Using Bayesian Structure Learning and Network Deconvolution to Uncover Direct Effects in Simulated Contagions

https://github.com/sjkenned/CS224W

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Abstract

This project evaluates the effectiveness of Bayesian Structure Learning with Network Deconvolution at uncovering direct effects in simulated contagions. In simulated contagions, the probabilities of individuals in a community contracting a contagion were modeled as random variables in a pseudo-randomly-generated Bayesian network. By forward-sampling the Bayesian network, samples outcomes for each node were generated that simulated the spread of the contagion over the population. K-2 Search Bayesian structure learning was applied to learn a directed graph structure from this data, and the results evaluated against the original Bayesian network structure for precision and recall of edges. Network Deconvolution via eigenvalue decomposition was then applied with the aim of pruning from the structure edges that represented indirect effects and were not there in the original graph. The improvement in F1 score from the deconvolution operation was compared against the baseline improvement that resulted from pruning edges that had the least impact on the Bayesian Score. On the large Bayesian Network, K-2 structure learning achieved an F1 score of .267 and when network deconvolution was applied, the F1 score improved by .53, compared to a .91 depreciation resulting from the baseline method. These results reflect the difficulty of making inferences from noisy data on a graph with many edges.

Introduction

Inferring the relationship between different variables from sampled values is a complex problem with many applications. Considering some population of variables, the joint probability distribution over all the variables specifies the likelihood of a given outcome for a given variable. A Bayesian network is a network representation of a joint probability distribution. Each node corresponds to a random variable, and a directed edge from one node to another represents a direct probabilistic relationship. Thus, the structure of the network encodes the inference rules for the distribution.

This project concerns a method of inferring the structure of a Bayesian Network, given enough data that comes from the equivalent distribution. The Bayesian Networks under inference all simulate the probabilities of individual members of a population contracting a contagion. Under the conditions of this experiment, forward-sampling any of the Bayesian Networks is very similar to modeling the spread of a contagion through a population (see Methods section). It is important to note, however, that the edges in the network in question technically encode only inference rules, and not vectors of direct contagion transmission. This distinction rests in part on the fact that a Bayesian Network must be acyclic.

Because structure learning algorithms do not account well for a distinction between direct and indirect effects, they often output graphs with many extra edges representing indirect effects. Consider members of a population A, B and C. In most samples where A acquires the contagion, C acquires it as well. A structure learning algorithm would likely infer an edge between A and C even if there was none, and A had only influenced C through B. See Appendix, fig.1 for an illustration of how indirect effects manifest from direct effects in a similar system with five nodes.

One effective method for removing indirect dependencies from a network is deconvolution. By abstractly decomposing the observed effects (edge weights) into direct effects (direct edges) and sums of indirect effects (paths of different lengths), deconvolution solves for the transitive closure of the true network. Here, deconvolution was applied to structures learned from contagion data with the hopes of uncovering the true network that generated the data and discarding the indirect effects. If the deconvolution works, the edge set of the graph afterwards should correspond much more closely to beforehand.

Related Work

This project's methods are based on a body of well-established algorithms. See Kochendorfer (2013) for an exploration of Bayesian Score, which quantifies the fit of a given graph to some data. *Ibid.* also includes the K2 search algorithm, which this project uses to explore the space of possible graphs for one that generates the highest Bayesian Score. P.35 includes the algorithm for direct sampling from a Bayesian network. Feizi et. Al (2013) introduces network convolution as a general method to distinguish direct dependencies in networks; which they describe as "a systematic method for inferring the direct dependencies in a network, corresponding to true interactions, and removing the effects of transitive relationships that result from indirect effects". Particularly critical is their method of eigenvalue decomposition for computing the deconvolution of a square matrix (see methods), which allows deconvolution to be applied to graphs of sizes that would previously render it computationally intractable. Feizi et. Al use deconvolution on graphs that model real-world phonomena, not abstracted inference effects – this project attempts to apply their work in a new area.

Methods

The experiment proceeded as follows, once for a small graph and then for a large one. First, a random Directed Acyclic Graph with a fixed number of nodes and edges was generated. Some nodes were made to have no in-edges so they could serve as priors. Then, the DAG was treated as a Bayesian Network, and forward sampling was carried out for a fixed number of iterations, according to the following algorithm (Kochendorfer 2013, Algorithm 2.4):

(1)

```
function DirectSample($B$)
    $X_{1:n} \leftarrow$ a topological sort of nodes in $B$
    for $i \leftarrow 1$ to $n$
        $x_i \leftarrow$ a random sample from $P(X_i \mid \mathrm{pa}_{x_i})$
    return $x_{1:n}$
```

At each iteration, this algorithm needs a value for the probability that the given node is a certain value, considering the values all other nodes. Luckily, a Bayesian network makes this easy, because $P(X_i|pa_{xi})$ at each iteration is determined directly by the current node's parents, so only those priors need to be considered. For all of the forward sampling carried out for this project, $P(X_i|pa_{xi})$ was based on some version of a contagion model. Ultimately the variation of the contagion model settled upon uses two different contagions, and the following probability that the current node *n* had contagion X:

(2)

$$P(n = X) \quad = \quad \frac{P_X}{P_{tot}}$$

Where P_x is the number of *n*'s parents who had contagion X, and P_{tot} was the total number of *n*'s parents. Because the graph is in topological order, we know that *n*'s parents have already been sampled. Thus, we proceed through the nodes in topological order, "spreading" the contagion as we go (of course, we are creating a sample based off a prior and not directly modeling contagion spread).

Once these samples were generated, a K-2 search was initiated over the space of possible graphs with the same number of nodes as there were sample variables (Kochendorfer 2013, Algorithm 2.8):

(3)

```
function K2SEARCH($f$)
    $X_{1:n} \leftarrow$ ordering of nodes
    $G' \leftarrow$ graph containing nodes $X_{1:n}$ and no edges
    for $i \leftarrow 1$ to $n$
        repeat
            $G \leftarrow G'$
            Add a parent to node $X_i$ in graph $G'$ that maximizes $f(G')$
        until $f(G') \leq f(G)$
    return $G$
```

Note that K2 search requires some scoring function *f(G)* to quantify the fit of the current graph structure to the data. Bayesian Scoring is particularly useful, as it directly calculates the probability that G fits:

(4)

$$\ln P(G \mid D) = \ln P(G) + \sum_{i=1}^{n}\sum_{j=1}^{q_i} \ln\left(\frac{\Gamma(\alpha_{ij0})}{\Gamma(\alpha_{ij0} + m_{ij0})}\right) + \sum_{k=1}^{r_i} \ln\left(\frac{\Gamma(\alpha_{ijk} + m_{ijk})}{\Gamma(\alpha_{ijk})}\right)$$

Where (G|D) is the probability that a given graphical structure represents the underlying relationship between the variables, given the observed data. α and *m* represent prior beliefs about the graph structure and occurrence counts for different values with respect to a variable's parent values, respectively. Thus, finding a graph structure that best fits the data is a matter of finding one that maximizes the Bayesian score.

Once the K2 search outputted the learned graph, its edges were compared to the edges of the original random Bayesian Network that generated the data, *and* compared to a version of that original network with new edges added for all indirect effects. Precision, recall, and F1 score were recorded for each comparison (see results). The difference in F1 scores between the two comparisons indicates whether the learned structure included edges that represented indirect effects. Next, two methods were tried to remove edges representing indirect effects from the learned network. In the first, baseline method, the edges that contribute the least to the Bayesian score of the graph were removed.

The second applied Network Deconvolution to the graph. Algorithm 5 uses eigen-decomposition to solve for the deconvolution of the graph (Feizi et al, 2007):

(5)

```
1: Decompose $G_{obs}$ into eigenvectors U and eigenvalues $\Sigma_{obs}$
2: Express each eigenvalue $\lambda_i^{dir}$ as a nonlinear function of a single corresponding
   eigenvalue $\lambda_i^{obs}$:
        $\lambda_i^{dir} = \lambda_i^{obs}(1 + \lambda_i^{obs})^{-1}$
3: Form a diagonal Matrix $\Sigma_{dir}$ such that $\Sigma_{dir}(i,i) = \lambda_i^{dir}$
4: Recover the true direct network as: $G_{dir=U\Sigma_{dir}U^{-1}}$
```

The output of both methods is once again compared with the initial graph for recall, precision, and F1.

Results (See fig.3)

Small Bayesian Network (nodes = 10, edges = 28, samples = 300) See fig. 2 for structure variants.

	Precision	Recall	F1
K-2 Search	0.227	0.357	0.277
K-2 (w/ indirect edges)	0.295	0.333	0.313
Pruned	0.200	0.214	0.206
Deconvolved	0.2922	0.3212	0.306

Large Bayesian Network (nodes = 30, edges = 260, samples = 8000)

	Precision	Recall	F1
K-2 Search	.192	.442	.267
K-2 (w/ indirect edges)	.181	.591	.277
Pruned	.168	.326	.229
Deconvolved	.261	.414	.320

Conclusion

Largely, these results were lower than expected across the board. This could owe to the noisiness of the datasets, which only had three possible values for each variable – structure learning often applies to more various distributions. Interestingly, F1 was significantly higher in both size settings for the K-2 learned graph compared to the original Bayesian Network with indirect edges added than it was for the K-2 learned graph compared to the original Bayesian Network alone. This suggests that K-2 does in fact learn indirect effects and reports them as edges, as expected. However, even for the case in which it was compared to the original *with* edges, an F1 score of .277. The deconvolution, though it did prune more invalid edges than valid edges in both cases, did not have the fully expected effect. F1 values increased as a result of deconvolution, but not to the degree that we would expect had all indirect effects been eliminated and only the direct effects remained. There are two factors which explain this outcome. The first is the failure of the K-2 search to consistently extract the direct edges at all – convolution can only uncover as many direct effects as exist in the graph it is applied to. The second is that there was insufficient data for the algorithms to extract a signal from all the noise generated by the randomness during sampling, which would suggest that increased sample sizes are necessary. Ultimately, deconvolution presents an intriguing tool that could still find application to Bayesian Networks with research that builds on these results.

Bibliography

1. Kochendorfer, M. (2013). *Probabilistic Models*. [online] Ieeexplore.ieee.org. Available at: https://ieeexplore.ieee.org/document/7288676/

2. S. Feizi, D. Marbach, M. Médard, and M. Kellis, “Network deconvolution as a general method to distinguish direct dependencies in networks,” *Nature Biotechnology*, vol. 33, no. 4, pp. 424–424, 2015.

3. Zhou and Yang, “Structure Learning of Probabilistic Graphical Models: A Comprehensive Survey,” *[astro-ph/0005112] A Determination of the Hubble Constant from Cepheid Distances and a Model of the Local Peculiar Velocity Field*, 29-Nov-2011. [Online]. Available: https://arxiv.org/abs/1111.6925. [Accessed: 10-Dec-2018]

Appendix

fig. 1: Direct and Indirect Effects in Observed Versus True Networks (CS224W Lec 4 Slide 50)

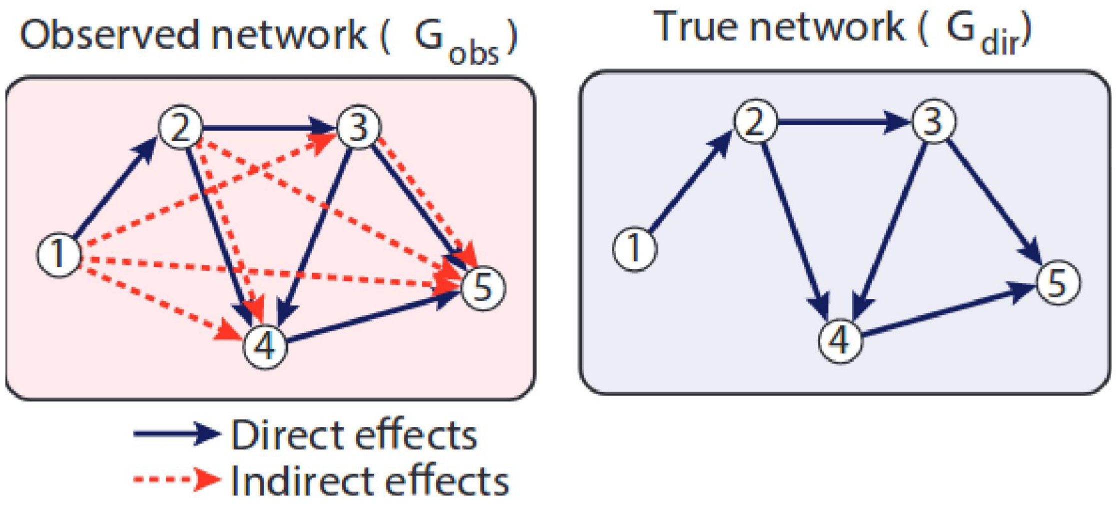


fig. 2: Small Dataset Graphs: (left to right) True Bayesian Network Structure; K2-Search learned Structure; K2-Search learned Structure after deconvolution

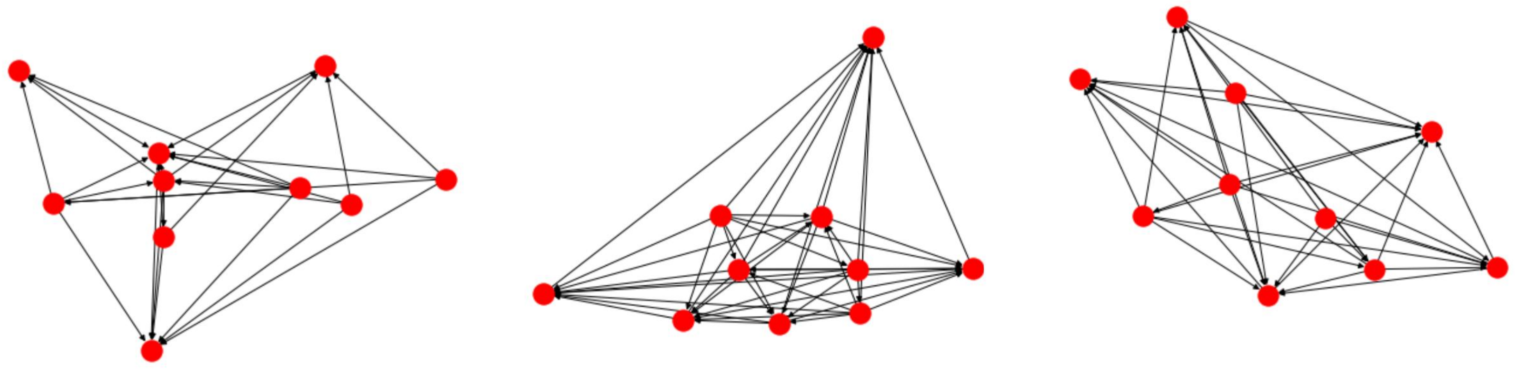
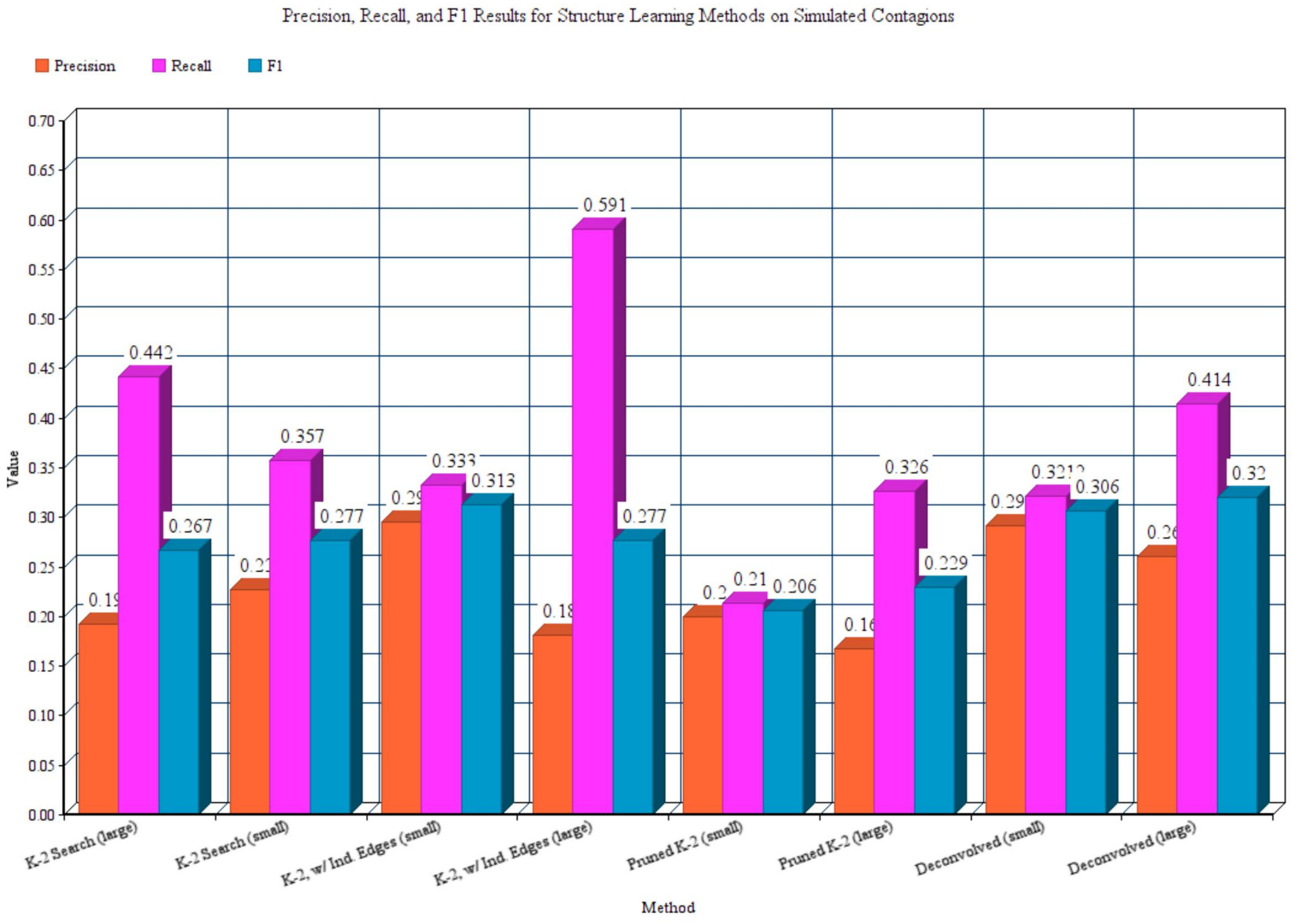


fig. 3 Plot of F1 values for modifications to the original learned graph


Precision, Recall, and F1 Results for Structure Learning Methods on Simulated Contagions
Precision
Recall
F1
Value
K-2 Search (large)
K-2 Search (small)
K-2, w/ Ind. Edges (small)
K-2, w/ Ind. Edges (large)
Pruned K-2 (small)
Pruned K-2 (large)
Deconvolved (small)
Deconvolved (large)
Method