Causal Identification with Matrix Equations

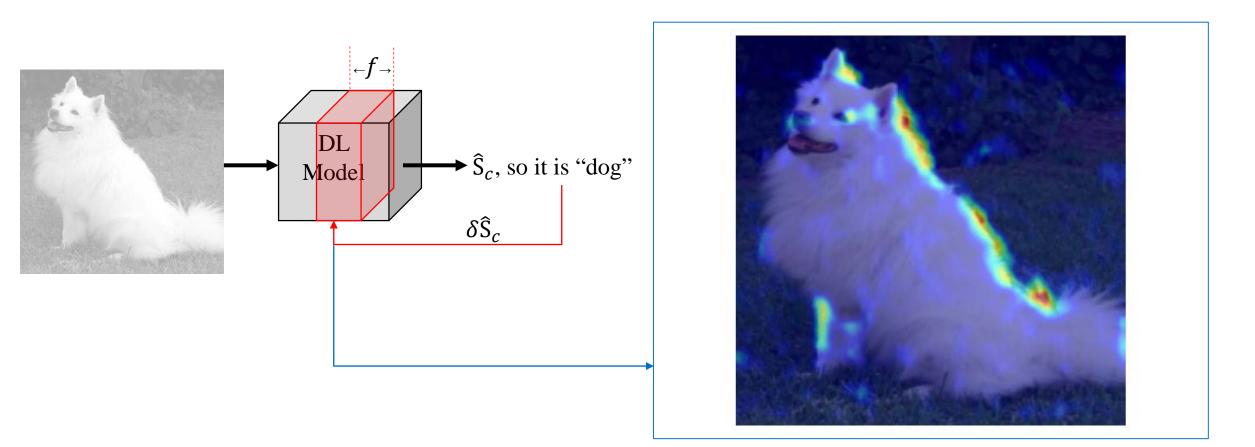
Sanghack Lee and Elias Bareinboin

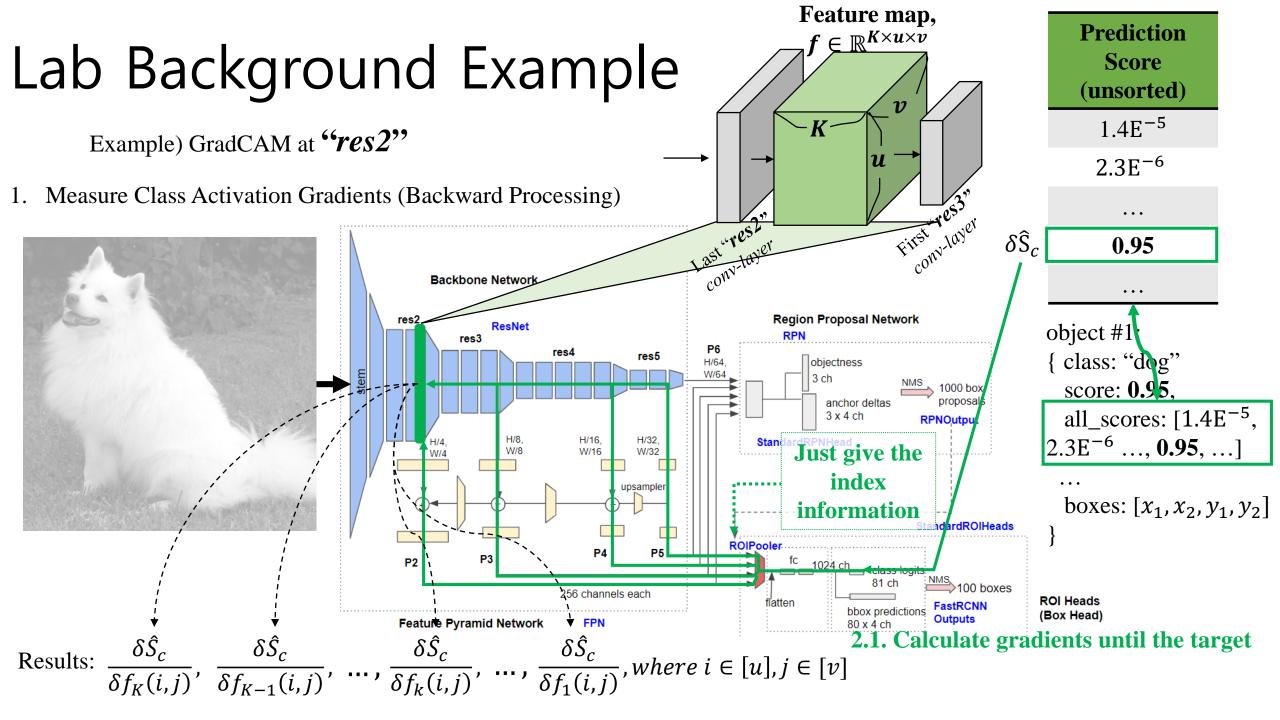
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Lab Background

• Class Activation Mapping (CAM)[1] and its variance Grad-CAM[2] gives importance pixels by estimating relations between a DL layer(=activation map f) and a output(=class \hat{S}_c).





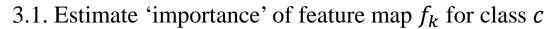
Lab Background Example $a_k^c = \frac{1}{Z} \sum_{i} \sum_{j} \frac{\partial S^c}{\partial f_k(i,j)}$ -Eq. (1)

Example) GradCAM at "res2"

 $\widehat{\delta}\widehat{S}_{c}$

Results:

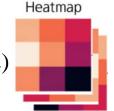
Generate "Localization Score(=Class Activation Mapping)"



$$\Rightarrow a_k^c = rac{1}{Z} \sum_i \sum_j rac{\partial S^c}{\partial f_k(i,j)}$$
 - Eq. (1)

3.2. Weighted Sum-up and ReLU

$$L^c_{Grad-CAM}(i,j) = ReLU(\sum_k a_k^c f_k(i,j))$$
 - Eq. (2)

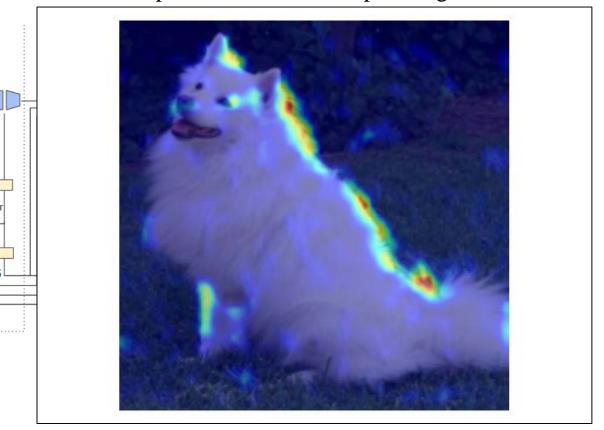


3.3. Visualization

res5

Feature Pyramid Network

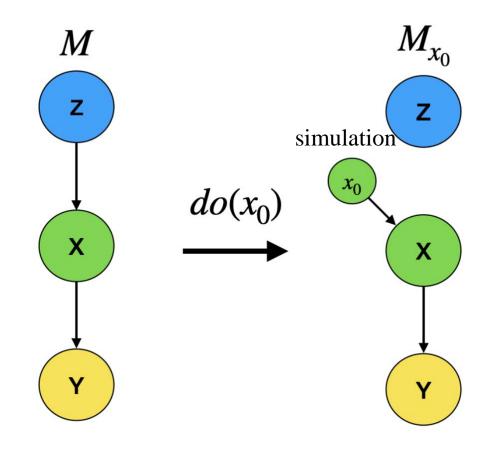
Then, Scale-up $L^c \in \mathbb{R}^{u \times v}$ to the input image size, $I \in \mathbb{R}^{H \times W}$



Background

- Basically,
- the inferential target usually appears as the effect of a set variables do(X = x) on another set of variables Y, which is written as P(y|do(x)) or $P_x(y)$ [3].

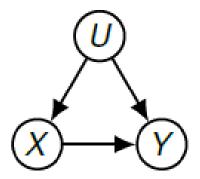
• Assumptions about the underlying DL processes are commonly expressed as a causal graph \mathcal{G} over variables V.



Background

How to estimate causality: The Baseline, factorization-based approach.

- If there is *non-parametric constraints* U encoded in G,
- A number of necessary and sufficient conditions were developed for determining the identifiability status of the query from observational data [3,4,5,6].
- For example, in Figure 1, the causal effect $P_x(y)$ is identified by a *back-door* criterion as $P_x(y) = \sum_{u \in U} P(y|x, u) P(u)$.



Assumption: all data (i.e., *U*, *X*, and *Y*) can be observed.

Figure 1. An example of back-door condition.

Background (About Confounder, exogeneous)

• Simple Example

	No Medicine (x ₀)		Medicine (x ₁)	
Gender (U)	Heart Attack	No Heart Attack	Heart Attack	No Heart Attack
	(y_0)	(y_1)	(y_0)	(y_1)
Female (u_0)	1(5%)	19	3 (7.5%)	37
Male (u_1)	12 (30%)	28	8 (40%)	12
Total	13 (27.7%)	47	11 (18.3%)	49

 $P_X(Y|U)$: Heart Attack Probability at given Gender According to Medicine:

Female: No Medicine $(5\%) \rightarrow$ With Medicine $(7.5\%) \rightarrow$ Wrong Interpretation: Increase Heart Attack by Medicine Male: No Medicine $(30\%) \rightarrow$ With Medicine $(40\%) \rightarrow$ Wrong Interpretation: Increase Heart Attack by Medicine Total: No Medicine $(27.7\%) \rightarrow$ With Medicine $(18.3\%) \rightarrow$ Right Interpretation: Decrease Heart Attack by Medicine

In this case, we call the variable, Gender={Female, Male}, is a **confounder** U (i.e. non-parametric constraints in previous).

Problem in Unobserved Confounders

How to estimate causality: proxy approach.

- Exploit assumptions about the relationship between *unobservable confounders U* and the observable variables, which will possibly lead to the invertibility of certain matrices, through the idea of *proxy variables* [8,9].
- For example, in Figure 2, there are an input X, outcome Y, and the proxies W, Z for the set of unobserved confounders U.

"Note that since U is unobserved, the effect of X on Y, i.e., $P_{\chi}(y)$ is provably not identifiable by previous approach"

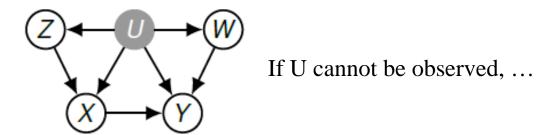


Figure 2. An example of proxy approach.

Appendix (Conditional Independencies)

This paper author refer [10], and call Figure 2, as the *identification condition MGT criterion*.

• [10] Miao, W., Geng, Z., & Tchetgen Tchetgen, E. J. (2018). Identifying causal effects with proxy variables of an unmeasured confounder. Biometrika, 105(4), 987-993.

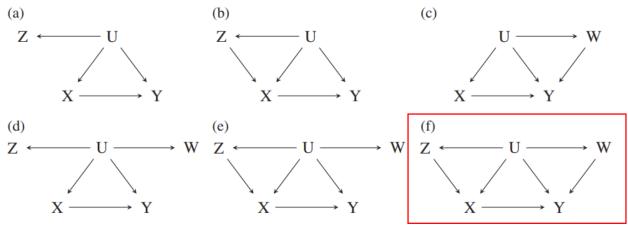


Fig. 1. Causal diagrams with confounder proxies.

MGT criterion (comes from Miao, Geng, Tchetgen **criterion**)

Table 1. Conditional independencies of the causal diagrams in Fig. 1

(a) $Z \perp \!\!\!\perp (X,Y) \mid U$

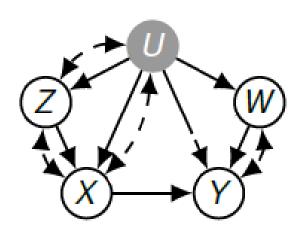
(b) $Z \perp \!\!\!\perp Y \mid (U,X)$

- (c) $W \perp \!\!\!\perp X \mid U$
- (d) $W \perp \!\!\!\perp (Z,X,Y) \mid U,Z \perp \!\!\!\perp (X,Y) \mid U$
- (e) $W \perp \!\!\!\perp (Z,X,Y) \mid U,Z \perp \!\!\!\perp Y \mid (U,X)$ (f) $W \perp \!\!\!\perp (Z,X) \mid U,Z \perp \!\!\!\perp Y \mid (U,X)$

Preliminary (1)

Causality (cambridge.org) (You can check book pdf)

- denote **a variable** by an upper case letter *X*, and its value is denoted by its corresponding lower case letter *x*.
- denote a set of variables by a bold capital letter X, with its value x.
- the union of *disjoint* sets; U not U
- Given $Z \subseteq W$, $W \setminus Z$ means all other variables excluding Z in W.
- Let $a/B = (A \cap B, a \setminus B)$ which retains B as a set of variables and values of a excluding B.
- observational: P(y|x)
- experimental or interventional: P(y|do(x))
- **❖** They may employ conditional $W \supseteq \emptyset$, experimental $Z \supseteq \emptyset$ compared to observational $Z = \emptyset$, and marginal if $Z \cup W \cup V' \subsetneq V$ (V' is a subset of V)



Preliminary (2)

To solve problem, use Structural Causal Models (SCMs)

• \mathcal{M} is a quadruple $\langle \mathbf{U}, \mathbf{V}, P(\mathbf{U}), \mathbf{F} \rangle$.

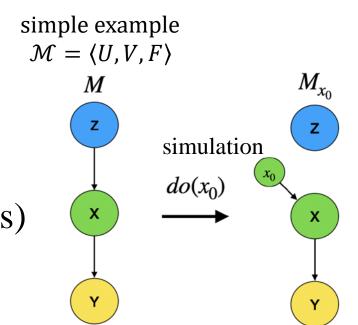
where



(ii) V is a set $\{V_1, ..., V_n\}$ of **endogenous** variables, that are determined by variables in the model (or functions) $F = \{f_i\}_{V_i \in V}$ such that $V_i \leftarrow f_i(\mathbf{pa_i}, \mathbf{u_i})$ where $\mathbf{PA_i} \subseteq \mathbf{V} \setminus \{V_i\}$ and $\mathbf{U_i} \subseteq \mathbf{U}$.

...(omitted)

 \mathbf{PA}_{i} means a parent set of V_{i} and its variables are \mathbf{pa}_{i} .



Goal 1. Characterizations of matrix equations with graphical constraints in a given causal diagram G.

- denote **P** the matrix notation of a distribution *P* where free outcomes are row and free condition or intervention are columns
- use ' and '' to represent two disjoint subsets such that $\mathbf{B} = \mathbf{B}' \dot{\cup} \mathbf{B}''$

Common Characterization.

Let $Q = P_r$ be an arbitrary interventional distribution. Let **A**, **B**, **C** and **R** be disjoint, a marginal probability is expressed as,

$$Q(\mathbf{a}, \mathbf{b}'|\mathbf{c}) = \sum_{\mathbf{b}''} Q(\mathbf{a}|\mathbf{b}, \mathbf{c}) Q(\mathbf{b}|\mathbf{c}) = \mathbf{Q}(\mathbf{a}|\mathbf{b}', \mathbf{B}'', \mathbf{c}) \mathbf{Q}(\mathbf{B}'', \mathbf{b}'|\mathbf{c}).$$

Chain Rule with Conditional Independence

- Considering conditional independence, we can enrich previous common characterization.
- Lemma 1. Given a causal diagram \mathcal{G} , let $Q = P_{\mathbf{r}}$ for some $\mathbf{r} \in \mathfrak{X}_{\mathbf{R}}$ where $\mathbf{R} \subsetneq \mathbf{V}$. Let $\mathbf{A}, \mathbf{B}, \mathbf{C}, \mathbf{D}, \mathbf{E}$ be disjoint subsets of $\mathbf{V} \backslash \mathbf{R}$. If $(\mathbf{D} \perp \mathbf{A} \mid \mathbf{B}, \mathbf{C}, \mathbf{E})$ and $(\mathbf{E} \perp \mathbf{B} \mid \mathbf{C}, \mathbf{D})$ in $\mathcal{G} \backslash \mathbf{R}$, then,

$$\mathbf{Q}(\mathbf{A}, \mathbf{b}' | \mathbf{c}, \mathbf{D}, \mathbf{e}) = \mathbf{Q}(\mathbf{A} | \mathbf{b}', \mathbf{B}'', \mathbf{c}, \mathbf{e}) \mathbf{Q}(\mathbf{B}'', \mathbf{b}' | \mathbf{c}, \mathbf{D}).$$

Adjustment Criteria

- It generalizes back-door criterion [3].
- Its matricized expression with employing $Q = P_{\mathbf{r}}$ is

$$Q_{\mathbf{x}}(\mathbf{y}) = \sum_{\mathbf{z}} Q(\mathbf{y}|\mathbf{x}, \mathbf{z})Q(\mathbf{z}) = \mathbf{Q}(\mathbf{y}|\mathbf{x}, \mathbf{Z})\mathbf{Q}(\mathbf{Z}).$$

C-Factorization

- also we did matricize C-Factorization [3].
- In Figure 3a. $P_{X_{ij}\setminus Y_{ij}}(Y_{ij}\setminus Z)$ can be obtained by multiplication of submatrices $P_{X_i}(Y_i)$ and $P_{X_j}(Y_j)$

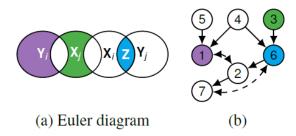


Figure 3: (a) set relationships, (b) a causal graph where the numbers correspond to the regions of (a) from the left to right.

• Lemma 2 (Matrix Equation of C-Factorization with Two-Factors)

Given a causal diagram \mathcal{G} and an experimental distribution $Q = P_{\mathbf{r}}$, if $\mathbf{Z} \subseteq \mathbf{X}_i \cap \mathbf{Y}_j$, a causal effect which is c-factorized as $Q_x(y) = \sum_z Q_{x_i}(y_i)Q_{x_j}(y_j)$ can be matricized by

$$\mathbf{Q}_{(\mathbf{x}_{ij} \setminus \mathbf{y}_{ij})/(\mathbf{X}_j \setminus \mathbf{X}_i \setminus \mathbf{Y}_i)}((\mathbf{y}_{ij} \setminus \mathbf{Z})/(\mathbf{Y}_i \setminus \mathbf{X}_j)) = \mathbf{Q}_{\mathbf{x}_i/\mathbf{Z}}(\mathbf{y}_i/(\mathbf{Y}_i \setminus \mathbf{X}_j))\mathbf{Q}_{\mathbf{x}_j/(\mathbf{X}_j \setminus \mathbf{X}_i \setminus \mathbf{Y}_i)}(\mathbf{y}_j/\mathbf{Z}).$$

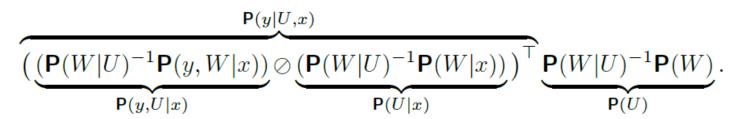
(a) $P_x(W)$

(b) $P_{x,y}(W)$

Goal 2. With the characterization from previous goal, the next goal is the generalization of single- and double-proxy settings [11].

Single-Proxy Setting

Figure 4. illustrate the available distributions and unknown distributions, considered in Figure 4b.



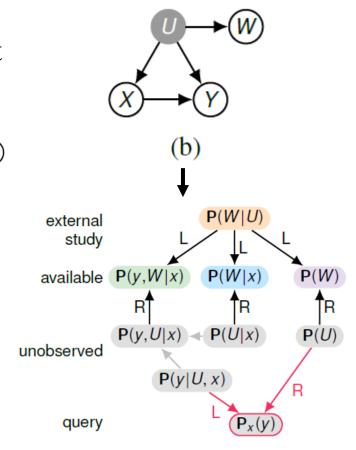


Figure 4: Schematic for a single proxy setting. Gray and red lines are for elementwise matrix multiplication and adjustment criterion, respectively.

(d) $P_z(W)$

Goal 2. With the characterization from previous goal, the next goal is the generalization of single- and double-proxy settings [11].

Double-Proxy Setting

Figure 5. illustrate the available distributions and unknown distributions, considered *MGT criterion* in Figure 2.

(c) $P_x(W)$

Theorem 2 (Generalized MGT Criterion). Given a causal graph \mathcal{G} , let $X, Y, Z, W, U, R \subset V$ be disjoint sets of variables where R can be empty. Let $Q = P_r$ for some $r \in \mathfrak{X}_R$ and $\mathcal{H} = \mathcal{G} \setminus R$. Let $S \subseteq X \cup Z$. A causal effect $Q_x(y) = P_{x,r}(y)$ is identifiable in \mathcal{G} if, for some z, (1) U is an adjustment set for $Q_x(y)$ in \mathcal{H} ; (2) $(Y \perp Z \mid U, X)_{\mathcal{H}}$; (3) $(W \perp S' \mid U, S)_{\mathcal{H}}$ where $S' = (X \cup Z) \setminus S$; (4) U is an adjustment set for $Q_{s'}(W)$ in \mathcal{H} ; (5) $Q(W \mid U, s')$ is invertible; (6) $Q(U \mid z/(S \cup Z'), x)$ is invertible for some $Z' \subseteq Z \setminus S$ and $Q(y \mid z/(S \cup Z'), x)$, $Q(W \mid z/(S \cup Z'), x)$, and $Q_{s'}(W)$ are available. Additionally, $Q(W \mid U, s'/Z')$ is available if $Z' \neq \emptyset$.

Remind Figure 2.

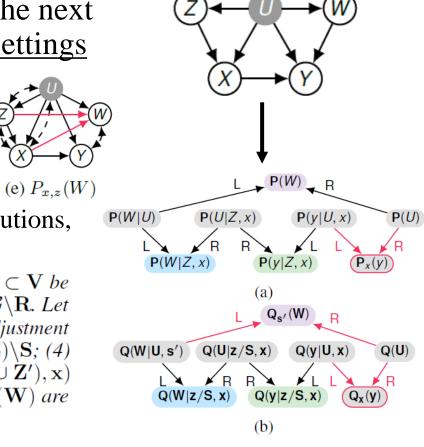


Figure 5: Schematics of (a) MGT criterion and (b) its generalization (simplified)

The paper suggest a novel identification condition(=intermediary criteria) for a challenging setting that neither previous matrical nor graphical approaches could handle.

Pseudoinverse

• First, they prove that the probability of interest is *identificable* through the *pseudoinverse* without invertibility assumption from proxy settings

Lemma 3 (Base Intermediary Criterion). Let $\{P_1, P_2, P_3, P_4\}$ be distributions. Let $\{P_i\}_{i=1}^4$ be their matrix representations. If submatrices $\{P_i'\}_{i=1}^4$ of $\{P_i\}_{i=1}^4$ satisfy $P_1' = P_2'P_3'P_4'$ and $P_2'P_3', P_3'P_4'$, and P_3' are given, then, $P_1' = (P_2'P_3')P_3'^{\dagger}(P_3'P_4')$.

Proof. By the given condition, the associativity of matrix multiplications, and the property of pseudoinverse $PP^{\dagger}P = P$, $P'_1 = P'_2P'_3P'_4 = P'_2(P'_3P'_3^{\dagger}P'_3)P'_4 = (P'_2P'_3)P'_3^{\dagger}(P'_3P'_4)$.

Intermediary Criterion

• Second, they characterize intermediary criterion from Chain-Rule to C-Factorization.

Lemma 4 (Chain-Rule Intermediary Criterion). Given a causal diagram \mathcal{G} , let \mathbf{A} , \mathbf{B} , \mathbf{C} , \mathbf{D} , and \mathbf{R} be disjoint subsets of \mathbf{V} with \mathbf{D} and \mathbf{R} can be empty. Let $\mathbf{B} = \mathbf{B}' \ \dot{\mathbf{D}}$ and $\mathbf{C} = \mathbf{C}' \ \dot{\mathbf{C}}$ where \mathbf{B}' and \mathbf{C}' are not empty. Given an interventional distribution $Q = P_{\mathbf{r}}$, if $(\mathbf{C}' \perp \mathbf{A} \mid \mathbf{B}, \mathbf{C}''\mathbf{D})$ in $\mathcal{G}\backslash\mathbf{R}$ and $Q(\mathbf{a}, \mathbf{b}'', \mathbf{c}''|\mathbf{d}) = \sum_{\mathbf{b}', \mathbf{c}'} Q(\mathbf{a}|\mathbf{b}, \mathbf{c}, \mathbf{d})Q(\mathbf{b}|\mathbf{c}, \mathbf{d})Q(\mathbf{c}|\mathbf{d})$, then,

$$\mathbf{Q}(\mathbf{A},\mathbf{b''},\mathbf{c''}|\mathbf{d}) = \mathbf{Q}(\mathbf{A},\mathbf{b''}|\mathbf{C'},\mathbf{c''},\mathbf{d}) \cdot \mathbf{Q}(\mathbf{B'},\mathbf{b''}|\mathbf{C'},\mathbf{c''},\mathbf{d})^{\dagger} \cdot \mathbf{Q}(\mathbf{B'},\mathbf{b''},\mathbf{c''}|\mathbf{d}).$$

Theorem 3 (C-Factorization Intermediary Criterion). Let \mathcal{G} be a causal diagram and $Q = P_{\mathbf{r}}$. Let $Q_{\mathbf{x}_{\ell}}(\mathbf{y}_{\ell})$ be c-factorized as Eq. (4). Let \mathbf{X}_{k}^{+} be a subset of \mathbf{X}_{k} excluding the rest five sets, $\{\mathbf{Y}_{i},\mathbf{Y}_{j},\mathbf{Y}_{k},\mathbf{X}_{i},\mathbf{X}_{j}\}$. \mathbf{Y}_{i}^{+} is similarly defined. If $\mathbf{Z} \subseteq (\mathbf{X}_{i} \cap \mathbf{Y}_{j}) \setminus \mathbf{X}_{k}$ and $\mathbf{W} \subseteq \mathbf{X}_{j} \cap \mathbf{Y}_{k}$, then $\mathbf{Q}_{\mathbf{x}_{\ell}/\mathbf{X}_{k}^{+}}(\mathbf{y}_{\ell}/\mathbf{Y}_{i}^{+})$, a submatrix of $\mathbf{Q}_{\mathbf{X}_{\ell}}(\mathbf{Y}_{\ell})$, becomes

$$\mathbf{Q}_{\mathbf{x}_{\ell}/\mathbf{X}_{k}^{+}}(\mathbf{y}_{\ell}/\mathbf{Y}_{i}^{+}) = \mathbf{Q}_{(\mathbf{x}_{ij}\backslash\mathbf{y}_{ij})/\mathbf{W}}((\mathbf{y}_{ij}\backslash\mathbf{Z})/\mathbf{Y}_{i}^{+}) \cdot \mathbf{Q}_{\mathbf{x}_{j}/\mathbf{W}}(\mathbf{y}_{j}/\mathbf{Z})^{\dagger} \cdot \mathbf{Q}_{(\mathbf{x}_{jk}\backslash\mathbf{y}_{jk})/\mathbf{X}_{k}^{+}}((\mathbf{y}_{jk}\backslash\mathbf{W})/\mathbf{Z}).$$

• Then, they suggest **ID-ME** (Identification with Matrix Equation) algorithm

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Algorithm 1 ID-ME
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function ID-ME(x, y, G, D)
    Input: x, y value assignments for a query P<sub>x</sub>(y); G a causal diagram; D a collection of distributions
    Output: a formula for P<sub>x</sub>(y) made with D or FAIL.
X, G' ← an Gx(Y) ∩ X, G[An G(Y)]

        D ← expand(G, D) unless D is unconditional
        F' ← F<sub>G'</sub> if D is unconditional and nonmarginal else ∪{F<sub>G'(V')</sub> | X ∪ Y ⊆ V' ⊆ V}
        F', F" ← empty dictionary, F<sup>+</sup>
        for all P<sub>Xi</sub>(Yi) ∈ F" and {P<sub>Z</sub>(V'|T) ∈ D | Yi ⊆ V', Xi ⊆ Z ∪ V' ∪ T} do
        update F', F" with ID-RC(P<sub>Xi</sub>(Yi), G', P<sub>Z</sub>(V'|T))
        for all P<sub>Xi</sub>(Yi) ∈ F" do update F', F" with PROXY(P<sub>Xi</sub>(Yi), G, D ∪ F')
        repeat update F', F" with CF-INT(G', F', F") and CF-INV(G', F', F") until F' not changed return exact-cover(G', P<sub>x</sub>(y), F')
```

expand: a procedure of chain rule closure with *chain-rule matrix inversion* and *chain-rule intermediary criterion* ID-RC: an identification module modified to hand a conditional distribution [12,13]

PROXY: generalized proxy criteria

CF-INT: Lemma 2 CF-INV: Theorem 3

Conclusion

- Characterize matrix equations made of distributions driven by graphical constraints
- Generalize proxy-based identification methods
- Develop novel intermediary criteria by utilizing pseudoinverse
- Suggest a causal identification algorithm for a causal query given a causal graph and distributions that can be marginal, experimental, and conditional harnessing the power of matrix equations and (pseudo)inverse.

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