# Causal Discovery: The secret to more promising data mining leads?

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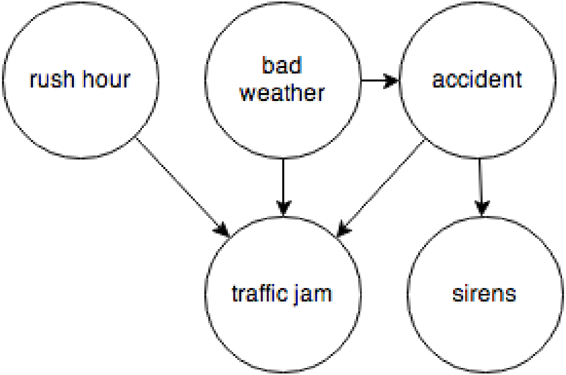
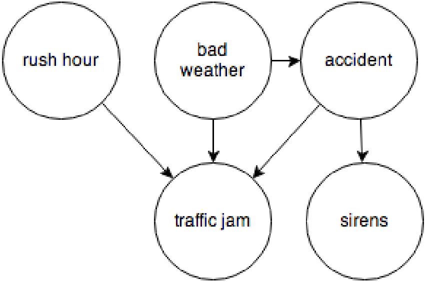
# Outline

# Bayesian Network/Causal Diagram



# Bayesian Network/Causal Diagram

**Motivation for Studying these Structures**: With observational data alone, causal inference using an accurate DAG has been shown to provide results that are up to par with the quintessential randomized controlled experiment (**do-calculus**)[1].




[1] Pearl, J., Glymour, M., and Jewell, N. P. *Causal Inference in Statistics, A Primer*. pgs. 118-124. 2016.

# Intervention Distribution From Observational Distribution

**Definition (Back-door Criterion)**

A set of variabiles $Z$ satisfies the back-door criterion relative to an ordered pair of variables $(X, Y)$ in a DAG $\mathcal{G}$ if:

- no nodes in $Z$ is a descendant of $X$, the intervention node.
- $Z$ blocks every path between $X$ and $Y$ that contains an arrow in $X$ (backdoor path).

$$
\begin{tikzcd}
 & & U \arrow[dl] \arrow[dr] & \\
V \arrow[r] & X \arrow[r] & M \arrow[r] & Y
\end{tikzcd}
$$

- $U$ satisfies the backdoor-criterion.

# Identifying Causal Effects Using a DAG and Observational Distribution

## Theorem (Back-door Adjustment)

*If $Z$ satisfies the back-door criterion relative to $(X, Y)$, then the causal effect of $X$ on $Y$ is given by:*

$$P(y|do(x)) = \sum_z P(y|x,z)P(z).$$

**Do-Operator:** Signifies an intervention on the node $X$, exogenous of the other nodes. $P(y|do(x))$ is the distribution of $Y$ given this intervention.
**Note:** The right-hand side is in terms of the observational distribution.

# Other Ways DAGs Help to Augment Causal Inference

Under a linearity assumption, $\gamma_{X \to Y} = \frac{\partial}{\partial x}\mathbb{E}[y|do(x)] = \alpha_2\alpha_3$ is a natural estimand of interest.

$$\begin{tikzcd} & & U \arrow[dl, "\theta_1"'] \arrow[dr, "\theta_2"] & \\ V \arrow[r, "\alpha_1"] & X \arrow[r, "\alpha_2"] & M \arrow[r, "\alpha_3"] & Y \end{tikzcd}$$

1. **Backdoor (Confounder) Adjustment:**

$$\gamma_{X \to Y} = \beta_X(Y \sim U + X),$$

   the coefficient of $X$ in the linear regression of $Y$ on $U$ and $X$.

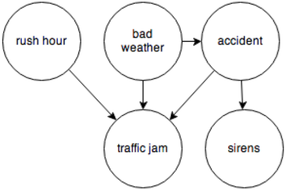
2. **Instrumental Variable Analysis**:

$$\gamma_{X \to Y} = \frac{\beta_V(Y \sim V)}{\beta_V(X \sim V)} = \frac{\alpha_1\alpha_2\alpha_3}{\alpha_1}.$$

3. **Mediation Analysis**:

$$\gamma_{X \to Y} = \beta_X(M \sim X) \times \beta_M(Y \sim X + M)$$

# Causal Discovery




**Challenge**: We do not always have the complete oracle-like knowledge about the graph structure, especially if many variables are involved.

**Research Goal**: Reconstructing a causal diagram with little to no prior knowledge for how things are related.

| Observation | Rush Hour | Bad Weather | Accident | Traffic Jam | Sirens |
|---|---|---|---|---|---|
| 1 | Yes | No | No | Yes | No |
| 2 | No | Yes | Yes | Yes | Yes |
| ⋮ | ⋮ | ⋮ | ⋮ | ⋮ | ⋮ |
| n | No | No | No | No | No |

# A Data Mining Use Case

1. Non-experimental data collected on $p$ variables $\mathrm{X} \in \mathbb{R}^p$.
2. We believe there is an underlying DAG $\mathcal{G}$ whose structure is fully or partially identifiable.
3. Before doing a potentially costly experiment, we want to estimate the causal effect of intervening on a set of variables $\mathcal{I} \subset \{1, 2, \ldots, p\}$.
4. We are interstested on its effect on a Response Set $\mathcal{R} \subset \{1, \ldots, p\} \backslash \mathcal{I}$, i.e.

$$P\left(X_{\mathcal{R}} | do(X_{\mathcal{I}})\right)$$

5. We may even wish to iterate our Inference Across different $\mathcal{I}$ or $\mathcal{R}$ using our estimated graphical model to see what experiments are "most promising."

# Related Other Work in this Setting

- Nandy et. al (2017)[2] extends the theory for the earlier method applied by Stekhoven et. al (2012)[3] to validate causal leads from an Arabidopsis Thaliana gene expression dataset.

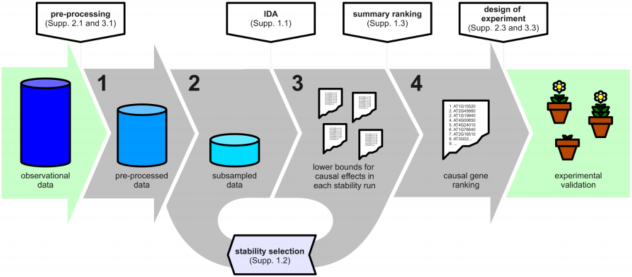



Figure: The causal discovery schema of Stekhoven et. al (2012).

[2] Preetam Nandy, Marloes H. Maathuis, and Thomas S. Richardson. "Estimating the effect of joint interventions from observational data in sparse high-dimensional settings." *The Annals of Statistics*. 2017.

[3] Stekhoven, Daniel & Moraes, Izabel & Sveinbjörnsson, Gardar & Hennig, Lars & Maathuis, Marloes & Bühlmann, Peter. "Causal Stability Ranking". *Bioinformatics*. 28. 2819-2823. 2012.

# Structure Identifiability

Without extra assumptions or prior knowledge (e.g. temporal order, past experiments), a DAG is generally only identifiable up to its **Markov equivalence class**: all DAGs which have the same skeleton and the same v-structures.


Figure: A DAG (left) and its corresponding CPDAG (right).

We can use prior knowledge, such as order in time, to eliminate DAGs in a Markov equivalence class, e.g. $U$ must precede $Y$:

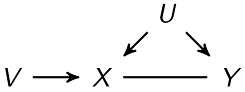



Figure: A CPDAG With Prior Knowledge.

So the only ambiguity left is whether $X \to Y$ or $X \leftarrow Y$.

# Structure Identifiability

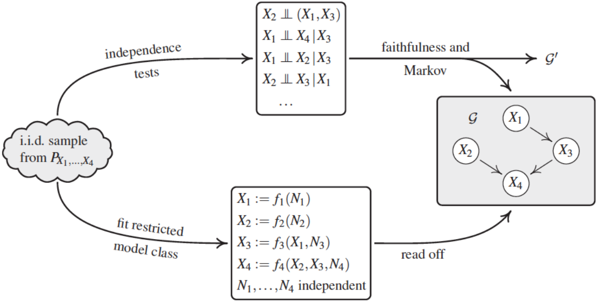
| $d$ | Number of DAGs with $d$ nodes |
|---|---|
| 1 | 1 |
| 2 | 3 |
| 3 | 25 |
| 4 | 543 |
| 5 | 29281 |
| 6 | 3781503 |
| 7 | 1138779265 |
| 8 | 783702329343 |
| 9 | 1213442454842881 |
| 10 | 4175098976430598143 |
| 11 | 31603459396418917607425 |
| 12 | 521939651343829405020504063 |
| 13 | 18676600744432035186664816926721 |
| 14 | 1439428141044398334941790719839535103 |
| 15 | 237725265553410354992180218286376719253505 |
| 16 | 83756670773733320287699303047996412235223138303 |
| 17 | 62707921196923889899446452602494921906963551482675201 |
| 18 | 99421195322159515895228914592354524516555026878588305014783 |
| 19 | 332771901227107591736177573311261125883583076258421902583546773505 |

Table B.1: The number of DAGs depending on the number $d$ of nodes, taken from `http://oeis.org/A003024` [OEIS Foundation Inc., 2017]. The length of the numbers grows faster than any linear term.

# Structure Identification

Idenitifying DAGs (or CPDAGs) is challenging and an open area of inquiry.

- Main methods (3+ variables)[4]




- Special methods (2 variables)
    - Direction-learning methods

[4]Peters, Jonas, et al. Elements of Causal Inference Foundations and Learning Algorithms. MIT Press. 2017

# Structure Learning By Conditional Independence Tests

Constraint based methods, e.g. the PC Algorithm[5,6]:

1. Find the Skeleton of $\mathcal{G}$ by CI tests: Check independence between every $X$ and $Y$ conditional on all $S \subseteq V \backslash \{X, Y\}$ of size at most $k$;
2. Identify v-structures: relations between triplets $(A, B, C)$ such that $A \to B \leftarrow C$ and $A, C$ not adjacent;
3. Orient other edges.
4. **Output:** CPDAG (or PDAG).

**R Package:** `pcalg`.

[5] Peter Spirtes and Clark Glymour. "An algorithm for fast recovery of sparse causal graphs." *Social Science Computer Review*, 9(1):62–72, 1991.

[6] P. Spirtes, C. Glymour, and R. Scheines. *Causation, Prediction, and Search.* Springer, 1993.

# Can we optimize a score function?

Score-based methods:

$$\hat{\mathcal{G}} = \arg \max_{G \in \{acyclic\}} S(G, \mathrm{D}_n).$$

1. $\mathrm{D}_n = (x_{ij})_{n \times p}$ iid data from $(\mathcal{G}, \mathbb{P})$.
2. $S(G, \mathrm{D}_n)$ is a scoring function, e.g.:

$$S_{BIC}(G, \mathrm{D}_n) = \log \; p(\mathrm{D}_n | \hat{\theta}, G) - \frac{d}{2} \log n,$$

$\hat{\theta}$ : MLE of parameters under $G$, $d =$ dimension of $\hat{\theta}$.

# Can we optimize a score function?

**Theorem (Chickering (2002))**

*Assume that $(\mathcal{G}, \mathbb{P})$ satisfies faithfulness. If the score function $S(G, \cdot)$ is consistent and score-equivalent, then:*

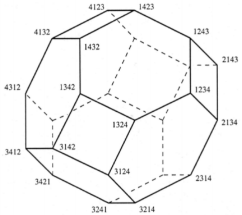
$$\lim_{n\to\infty} \mathbb{P}\left\{\arg\max_{G} S(G, \mathrm{D}_n) \in [\mathcal{G}]\right\} = 1,$$

*where $[\mathcal{G}] := \{G : G \sim \mathcal{G}\}$ is the MEC of the true $\mathcal{G}$.*

**Consistency** roughly says that a DAG $G$ gives the the optimal score with probability $\to 1$ only if it is faithful to the underlying distribution and is sparsest among all faithful DAGs.

# Notable Score-based methods

edges in polytope of permutations (i.e., permutohedron) connect neighboring transpositions, e.g. $(3,1,4,2) - (3,4,1,2)$




- Solus et. al (2018) search across a permutohedron and simply use the number of edges in the DAG as the score $S(G, D_n)$[7].
- Ye et. al (2020) use a Gaussian regularized likelihood score and Simulated Annealing to search permutations of nodes[8].

[7] Solus, L., Wange, Y., Uhler, C. "Consistency Guarantees for Greedy Permutation-Based Causal Inference Algorithms." arXiv:1702.03530, 2018.

[8] Ye, Q., Amini, A.A., and Zhou, Q. "Optimizing regularized Cholesky score for order-based learning of Bayesian networks." *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 2020.

# What if a CPDAG is not informative enough?

**Identifiability Problem**: Nandy et. al (2017) use the PC Algorithm (or similar) which outputs an equivalence class, so a given causal effect can be trivially lower bounded by zero.

**Linear Non-Gaussian Acyclic Model** (LiNGAM): Shimizu et. al (2011) propose an unconfounded linear Bayesian network with non-gaussian errors whose DAG structure (and causal ordering) is identifiable[9].

**Our Structural Causal Model**:

$$X = B_{p \times p}^{\top} X_{p \times 1} + \epsilon \in \mathbb{R}^{p};$$

$B$ acyclic, $\epsilon_j \sim \mathbb{P}(\epsilon_j; \theta_j)$ independent non-Gauassian entries.

**In terms of a Mixing Matrix:** Let $M := (\mathbb{I}_p - B)^{-T}$

$$X = M\epsilon \implies X_k = \epsilon_k + \sum_{j \in AN(k)} M_{kj}\epsilon_j.$$

[9] Shimizu, S., Inazumi, T., Sogawa, Y., Hyvärinen, A., Kawahara, Y., Washio, T., Hoyer, P. O., and Bollen, K., "DirectLiNGAM: a direct method for learning a linear non-Gaussian

# Topological Ordering of a DAG

**Goal**: Do inference using the topological ordering.

## Definition: Topological Ordering via a Permutation

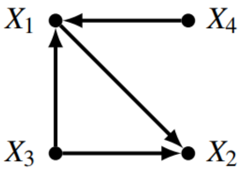
1. A bijective function (permutation)

$$\pi : \{1, 2, \ldots, p\} \mapsto \{\pi(1), \pi(2), \ldots, \pi(j), \ldots, \pi(p)\}$$

2. $\pi(1), \pi(2), \ldots, \pi(p)$ are the observed node labels.
3. Every parent node precedes its child in the ordering via $\pi$:

$$j \in PA_k \implies \pi^{-1}(j) < \pi^{-1}(k).$$

# Topological Ordering of a DAG: An Example




$$X_3 = f_3(U_3)$$
$$X_4 = f_4(U_4)$$
$$X_1 = f_1(X_3, X_4, U_1)$$
$$X_2 = f_2(X_1, X_3, U_2)$$

**A Possible Permutation**:

- $\pi(1) = X_3$,
- $\pi(2) = X_4$,
- $\pi(3) = X_1$, and
- $\pi(4) = X_2$.

# A Generic Algorithm

Let

- $\hat{\pi}$ be our estimate of a topological ordering for DAG $\mathcal{G}$.
- $\mathcal{A}_t = \{\hat{\pi}(1), \ldots, \hat{\pi}(t-1)\}$

**Algorithm: Continuing an Estimate Ordering**

1. $$\hat{\pi}(t) \leftarrow \arg\min_{k \notin \mathcal{A}_t} \mathcal{S}\left(k, \mathcal{A}_t; \mathrm{X}\right)$$

   for summary statistic $\mathcal{S}$ comparable between different nodes.
2. The continued Partial Ordering: $\mathcal{A}_{t+1} \leftarrow \mathcal{A}_t \cup \{\hat{\pi}(t)\}$.

We apply this algorithm sequentially for $t = 1, 2, \ldots$ until completion.

# Linear Non-Gaussian Acylcic Model

We have:

$$X = B_{p\times p}^{\top} X_{p\times 1} + \epsilon = M\epsilon \implies X_k = \epsilon_k + \sum_{j\in AN(k)} M_{kj}\epsilon_j.$$

Shimizu et. al (2011) show that node $j \notin \mathcal{A}_t$ is a valid node to append to $\mathcal{A}_t$ if and only if

$$X_k - \mathbb{E}[X_k | X_j, X_{\mathcal{A}_t}]$$

is independent of $X_j - \mathbb{E}[X_j|X_{\mathcal{A}_t}]$ for each $k \notin \mathcal{A}_t \cup \{j\}$.

**Intuition:** If $PA(j) \subseteq \mathcal{A}_t$, then $X_j - \mathbb{E}[X_j|X_{\mathcal{A}_t}] = \epsilon_j$. Also,

$$X_{\mathcal{A}_{tj}} = M_{\mathcal{A}_{tj},\mathcal{A}_{tj}}\epsilon_{\mathcal{A}_{tj}};\ \mathcal{A}_{tj} = \mathcal{A}_t \cup \{j\}.$$

So

$$X_k - \mathbb{E}[X_k|X_j, X_{\mathcal{A}_t}] = X_k - \mathbb{E}[X_k|\epsilon_{\mathcal{A}_t \cup \{j\}}] = \sum_{l \notin \mathcal{A}_t \cup \{j\}} M_{kl}\epsilon_l.$$

# Conclusion

**Takeaway:** Causal discovery–a small initial step in the scientific pipeline–should be used with caution.

- The idea behind Causal Discovery is appealing, but it is a bit difficult. Nonetheless, there has been progress.
- We have a trade-off between generality (e.g. equivalence class estimation which gives ambiguity of causal effects) and stronger assumptions which may or not be realistic.
- What about unobserved confounders? What about non-iid data, such as a system of variables that varies in time?[10].

[10] Glymour, C., Zhang, K., & Spirtes, P. (2019). Review of Causal Discovery Methods Based on Graphical Models. Frontiers in genetics, 10, 524. https://doi.org/10.3389/fgene.2019.00524

# Acknowledgements

Qing, Oscar

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