin{aligned} & Q(g, y_i = y_1, Y_{-i}, X) - Q(g, y_i = y_0, Y_{-i}, X) \\ &= b(X_i)(y_1 - y_0) + \lambda(y_1 - y_0) \sum_{j \in \mathcal{N}} g_{ij} y_j - \frac{1}{2}(y_1^2 - y_0^2) \\ &= U_i(g, y_i = y_1, Y_{-i}, X) - U_i(g, y_i = y_0, Y_{-i}, X). \end{aligned}$$

Next, we consider the case where the network is updated from  $g_0 = \{g_{ij} = 0, g_{-ij}\}$  to  $g_1 = \{g_{ij} = 1, g_{-ij}\}$ , while  $Y$  remains unchanged. In this case,

$$Q(g_1, Y, X) - Q(g_0, Y, X) = a(g_1, X) - a(g_0, X) + \lambda y_i y_j.$$

As

$$\begin{aligned} a(g_1, X) - a(g_0, X) &= \delta_0 + h_{ij}(\delta_1) + \delta_2 \sum_{k \in \mathcal{N} \setminus \{i, j\}} (g_{ik} + g_{jk}) + 2\delta_3 \sum_{k \in \mathcal{N} \setminus \{i, j\}} g_{ik} g_{jk} \\ &= \frac{1}{2}[a_i(g_1, X) + a_j(g_1, X)] - \frac{1}{2}[a_i(g_0, X) + a_j(g_0, X)], \end{aligned}$$

we have

$$Q(g_1, Y, X) - Q(g_0, Y, X) = \bar{U}_{ij}(g_1, Y, X) - \bar{U}_{ij}(g_0, Y, X).$$

Therefore,  $Q(g, Y, X)$  defined in Equation (7) is the potential function.

(II) The sequence  $\{(g_t, Y_t)\}$  is a Markov chain. A sufficient condition for the stationarity of the Gibbs measure given in Equation (8) is the detailed balance condition, i.e.,  $\pi(\omega_0)p(\omega_0, \omega_1) = \pi(\omega_1)p(\omega_1, \omega_0)$ , where  $p(\omega_0, \omega_1)$  is the transition density from state  $\omega_0$  to state  $\omega_1$ . Here, we only need to verify the detailed balance condition for (i)  $\omega_0$  and  $\omega_1$  differ by only one element of  $g$  and (ii)  $\omega_0$  and  $\omega_1$  differ by only one element of  $Y$ , since the transition density for other cases is zero.

(i)  $\omega_0$  and  $\omega_1$  differ by only one element of  $g$ . Let  $\omega_0 = (g_{ij} = 0, g_{-ij}, Y)$  and  $\omega_1 = (g_{ij} = 1, g_{-ij}, Y)$ . Then,

$$\begin{aligned} & \pi(\omega_0)p(\omega_0, \omega_1) \\ = & \pi(\omega_0)\rho_0\rho(g_{t-1}, X_i, X_j) \frac{\exp[\sigma^{-2}Q(g_{ij} = 1, g_{-ij}, Y)]}{\exp[\sigma^{-2}Q(g_{ij} = 0, g_{-ij}, Y)] + \exp[\sigma^{-2}Q(g_{ij} = 1, g_{-ij}, Y)]} \\ = & \pi(\omega_1)\rho_0\rho(g_{t-1}, X_i, X_j) \frac{\exp[\sigma^{-2}Q(g_{ij} = 0, g_{-ij}, Y)]}{\exp[\sigma^{-2}Q(g_{ij} = 0, g_{-ij}, Y)] + \exp[\sigma^{-2}Q(g_{ij} = 1, g_{-ij}, Y)]} \\ = & \pi(\omega_1)p(\omega_1, \omega_0). \end{aligned}$$

(ii)  $\omega_0$  and  $\omega_1$  differ by only one element of  $Y$ . Let  $\omega_0 = (g, y_0, Y_{-i})$  and  $\omega_1 = (g, y_1, Y_{-i})$ .

Then,

$$\begin{aligned}
& \pi(\omega_0)p(\omega_0, \omega_1) \\
= & \pi(\omega_0)(1 - \rho_0)\rho(X_i) \frac{\exp[\sigma^{-2}U_i(g, y_1, Y_{-i})]}{\int_{\mathcal{Y}} \exp[\sigma^{-2}U_i(g, y, Y_{-i,t-1})]dy} \\
= & \pi(\omega_0)(1 - \rho_0)\rho(X_i) \frac{\exp[\sigma^{-2}Q(g, y_1, Y_{-i})]}{\int_{\mathcal{Y}} \exp[\sigma^{-2}Q(g, y, Y_{-i,t-1})]dy} \\
= & \pi(\omega_1)(1 - \rho_0)\rho(X_i) \frac{\exp[\sigma^{-2}Q(g, y_0, Y_{-i})]}{\int_{\mathcal{Y}} \exp[\sigma^{-2}Q(g, y, Y_{-i,t-1})]dy} \\
= & \pi(\omega_1)(1 - \rho_0)\rho(X_i) \frac{\exp[\sigma^{-2}U_i(g, y_0, Y_{-i})]}{\int_{\mathcal{Y}} \exp[\sigma^{-2}U_i(g, y, Y_{-i,t-1})]dy} \\
= & \pi(\omega_1)p(\omega_1, \omega_0).
\end{aligned}$$

The desired result follows by the reversibility, irreducibility, and Harris recurrence of the Markov chain. ■

*Proof of Proposition 2.* To show  $p(\theta|g, Y)$  is the stationary distribution, we need to check the detailed balance condition, i.e.,  $p(\theta|g, Y)p(\tilde{\theta}|\theta) = p(\tilde{\theta}|g, Y)p(\theta|\tilde{\theta})$  where

$$p(\tilde{\theta}|\theta) = q_{\theta}(\tilde{\theta}|\theta)\pi(\tilde{g}, \tilde{Y}|\tilde{\theta}) \min \left\{ 1, \frac{p(\tilde{\theta}|g, Y)q_{\theta}(\theta|\tilde{\theta})\pi(\tilde{g}, \tilde{Y}|\theta)}{p(\theta|g, Y)q_{\theta}(\tilde{\theta}|\theta)\pi(\tilde{g}, \tilde{Y}|\tilde{\theta})} \right\}.$$

Indeed,

$$\begin{aligned}
p(\theta|g, Y)p(\tilde{\theta}|\theta) &= p(\theta|g, Y)q_{\theta}(\tilde{\theta}|\theta)\pi(\tilde{g}, \tilde{Y}|\tilde{\theta}) \min \left\{ 1, \frac{p(\tilde{\theta}|g, Y)q_{\theta}(\theta|\tilde{\theta})\pi(\tilde{g}, \tilde{Y}|\theta)}{p(\theta|g, Y)q_{\theta}(\tilde{\theta}|\theta)\pi(\tilde{g}, \tilde{Y}|\tilde{\theta})} \right\} \\
&= \min \left\{ p(\theta|g, Y)q_{\theta}(\tilde{\theta}|\theta)\pi(\tilde{g}, \tilde{Y}|\tilde{\theta}), p(\tilde{\theta}|g, Y)q_{\theta}(\theta|\tilde{\theta})\pi(\tilde{g}, \tilde{Y}|\theta) \right\} \\
&= \min \left\{ \frac{p(\theta|g, Y)q_{\theta}(\tilde{\theta}|\theta)\pi(\tilde{g}, \tilde{Y}|\tilde{\theta})}{p(\tilde{\theta}|g, Y)q_{\theta}(\theta|\tilde{\theta})\pi(\tilde{g}, \tilde{Y}|\theta)}, 1 \right\} p(\tilde{\theta}|g, Y)q_{\theta}(\theta|\tilde{\theta})\pi(\tilde{g}, \tilde{Y}|\theta) \\
&= p(\tilde{\theta}|g, Y)p(\theta|\tilde{\theta}).
\end{aligned}$$

The desired result follows by the reversibility, irreducibility, and Harris recurrence of the Markov chain. ■

*Proof of Proposition 3.* To show  $\pi(g, Y|\theta)$  is the stationary distribution, we need to check the detailed balance condition, i.e.,  $\pi(g, Y|\theta)p(\tilde{g}, \tilde{Y}|g, Y) = \pi(\tilde{g}, \tilde{Y}|\theta)p(g, Y|\tilde{g}, \tilde{Y})$  where

$$p(\tilde{g}, \tilde{Y}|g, Y) = p_Y(\tilde{Y}|\tilde{g})q_g(\tilde{g}|g) \min \left\{ 1, \frac{\pi(\tilde{g}, \tilde{Y}|\theta)p_Y(Y|g)q_g(g|\tilde{g})}{\pi(g, Y|\theta)p_Y(\tilde{Y}|\tilde{g})q_g(\tilde{g}|g)} \right\}.$$

Indeed,

$$\begin{aligned} & \pi(g, Y|\theta)p(\tilde{g}, \tilde{Y}|g, Y) \\ &= c(\theta)^{-1} \exp[\sigma^{-2}Q(g, Y|\gamma)]p_Y(\tilde{Y}|\tilde{g})q_g(\tilde{g}|g) \min \left\{ 1, \frac{\exp[\sigma^{-2}Q(\tilde{g}, \tilde{Y}|\gamma)]p_Y(Y|g)q_g(g|\tilde{g})}{\exp[\sigma^{-2}Q(g, Y|\gamma)]p_Y(\tilde{Y}|\tilde{g})q_g(\tilde{g}|g)} \right\} \\ &= c(\theta)^{-1} \min \left\{ \exp[\sigma^{-2}Q(g, Y|\gamma)]p_Y(\tilde{Y}|\tilde{g})q_g(\tilde{g}|g), \exp[\sigma^{-2}Q(\tilde{g}, \tilde{Y}|\gamma)]p_Y(Y|g)q_g(g|\tilde{g}) \right\} \\ &= \min \left\{ \frac{\exp[\sigma^{-2}Q(g, Y|\gamma)]p_Y(\tilde{Y}|\tilde{g})q_g(\tilde{g}|g)}{\exp[\sigma^{-2}Q(\tilde{g}, \tilde{Y}|\gamma)]p_Y(Y|g)q_g(g|\tilde{g})}, 1 \right\} c(\theta)^{-1} \exp[\sigma^{-2}Q(\tilde{g}, \tilde{Y}|\gamma)]p_Y(Y|g)q_g(g|\tilde{g}) \\ &= \pi(\tilde{g}, \tilde{Y}|\theta)p(g, Y|\tilde{g}, \tilde{Y}). \end{aligned}$$

The desired result follows by the reversibility, irreducibility, and Harris recurrence of the Markov chain. ■

## B Implementation Details

### B.1 MCMC

In our empirical study of R&D collaboration networks, we want to estimate the spillover effect parameter  $\lambda$ , parameters in the marginal cost of production  $\beta = (\beta_0, \beta'_1, \beta_2)'$  (with the dimension denoted by  $K$ ), parameters in the collaboration cost  $\delta = (\delta_0, \delta'_1, \delta_2, \delta_3)'$  (with the dimension denoted by  $S$ ), and the noise parameter  $\sigma^2$ . These parameters are denoted by  $\theta = (\lambda, \beta', \delta', \sigma^2)'$ . Other than  $\theta$ , there are also unobservable individual-specific random variables  $x^U = (x_1^U, \dots, x_n^U)'$ , which are regarded as individual random effects, in the model.

We assign the prior distributions of model parameters and unknown variables as follows:

1. Individual latent variable:  $x^U \sim N(0, \varsigma_x^2 I_n)$ , with  $\varsigma_x^2 \sim \kappa \text{Inv}\chi^2(\alpha)$ .
2. Spillover effect parameter:  $\lambda \sim U(-\|G\|_\infty^{-1}, \|G\|_\infty^{-1})$ .
3. Parameters in the marginal cost of production:  $\beta \sim N(\mu_\beta, \varsigma_\beta^2 I_K)$ .
4. Parameters in the collaboration cost:  $\delta \sim N(\mu_\delta, \varsigma_\delta^2 I_S)$ .
5. Noise parameter:  $\sigma^2 \sim N_{[0, \infty)}(\mu_\sigma, \varsigma_\sigma^2)$ .

The above prior distributions are conjugate priors commonly used in the Bayesian literature. First, treating  $x_i^U$  as an individual random effect, we specify a hierarchical prior for  $x_i^U$  with a prior for the variance given by  $\varsigma_x^2 \sim \kappa \text{Inv}\chi^2(\alpha)$ . The hyper-parameters  $\kappa$  and  $\alpha$  are to be specified by the user. The spillover effect parameter  $\lambda$  shares similar properties as the spatial lag parameter in the spatial econometrics literature and we use a uniform prior for  $\lambda$  following Smith and LeSage (2004) and assume  $\lambda \in (-\|G\|_\infty^{-1}, \|G\|_\infty^{-1})$  to guarantee that the best response function (3) has a unique equilibrium. Finally, to guarantee that  $\sigma^2$  is non-negative, we assume it follows a truncated normal distribution on  $[0, \infty)$ . We also assume independence across prior distributions of parameters and latent variables. We set  $\mu_\beta = 0$ ,  $\mu_\delta = 0$ ,  $\mu_\sigma = 0$ ,  $\varsigma_\beta^2 = \varsigma_\delta^2 = \varsigma_\sigma^2 = 100$ ,  $\kappa = 1$  and  $\alpha = 2$  to ensure our prior distributions cover a wide range of parameter spaces and thus be uninformative in our empirical analysis.

We adopt the Bayesian data augmentation approach (Tanner and Wong, 1987; Albert and Chib, 1993) to sample  $\theta$  together with  $x^U$  from the joint posterior distribution by the MCMC procedure. In an iteration of the MCMC procedure with the current values of the parameters and individual latent variables denoted by  $\theta$  and  $x^U$ , we perform the following steps sequentially. Let  $x_{-i}^U = (x_1^U, \dots, x_{i-1}^U, x_{i+1}^U, \dots, x_n^U)'$ .

Step I. Simulate  $\tilde{x}_i^U$  from  $p(\tilde{x}_i^U | g, Y, x_{-i}^U, \theta)$  by the DMH algorithm, for  $i = 1, \dots, n$ .

I.1. Propose  $\tilde{x}_i^U$  from a random walk proposal density  $q_x(\tilde{x}_i^U | x_i^U)$ .

- I.2. Simulate auxiliary data  $(\tilde{g}, \tilde{Y})$  by  $R$  runs of Algorithm 2 defined in Section 3.2, starting from the observed  $(g, Y)$ . In the first step of Algorithm 2, we allow for both a “local update” (with probability  $1 - p_{global}$ ), where only one link is flipped, and a “global update” (with probability  $p_{global}$ ), where all links are flipped.<sup>1</sup>
- I.3. Accept  $\tilde{x}_i^U$  according to the acceptance probability

$$\begin{aligned} \alpha_x &= \min \left\{ 1, \frac{\pi(g, Y | \theta, \tilde{x}^U)}{\pi(g, Y | \theta, x^U)} \cdot \frac{p(\tilde{x}_i^U | \varsigma_x^2)}{p(x_i^U | \varsigma_x^2)} \cdot \frac{\pi(\tilde{g}, \tilde{Y} | \theta, x^U)}{\pi(\tilde{g}, \tilde{Y} | \theta, \tilde{x}^U)} \right\} \\ &= \min \left\{ 1, \frac{\exp[\sigma^{-2}Q(g, Y | \gamma, \tilde{x}^U)]}{\exp[\sigma^{-2}Q(g, Y | \gamma, x^U)]} \cdot \frac{p(\tilde{x}_i^U | \varsigma_x^2)}{p(x_i^U | \varsigma_x^2)} \cdot \frac{\exp[\sigma^{-2}Q(\tilde{g}, \tilde{Y} | \gamma, x^U)]}{\exp[\sigma^{-2}Q(\tilde{g}, \tilde{Y} | \gamma, \tilde{x}^U)]} \right\}, \end{aligned}$$

where  $p(x_i^U | \varsigma_x^2)$  denotes the density function of  $N(0, \varsigma_x^2 I_n)$ . Otherwise, set  $\tilde{x}_i^U = x_i^U$ .

Step II. Simulate  $\tilde{\varsigma}_x^2$  from  $[\kappa + \sum_{i=1}^n (\tilde{x}_i^U)^2] \text{Inv}\chi^2(\alpha + n)$  by a standard Gibbs sampler.

Step III. Simulate  $\tilde{\theta}$  from  $p(\tilde{\theta} | g, Y, \tilde{x}^U)$  by the DMH algorithm.

III.1. Propose  $\tilde{\theta}$  from a random walk proposal density  $q_\theta(\tilde{\theta} | \theta)$ .

III.2. Simulate auxiliary data  $(\tilde{g}, \tilde{Y})$  by  $R$  runs of Algorithm 2 defined in Section 3.2, starting from the observed  $(g, Y)$  and allowing for both local and global updates as described in Step I.2.

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<sup>1</sup>Similar local and global updates are suggested in Snijders (2002) and Mele (2017) to improve the convergence of graph sampling, particularly when the graph distribution exhibits a bimodal shape, one mode having low and the other high graph densities. In the simulation and empirical studies, we set the probability of global update  $p_{global} = 0.01$ .



III.3. Accept  $\tilde{\theta}$  according to the acceptance probability

$$\begin{aligned}\alpha_\theta &= \min \left\{ 1, \frac{\pi(g, Y|\tilde{\theta}, \tilde{x}^U)}{\pi(g, Y|\theta, \tilde{x}^U)} \cdot \frac{p(\tilde{\theta})}{p(\theta)} \cdot \frac{\pi(\tilde{g}, \tilde{Y}|\theta, \tilde{x}^U)}{\pi(\tilde{g}, \tilde{Y}|\tilde{\theta}, \tilde{x}^U)} \right\} \\ &= \min \left\{ 1, \frac{\exp[\tilde{\sigma}^{-2}Q(g, Y|\tilde{\gamma}, \tilde{x}^U)]}{\exp[\sigma^{-2}Q(g, Y|\gamma, \tilde{x}^U)]} \cdot \frac{p(\tilde{\theta})}{p(\theta)} \cdot \frac{\exp[\sigma^{-2}Q(\tilde{g}, \tilde{Y}|\gamma, \tilde{x}^U)]}{\exp[\tilde{\sigma}^{-2}Q(\tilde{g}, \tilde{Y}|\tilde{\gamma}, \tilde{x}^U)]} \right\},\end{aligned}$$

where  $\tilde{x}^U = (\tilde{x}_1^U, \dots, \tilde{x}_n^U)'$ . Otherwise, set  $\tilde{\theta} = \theta$ .

## B.2 Matrix Perturbation

In the MCMC algorithm, we need to evaluate  $(I_n - \lambda G)^{-1}$  and  $\det(I_n - \lambda G)$  whenever a link is added or removed in the network  $g$ . The following lemma is helpful for this purpose.

**Lemma 1.** *Let  $e_i$  be the  $i$ th unit basis vector in  $\mathbb{R}^n$ . Let  $A$  denote an  $n \times n$  matrix and*

$$B_{ij} = \frac{A^{-1}e_i e_j' A^{-1}}{1 + \alpha e_j' A^{-1} e_i}.$$

*Adding a perturbation  $\alpha$  to the matrix  $A$  in the  $(i, j)$ th and the  $(j, i)$ th position can be written as  $A + \alpha e_i e_j' + \alpha e_j e_i'$ .*

(i) *The inverse of the perturbed matrix can be written as*

$$(A + \alpha e_i e_j' + \alpha e_j e_i')^{-1} = A^{-1} - \alpha B_{ij} - \alpha \frac{(A^{-1} - \alpha B_{ij})e_j e_i' (A^{-1} - \alpha B_{ij})}{1 + \alpha e_i' (A^{-1} - \alpha B_{ij}) e_j}. \quad (1)$$

(ii) *The determinant of the perturbed matrix can be written as*

$$\det(A + \alpha e_i e_j' + \alpha e_j e_i') = [1 + \alpha e_i' (A^{-1} - \alpha B_{ij}) e_j] (1 + \alpha e_j' A^{-1} e_i) \det(A). \quad (2)$$

*Proof.* We first prove part (i) of Lemma 1. By the Sherman-Morrison formula (Meyer, 2000),

$$(A + \alpha e_i e_j')^{-1} = A^{-1} - \alpha \frac{A^{-1} e_i e_j' A^{-1}}{1 + \alpha e_j' A^{-1} e_i} = A^{-1} - \alpha B_{ij}.$$

Therefore,

$$(A + \alpha e_i e_j' + \alpha e_j e_i')^{-1} = [(A^{-1} - \alpha B_{ij})^{-1} + \alpha e_j e_i']^{-1} = A^{-1} - \alpha B_{ij} - \alpha \frac{(A^{-1} - \alpha B_{ij}) e_j e_i' (A^{-1} - \alpha B_{ij})}{1 + \alpha e_i' (A^{-1} - \alpha B_{ij}) e_j},$$

where the last equality holds by the Sherman-Morrison formula.

We next prove part (ii) of Lemma 1. By the matrix determinant lemma (Horn and Johnson, 1985),

$$\begin{aligned} \det(A + \alpha e_i e_j' + \alpha e_j e_i') &= \det[(A + \alpha e_i e_j') + \alpha e_j e_i'] \\ &= [1 + \alpha e_i' (A + \alpha e_i e_j')^{-1} e_j] \det(A + \alpha e_i e_j') \\ &= [1 + \alpha e_i' (A + \alpha e_i e_j')^{-1} e_j] (1 + \alpha e_j' A^{-1} e_i) \det(A) \\ &= [1 + \alpha e_i' (A^{-1} - \alpha B_{ij}) e_j] (1 + \alpha e_j' A^{-1} e_i) \det(A), \end{aligned}$$

where the last equality holds by the Sherman-Morrison formula. ■

With Lemma 1 the inverse and determinant of the perturbed matrix  $A + \alpha e_i e_j' + \alpha e_j e_i'$  can be easily computed if the inverse and determinant of  $A$  are known.

## C Additional Monte Carlo Experiments

We conduct additional Monte Carlo experiments to investigate the performance of the proposed MCMC procedure. We consider a model misspecification scenario where the DGP does not include any externality effect from network structure, but we estimate the model in Equation (7) with both congestion and cyclic triangle effects. In other words, compared to the Monte Carlo study setting in Section 3.4, we change the true parameter values of  $\delta_3$  from -0.25 to 0, and  $\delta_4$  from 0.15 to 0. Meanwhile, we also change  $\delta_0$  from -2.5 to -5 and  $\delta_1$  from 0.5 to 0.25 in order to maintain similar network statistics as in Section 3.4. We maintain network size at  $n = 100$ .

The estimation results across 100 repetitions are reported in the second column of Table C1. One can see that our proposed MCMC estimation procedure is able to identify zero effects from network congestion and cyclic triangle terms as the estimates of  $\delta_2$  and  $\delta_3$  are small and insignificant. The estimate of other parameters are close to their true values. This simulation study demonstrates that our estimation procedure will not generate spurious network externality effects if these effects are indeed non-existent in the real data.

## D Spectral Goodness of Fit

We follow Shore and Lubin (2015) to compute the spectral goodness of fit (SGOF) to measure how well a network model explains the structure of an observed network. For an undirected network represented by an adjacency matrix  $G = [g_{ij}]$ , where  $g_{ij} = g_{ji} = 1$  if agents  $i$  and  $j$  form a link and  $g_{ij} = 0$  otherwise, a Laplacian matrix  $L$  is defined as  $L = D - G$ , where  $D$  is the “degree matrix” containing the row sums of  $G$  on its diagonal and zero elsewhere. The spectrum of  $L$  is the set of ordered eigenvalues,  $\boldsymbol{\nu} = (\nu_0, \nu_1, \dots, \nu_n)$ , such that  $\nu_0 \leq \nu_1 \leq \dots \leq \nu_n$ . We normalize all spectra to sum to unity:  $\hat{\nu}_i = \frac{1}{\sum_{j=1}^n \nu_j} \nu_i$ .

Given the structural information contained in the spectrum, the Euclidean spectral distance (ESD) between two spectra,  $\|\boldsymbol{\nu}^A - \boldsymbol{\nu}^B\|$  is used as a measure of the structural similarity of two adjacency matrices A and B. From our estimated network model we can simulate a number of artificial networks and calculate the ESD for the  $k$ th simulated network as

$$\text{ESD}_{obs, sim_k} = \|\boldsymbol{\nu}^{obs} - \boldsymbol{\nu}^{sim_k}\| = \sqrt{\sum_{i=1}^n (|\hat{\nu}_i^{obs} - \hat{\nu}_i^{sim_k}|)^2}.$$

In the paper we consider two empirical network models, Model 1 that ignores unobserved heterogeneity and Model 2 that controls for unobserved heterogeneity. The SGOF is computed by

$$SGOF_{12} = 1 - \frac{\overline{ESD}_{obs, Model_1}}{\overline{ESD}_{obs, Model_2}},$$

where  $\overline{ESD}_{obs,Model_s} = \frac{1}{K_{sim}} \sum_{k=1}^{K_{sim}} ESD_{obs,Model_{s,k}}$  is the arithmetic mean of the ESDs from each of individual simulated networks based on Model  $s$ , for  $s = 1, 2$ . In practice, we set the number of simulated networks  $K_{sim} = 1000$ . Other than checking the SGOF evaluated at the mean ESD values, it is also important to examine the SGOF with the 2.5th and 97.5th percentile results of  $ESD$  to get a quantitative sense of the range of networks that a given network model produces. Based on the simulation from the estimated Model 1 and Model 2, we obtain the value of  $SGOF_{12}$  equals 0.5050, and the 2.5th and 97.5th percentile results equal (0.0869, 0.7589), which implies that Model 2 improves the goodness of fit of Model 1 by 51% and this improvement is significant at the 5% level.

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Table C1: Monte Carlo simulation results  
(Part III)

	True value	Estimation result	
$\lambda$	0.0300	0.0291	(0.0047)
.....			
$\beta_1$	0.5000	0.5023	(0.0194)
$\beta_2$	0.5000	0.4950	(0.0682)
.....			
$\delta_0$	-5.0000	-5.0221	(0.2413)
$\delta_1$	0.2500	0.2629	(0.0846)
$\delta_2$	0.0000	-0.0173	(0.0558)
$\delta_3$	0.0000	0.0004	(0.0570)
.....			
$\sigma^2$	0.5000	0.5001	(0.0751)
$\zeta_x^2$	1.0000	1.1317	(0.2194)