WEB MATERIAL

Assortativity and Bias in Epidemiologic Studies of Contagious Outcomes: A Simulated Example in the Context of Vaccination

Paul N. Zivich, Alexander Volfovsky, James Moody, Allison E. Aiello

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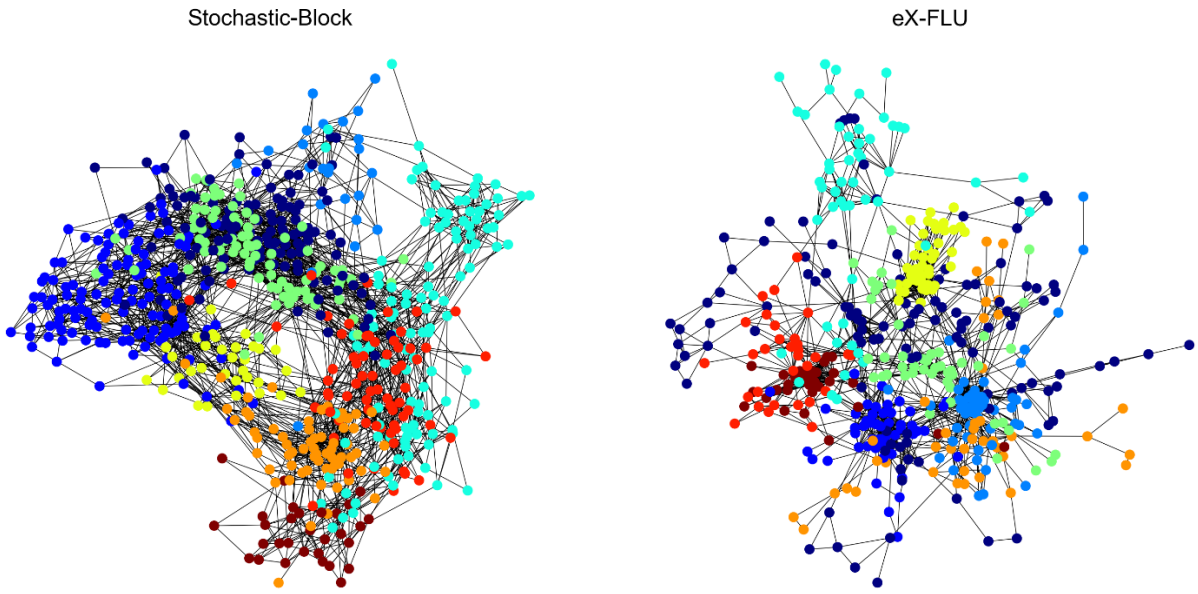
Web Figure 1: Stochastic-block and eX-FLU networks



Node color indicates community or cluster membership of nodes based on Louvain's community detection algorithm. The mean clustering coefficient is the average of the clustering coefficient, which measures the extent a node's contacts have an edge with each other.

The Stochastic-block network (nodes: 658, edges: 2258, mean clustering coefficient: 0.06) is a randomly generated network from a stochastic block model.

The eX-FLU network (nodes: 467, edges: 1818, mean clustering coefficient: 0.48) comes from the eX-FLU study, a cluster randomized trial on three-day self-isolation for respiratory illness mitigation among university students. Dark blue nodes in the eX-FLU network are six disparate communities considered as a single cluster in simulations.

Web Appendix 1

Networks generated from a stochastic block model produce networks with underlying community structures, and is commonly used as a benchmark for community detection algorithms. Stochastic block models generate networks by partitioning nodes into distinct sets. Nodes within the same set have a specified probability for an edge existing. Edges between nodes in discordant sets have a different probability. Probabilities are specified for each combination of node sets.

A single network from the stochastic block model was generated using R's `igraph` library. The stochastic block model was partitioned into 20 different sets, with each set having between 20 to 50 nodes with that set. A matrix of probabilities was specified, corresponding to the probabilities of edges between each distinct set. The diagonal of the matrix was probabilities of edges within each set. Below is the R code used to generate the network

```
library(igraph)

# Stochastic Block Probability Matrix
pm <- cbind( c(.12, .03, .00, .02, .00, .00, .00, .00, .00, .00, .00, .00, .00, .03, .00, .00, .00, .00, .03, .00),
             c(555, .11, .00, .00, .02, .00, .00, .00, .03, .00, .00, .00, .00, .00, .00, .00, .00, .01, .00, .00),
             c(555, 555, .12, .04, .00, .00, .00, .00, .00, .02, .00, .00, .00, .00, .00, .01, .00, .02, .00, .00, .00),
             c(555, 555, 555, .15, .00, .02, .04, .00, .00, .00, .00, .02, .00, .00, .00, .00, .00, .00, .00, .00, .00),
             c(555, 555, 555, 555, .10, .00, .00, .02, .00, .00, .03, .02, .00, .02, .00, .02, .00, .00, .00, .00, .00),
             c(555, 555, 555, 555, 555, .13, .00, .00, .02, .00, .00, .00, .02, .00, .00, .00, .00, .00, .00, .00, .03),
             c(555, 555, 555, 555, 555, 555, .14, .02, .00, .00, .00, .00, .00, .02, .00, .00, .00, .00, .00, .00, .00),
             c(555, 555, 555, 555, 555, 555, 555, .10, .00, .00, .02, .00, .00, .03, .00, .00, .00, .05, .00, .00),
             c(555, 555, 555, 555, 555, 555, 555, 555, .09, .00, .00, .00, .00, .00, .00, .00, .00, .00, .00, .00),
             c(555, 555, 555, 555, 555, 555, 555, 555, 555, .15, .00, .00, .02, .00, .00, .00, .00, .00, .00, .00),
             c(555, 555, 555, 555, 555, 555, 555, 555, 555, 555, .11, .00, .00, .00, .00, .00, .00, .00, .00, .00),
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             c(555, 555, 555, 555, 555, 555, 555, 555, 555, 555, 555, 555, .13, .00, .01, .00, .00, .00, .00, .00),
             c(555, 555, 555, 555, 555, 555, 555, 555, 555, 555, 555, 555, 555, .09, .00, .00, .00, .03, .00, .00),
             c(555, 555, 555, 555, 555, 555, 555, 555, 555, 555, 555, 555, 555, 555, .10, .05, .00, .00, .00, .02),
             c(555, 555, 555, 555, 555, 555, 555, 555, 555, 555, 555, 555, 555, 555, 555, .11, .00, .01, .00, .00),
             c(555, 555, 555, 555, 555, 555, 555, 555, 555, 555, 555, 555, 555, 555, 555, 555, .12, .00, .00, .00),
             c(555, 555, 555, 555, 555, 555, 555, 555, 555, 555, 555, 555, 555, 555, 555, 555, 555, .08, .01, .00),
             c(555, 555, 555, 555, 555, 555, 555, 555, 555, 555, 555, 555, 555, 555, 555, 555, 555, 555, .11, .03),
             c(555, 555, 555, 555, 555, 555, 555, 555, 555, 555, 555, 555, 555, 555, 555, 555, 555, 555, 555, .15) )
pm[upper.tri(pm)] = t(pm)[upper.tri(pm)] # Fills in the `555` with the corresponding probabilities

# Generating the network
n = c(40,30,40,30,50,20,40,20,30,30,
      40,30,40,30,50,20,40,20,30,30)
g <- sample_sbm(sum(n), pref.matrix=pm, block.sizes=n)

# Selecting only the largest component of the graph
dg <- decompose.graph(g)
g <- dg[[1]]
```

The generated network used for simulations is available in Supplementary File 2, along with the Python code used for simulations.

The eX-FLU network comes from the eX-FLU cluster randomized trial. Students were recruited from one of six dormitories, with dormitories selected based on their proximity to each other and their representativeness of the overall undergraduate student population. To identify participants (or generate the *roster* of students), students were recruited through a chain referral sampling procedure; with seed students recruited through informational flyers, emails, and in-person informational tables at the dormitories. Students were asked to nominate other students to participate in the study. In total there were 262 seed students and 328 nominees enrolled. Among all enrolled students, contacts were collected via self-report each week over the follow-up period. To enhance participant recall, previously reported contacts were listed.

Web Table 1: Summary network characteristics for networks used for simulations

	Stochastic-block*	eX-FLU†
Nodes	658	467
Edges	2258	1818
Degree (SD)	6.86 (2.68)	7.79 (7.06)
Diameter	9	14
Radius	5	7
Density	0.01	0.02
Cluster Coefficient (SD)	0.06 (0.07)	0.48 (0.32)
Average Shortest Path	4.24	4.90
Degree Assortativity	0.11	0.47
Clusters	9	9

SD: standard deviation, Degree: number of edges an individual has, Diameter: maximum eccentricity (greatest distance between one node to any other node in the network), Radius: minimum eccentricity, Density: number of actual edges relative to the maximum number of potential edges for the entire network, Clustering coefficient: measure of extent to which node's neighbors connect to each other, Average Shortest Path: average of the all shortest paths between all combinations of nodes, Degree assortativity: measure of node connections to other nodes with a similar degree

* The Stochastic-block model was a randomly generated network

† The eX-FLU network is a real-world contact network obtained from the eX-FLU study. The study was a cluster-randomized trial assessing the efficacy of three-day self-isolation on mitigating spread of respiratory illness among university students over a ten-week period. Louvain's algorithm detected 15 clusters (i.e., communities). Seven of these were collapsed into a single cluster because of size and were similar in that they lay on paths between the major clusters.

Web Appendix 2

Infection transmission simulation procedure

To simulate infection spread in the networks, we used the following procedure based on a stochastic Susceptible-Infected-Recovered network model:

1. Two individuals were chosen at random to be infected at baseline (t_0). Vaccinated individuals were selected at the same probability as unvaccinated individuals in all scenarios.
2. For 20 discrete time steps, the following procedure was used to simulate spread within the network.
   2.1. Nodes of the network were put into a random order.
   2.2. For node n_i:
      2.2.1. If n_i was infected, their infection duration counter increased by one
      2.2.2. If the duration counter for n_i was greater than the maximum infection time, then n_i moved to a recovered status. n_i could no longer become infected or infect their contacts in future time steps.
      2.2.3. For each of n_i's immediate contacts:
         2.2.3.1. n_i attempted to transmit their infection to un-infected and un-recovered neighbor n_j. Infections were based on a Bernoulli random variable dependent on n_i's vaccination status and their neighbor's vaccination status.
3. If the incidence of disease by 20 discrete time steps was between 0.05 and 0.95, then the simulation procedure continued. Otherwise, the previous outbreak steps were repeated.

Truth value simulation procedure

In compartmental models with multiple groups, the population is broken into subgroups where the contact rate between intragroup individuals is constant, and either no or some constant contact rate with intergroup individuals (1, 2). The set simulation parameters (transmission probability given a single exposure, duration of infection, contact rate) can then be converted to the unit-treatment RR (2). Unlike compartmental models, network models explicitly state whether each potential contact exists, rather than some random possibility of contact between any two individuals in the population/group. The explicit specification of contacts within a network complicates the computation from transmission probabilities. Previous network-based simulations that compared regression model estimates have avoided this issue by focusing on confidence interval coverage of null relationships, where the true effect is explicitly known (3, 4). For situations where effects were non-null, the focus was on rejection of the null hypothesis (3). However, our interest was in correct point estimation for null and non-null unit-treatment RR. Under a Bernoulli randomization procedure with the same expectation for each individual, the average assortativity coefficient is zero in expectation. As shown in Hudgens and Halloran (2008), $\frac{\sum Y_i I(V_i=v)}{\sum I(V_i=v)}$ for $v = \{0,1\}$ is an unbiased estimator for $\Pr(Y|V = v, \alpha)$ under the design α (5). Eck, Morozova, and Crawford (2018) show that this is limited to Bernoulli randomization designs (as opposed to cluster or block randomizations) (4). Therefore, the estimated unit-treatment effect in our simulations will be unbiased for the true unit-treatment effect.

To obtain the true RR for non-null unit-treatment effects, the following simulation procedure was used:

1. Vaccination was randomly assigned based on a Bernoulli random variable. Each individual had the same expected value.
2. The infection transmission simulation procedure was conducted for the 20 discrete time-steps.
3. The risk ratio was calculated by taking the incidence proportion in the vaccinated divided by the incidence proportion in the unvaccinated.
4. Steps 1-3 were repeated 50,000 times.

The true unit-treatment effect was defined as the mean of the log-transformed unit-treatment effects.

Simulation Procedure

To simulate the performance for each of the proposed models, the following procedure was used:

1. Vaccination was assigned randomly based on a Bernoulli random variable. Different clusters (as defined by Louvain's algorithm) had different proportions of vaccinated individuals in expectation. The expectations for clusters were based on values that resulted in a specific assortativity value on average.
2. The infection transmission simulation procedure was conducted
3. Each of the proposed regression models (traditional, cluster, one-step, two-step) was fit to the data.
   3.1. The corresponding unit-treatment effect was extracted from each model and stored.
4. Steps 1-3 were repeated 10,000 times.

Web Table 2: Simulation parameters for combinations of direct and indirect effects

	Unvaccinated individuals		Vaccinated individuals		
	B	t	V	t	R
No direct effect					
No indirect effect	0.07	5	1.0	5	1
Weak indirect effect	0.07	5	1.0	4	0.90
Moderate indirect effect	0.07	5	1.0	3	0.75
Weak direct effect					
No indirect effect	0.07	5	0.7	5	1
Weak indirect effect	0.07	5	0.7	4	0.90
Moderate indirect effect	0.07	5	0.7	3	0.75
Moderate direct effect					
No indirect effect	0.07	5	0.4	5	1
Weak indirect effect	0.07	5	0.4	4	0.90
Moderate indirect effect	0.07	5	0.4	3	0.75

B: transmission probability given a single exposure to the infectious agent.
t: number of simulation steps an individual was infected and could transmit the infection R: relative reduction in transmission probability for an infected individual
V: relative reduction in infection probability for an uninfected individual. Vaccination followed the "leaky vaccine" model.

Web Table 3: Simulated reference values for direct effects across scenario combinations and networks

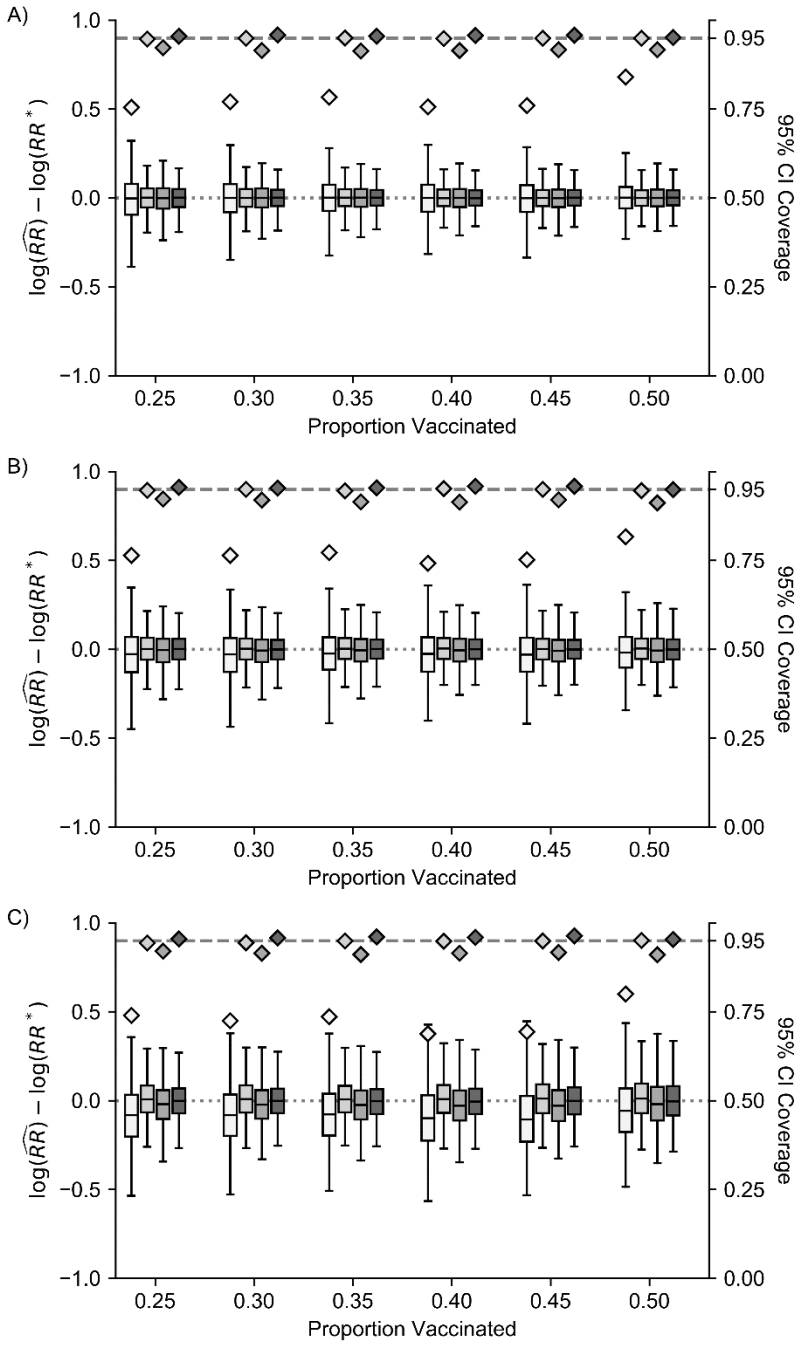
	Stochastic Block Model			eX-FLU		
	None†	Weak	Moderate	None†	Weak	Moderate
No individual effect*						
25%	1	1	1	1	1	1
30%	1	1	1	1	1	1
35%	1	1	1	1	1	1
40%	1	1	1	1	1	1
45%	1	1	1	1	1	1
50%	1	1	1	1	1	1
Weak individual effect*						
25%	0.8053	0.7969	0.7883	0.8688	0.8636	0.8612
30%	0.8038	0.7932	0.7837	0.8693	0.8624	0.8578
35%	0.8019	0.7903	0.7788	0.8683	0.8631	0.8591
40%	0.7996	0.7875	0.7744	0.8680	0.8628	0.8569
45%	0.7976	0.7826	0.7691	0.8697	0.8621	0.8579
50%	0.7956	0.7812	0.7666	0.8697	0.8624	0.8565
Moderate individual effect*						
25%	0.5171	0.5098	0.5024	0.6584	0.6500	0.6431
30%	0.5100	0.5020	0.4947	0.6547	0.6478	0.6381
35%	0.5057	0.4959	0.4864	0.6550	0.6452	0.6355
40%	0.5007	0.4907	0.4807	0.6536	0.6435	0.6330
45%	0.4963	0.4860	0.4748	0.6540	0.6423	0.6279
50%	0.4924	0.4813	0.4672	0.6528	0.6405	0.6238

In the no individual effect scenario, the reference value (RR = 1) was *a priori* known. For the other scenario combinations, simulations were used to determine reference values. Outbreaks were simulated where the full network was randomly vaccinated (assortativity was zero). Outbreak simulations were repeated 50,000 times, with the reference value defined as the mean of the log-transformed risk ratio.

* The individual effect of the vaccines followed the “leaky vaccine” model, where the vaccine reduced the probability of infection given a single exposure to the contagious agent. Weak individual effect was a reduction in the relative probability of infection by 70%. The moderate individual effect was a reduction in the relative probability of infection by 40%

† Columns are stratified by the strength of indirect effects. No spillover effect meant the same duration of infection (five-time steps) and probability of transmitting (p=0.07) between unvaccinated-and-infected and vaccinated-but-infected individuals. Weak spillover effect reduced the duration of infectiousness to four-time steps and reduced relative infectiousness by 10%. Moderate spillover effect reduced the duration of infectiousness to three-time steps and reduced infectiousness by 25%

Web Figure 2: Stochastic-block simulation results for hypothetical vaccine with no unit-treatment effect



A) no spillover B) weak infectiousness effect C) moderate infectiousness effect. From light to dark gray (left to right): traditional model, cluster model, one-step model, two-step model. RR: risk ratio, 95% CI: 95% confidence interval.
Left y-axes and box plots correspond to bias, defined as the difference between the regression model log-transformed risk ratio minus the true log-transformed risk ratio. Whiskers indicate the 2.5th and 97.5th percentiles. The right y-axes and diamonds correspond to 95% CI coverage, defined as the proportion of 95% CI that contained the true value. The x-axis indicates the overall proportion vaccinated in the population in expectation.

Web Table 4: eX-FLU root mean squared error results for hypothetical vaccine with no unit-treatment effect

	Proportion vaccinated					
	0.25	0.3	0.35	0.4	0.45	0.5
No infectiousness effect						
Traditional model	0.241	0.229	0.213	0.208	0.206	0.198
Cluster model	0.128	0.117	0.106	0.107	0.103	0.103
One-step model	0.155	0.139	0.125	0.121	0.124	0.120
Two-step model	0.133	0.118	0.108	0.106	0.109	0.104
Weak infectiousness effect						
Traditional model	0.245	0.244	0.241	0.236	0.231	0.228
Cluster model	0.131	0.122	0.117	0.118	0.116	0.113
One-step model	0.152	0.146	0.141	0.135	0.135	0.130
Two-step model	0.134	0.123	0.122	0.119	0.117	0.116
Moderate infectiousness effect						
Traditional model	0.270	0.278	0.283	0.276	0.273	0.285
Cluster model	0.142	0.138	0.138	0.134	0.131	0.137
One-step model	0.163	0.164	0.158	0.156	0.153	0.162
Two-step model	0.146	0.140	0.141	0.137	0.133	0.144

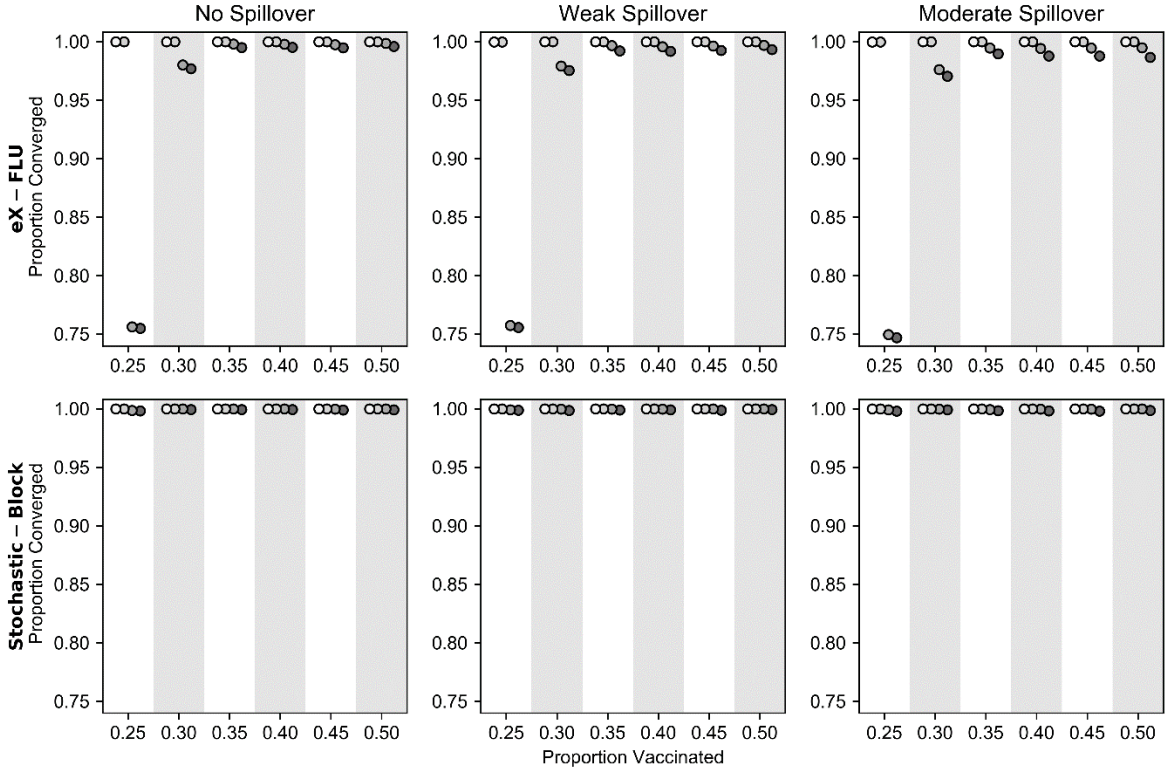
Extreme outliers (log(RR)> ±15) were removed.

Web Table 5: Stochastic-Block root mean squared error results for hypothetical vaccine with no unit-treatment effect

	Proportion vaccinated					
	0.25	0.3	0.35	0.4	0.45	0.5
No infectiousness effect						
Traditional model	0.176	0.168	0.154	0.160	0.154	0.127
Cluster model	0.096	0.096	0.092	0.086	0.085	0.083
One-step model	0.113	0.113	0.107	0.105	0.102	0.097
Two-step model	0.093	0.090	0.087	0.083	0.082	0.082
Weak infectiousness effect						
Traditional model	0.201	0.201	0.188	0.188	0.191	0.168
Cluster model	0.114	0.114	0.110	0.106	0.108	0.109
One-step model	0.133	0.134	0.131	0.124	0.125	0.130
Two-step model	0.112	0.107	0.106	0.102	0.102	0.109
Moderate infectiousness effect						
Traditional model	0.238	0.239	0.234	0.258	0.258	0.230
Cluster model	0.139	0.141	0.135	0.144	0.147	0.149
One-step model	0.158	0.159	0.162	0.168	0.166	0.179
Two-step model	0.135	0.133	0.132	0.137	0.138	0.152

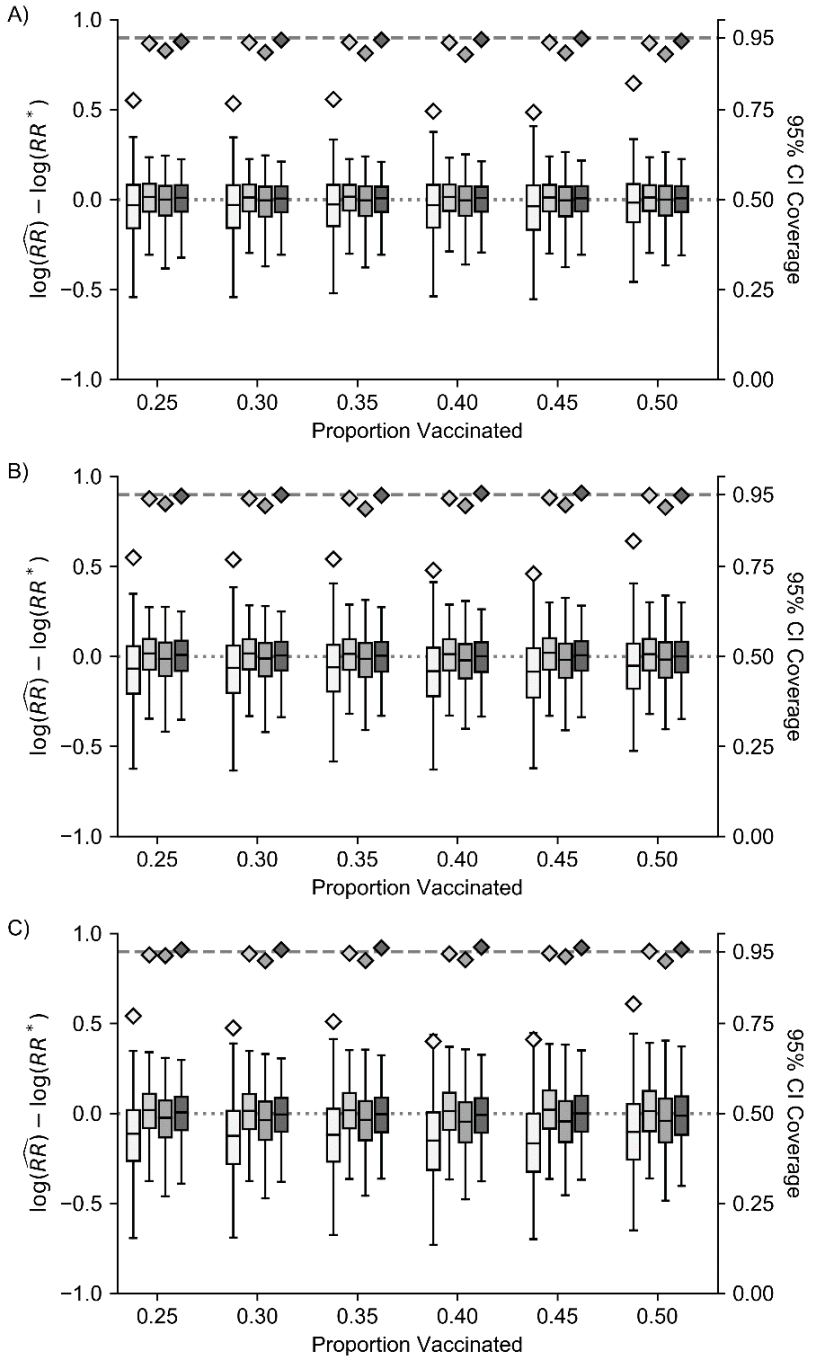
Extreme outliers (log(RR)> ±15) were removed.

Web Figure 3: Convergence proportions for the vaccine with no unit-treatment effect



The y-axis is the proportion of the 10,000 models that converged. Outliers (i.e. log(RR) > ±15) were considered as non-converging. From light to dark gray (left to right): traditional model, cluster model, one-step model, two-step model.

Web Figure 4: Stochastic-block simulation results for hypothetical vaccine with weak unit-treatment effect



A) no infectiousness effect B) weak infectiousness effect C) moderate infectiousness effect. From light to dark gray (left to right): traditional model, cluster model, one-step model, two-step model. RR: risk ratio, 95% CI: 95% confidence interval.
Left y-axes and box plots correspond to bias, defined as the difference between the regression model log-transformed risk ratio minus the true log-transformed risk ratio. Whiskers indicate the 2.5th and 97.5th percentiles. The right y-axes and diamonds correspond to 95% CI coverage, defined as the proportion of 95% CI that contained the true value. The x-axis indicates the overall proportion vaccinated in the population in expectation.

Web Table 6: eX-FLU root mean squared error results for hypothetical vaccine with a weak unit-treatment effect

	Proportion vaccinated					
	0.25	0.3	0.35	0.4	0.45	0.5
No infectiousness effect						
Traditional model	0.274	0.270	0.262	0.260	0.259	0.257
Cluster model	0.149	0.140	0.132	0.129	0.130	0.129
One-step model	0.175	0.164	0.153	0.155	0.154	0.150
Two-step model	0.153	0.144	0.137	0.136	0.137	0.132
Weak infectiousness effect						
Traditional model	0.286	0.295	0.292	0.279	0.281	0.284
Cluster model	0.157	0.153	0.147	0.142	0.139	0.139
One-step model	0.179	0.178	0.165	0.163	0.159	0.160
Two-step model	0.162	0.156	0.144	0.144	0.140	0.145
Moderate infectiousness effect						
Traditional model	0.311	0.319	0.328	0.316	0.329	0.341
Cluster model	0.165	0.163	0.161	0.154	0.155	0.161
One-step model	0.194	0.191	0.183	0.176	0.183	0.190
Two-step model	0.177	0.168	0.163	0.157	0.162	0.169

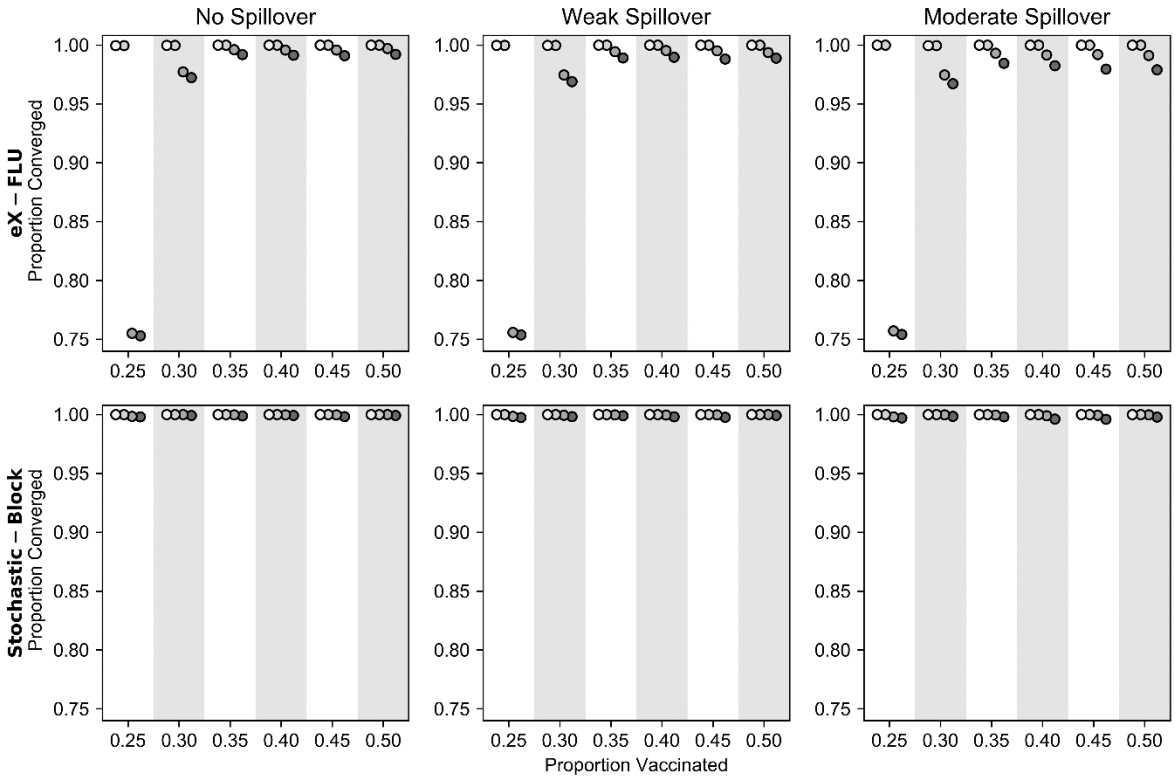
Extreme outliers (log(RR)> ±15) were removed.

Web Table 7: Stochastic-Block root mean squared error results for hypothetical vaccine with a weak unit-treatment effect

	Proportion vaccinated					
	0.25	0.3	0.35	0.4	0.45	0.5
No infectiousness effect						
Traditional model	0.234	0.228	0.217	0.234	0.237	0.198
Cluster model	0.143	0.137	0.134	0.133	0.135	0.133
One-step model	0.162	0.159	0.156	0.160	0.159	0.157
Two-step model	0.140	0.135	0.132	0.132	0.131	0.135
Weak infectiousness effect						
Traditional model	0.259	0.266	0.251	0.268	0.272	0.235
Cluster model	0.158	0.157	0.153	0.154	0.156	0.156
One-step model	0.177	0.180	0.180	0.179	0.180	0.185
Two-step model	0.153	0.150	0.151	0.148	0.150	0.161
Moderate infectiousness effect						
Traditional model	0.291	0.298	0.292	0.323	0.321	0.285
Cluster model	0.180	0.178	0.176	0.183	0.186	0.188
One-step model	0.199	0.200	0.204	0.209	0.207	0.220
Two-step model	0.176	0.170	0.172	0.173	0.176	0.189

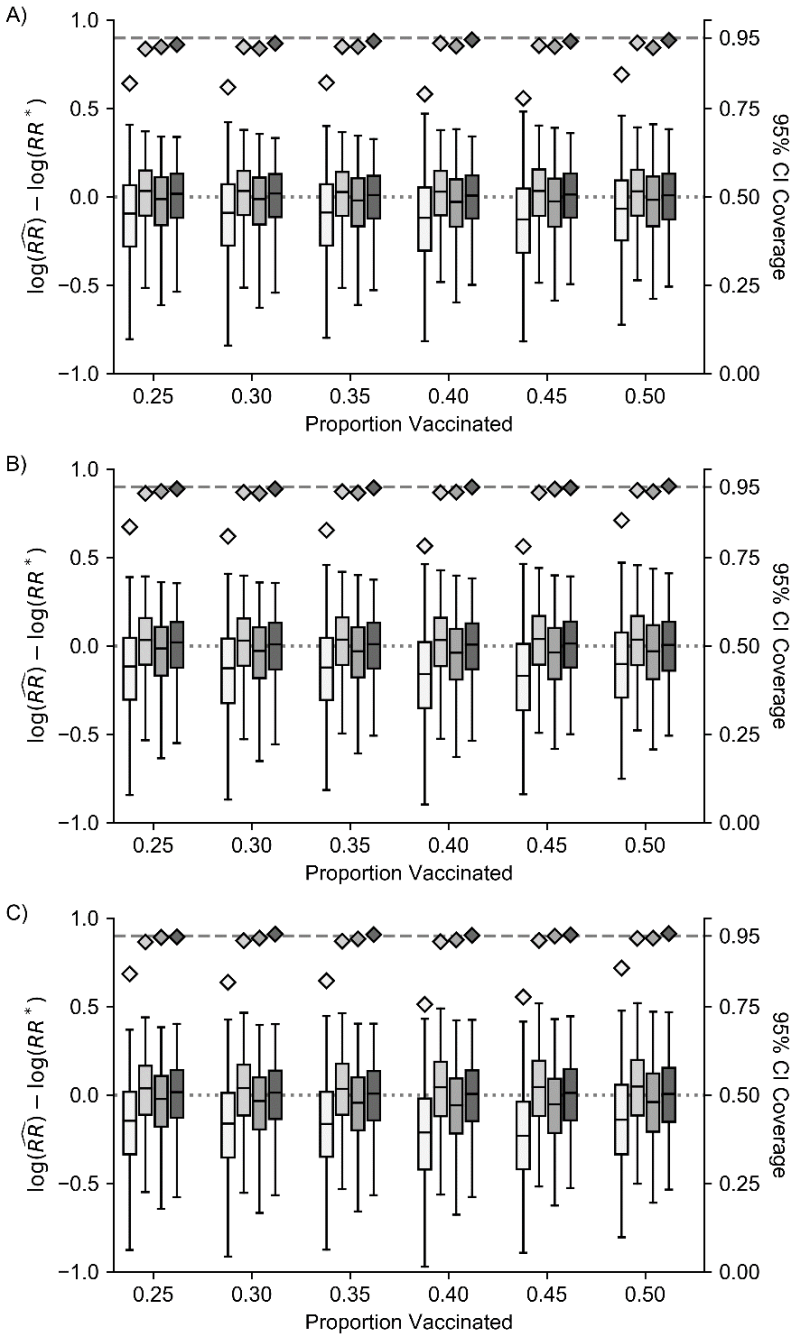
Extreme outliers (log(RR)> ±15) were removed.

Web Figure 5: Convergence proportions for the vaccine with a weak unit-treatment effect



The y-axis is the proportion of the 10,000 models that converged. Outliers (i.e. log(RR) > ±15) were considered as non-converging. From light to dark gray (left to right): traditional model, cluster model, one-step model, two-step model.

Web Figure 6: Stochastic-Block simulation results for hypothetical vaccine with moderate unit-treatment effect



A) no infectiousness effect B) weak infectiousness effect C) moderate infectiousness effect. From light to dark gray (left to right): traditional model, cluster model, one-step model, two-step model. RR: risk ratio, 95% CI: 95% confidence interval.
Left y-axes and box plots correspond to bias, defined as the difference between the regression model log-transformed risk ratio minus the true log-transformed risk ratio. Whiskers indicate the 2.5th and 97.5th percentiles. The right y-axes and diamonds correspond to 95% CI coverage, defined as the proportion of 95% CI that contained the true value. The x-axis indicates the overall proportion vaccinated in the population in expectation.

Web Table 8: eX-FLU root mean squared error results for hypothetical vaccine with a moderate unit-treatment effect

	Proportion vaccinated					
	0.25	0.3	0.35	0.4	0.45	0.5
No infectiousness effect						
Traditional model	0.342	0.340	0.355	0.338	0.341	0.352
Cluster model	0.203	0.194	0.191	0.185	0.179	0.185
One-step model	0.236	0.219	0.214	0.208	0.205	0.212
Two-step model	0.216	0.195	0.192	0.189	0.185	0.193
Weak infectiousness effect						
Traditional model	0.347	0.358	0.374	0.361	0.369	0.375
Cluster model	0.204	0.204	0.200	0.196	0.197	0.196
One-step model	0.232	0.230	0.228	0.219	0.220	0.225
Two-step model	0.214	0.210	0.208	0.200	0.199	0.204
Moderate infectiousness effect						
Traditional model	0.357	0.372	0.383	0.391	0.398	0.415
Cluster model	0.218	0.213	0.207	0.211	0.211	0.221
One-step model	0.239	0.238	0.231	0.231	0.231	0.240
Two-step model	0.222	0.219	0.210	0.210	0.210	0.221

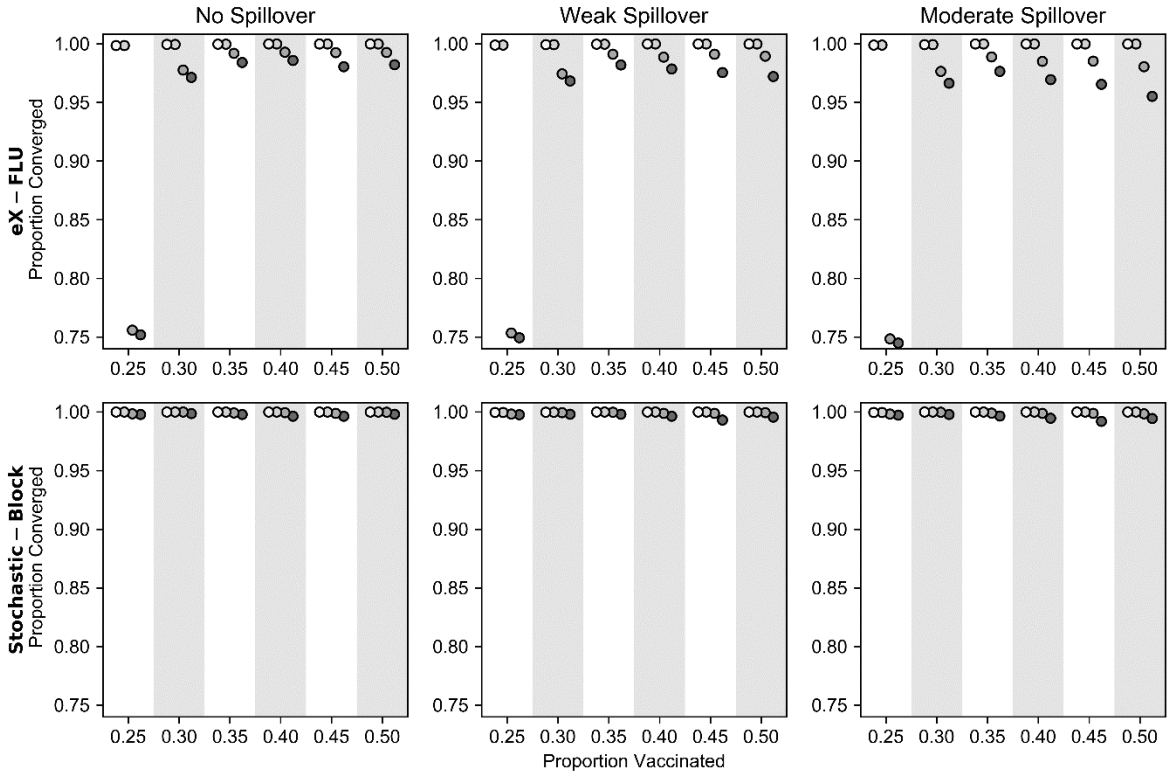
Extreme outliers (log(RR)> ±15) were removed.

Web Table 9: Stochastic-Block root mean squared error results for hypothetical vaccine with a moderate unit-treatment effect

	Proportion vaccinated					
	0.25	0.3	0.35	0.4	0.45	0.5
No infectiousness effect						
Traditional model	0.328	0.338	0.325	0.342	0.346	0.305
Cluster model	0.228	0.231	0.220	0.216	0.223	0.217
One-step model	0.245	0.253	0.245	0.244	0.242	0.247
Two-step model	0.223	0.225	0.216	0.212	0.216	0.220
Weak infectiousness effect						
Traditional model	0.342	0.353	0.340	0.373	0.365	0.327
Cluster model	0.236	0.234	0.233	0.240	0.237	0.235
One-step model	0.256	0.258	0.256	0.260	0.252	0.260
Two-step model	0.233	0.230	0.229	0.229	0.226	0.232
Moderate infectiousness effect						
Traditional model	0.357	0.376	0.370	0.414	0.399	0.350
Cluster model	0.252	0.253	0.251	0.262	0.258	0.255
One-step model	0.265	0.272	0.273	0.283	0.268	0.274
Two-step model	0.246	0.244	0.244	0.249	0.242	0.249

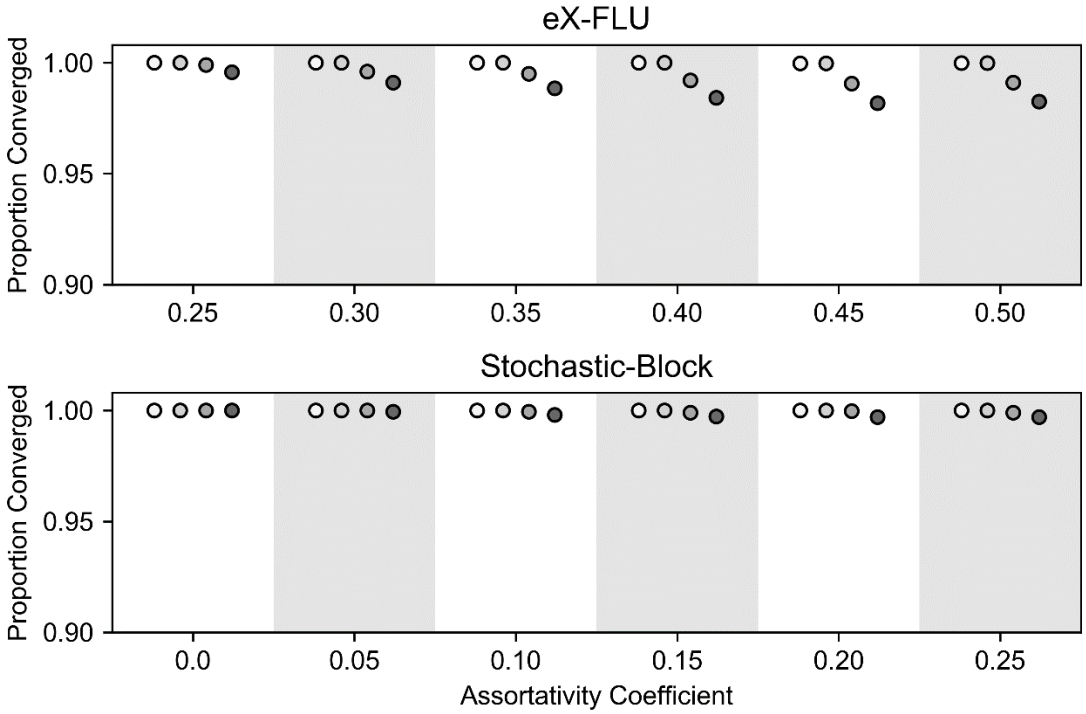
Extreme outliers (log(RR)> ±15) were removed.

Web Figure 7: Convergence proportions for the vaccine with a moderate unit-treatment effect



The y-axis is the proportion of the 10,000 models that converged. Outliers (i.e. log(RR) > ±15) were considered as non-converging. From light to dark gray (left to right): traditional model, cluster model, one-step model, two-step model.

Web Figure 8: Convergence proportions for the vaccine with a moderate unit-treatment effect



The y-axis is the proportion of the 10,000 models that converged. Outliers (i.e. log(RR) > ±15) were considered as non-converging. From light to dark gray (left to right): traditional model, cluster model, one-step model, two-step model.

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