Supplement to "Interpreting and using CPDAGs with background knowledge"

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This is the supplement of the paper "Interpreting and using CPDAGs with background knowledge", which we refer to as the "main text".

A PRELIMINARIES

Paths. If $p = \langle X_1, X_2, \dots, X_k, \rangle, k \geq 2$ is a path, then with -p we denote the path $\langle X_k, \dots, X_2, X_1 \rangle$. The *length* of a path equals the number of edges on the path. We denote the concatenation of paths by \oplus , so that for example $p = p(X_1, X_m) \oplus p(X_m, X_k)$ for $1 \leq m \leq k$.

Definition A.1. (*Distance-from-Z*) Let \mathbf{X} , \mathbf{Y} and \mathbf{Z} be pairwise disjoint node sets in a maximal PDAG \mathcal{G} . Let p be a path from \mathbf{X} to \mathbf{Y} in \mathcal{G} such that every collider C on p has a b-possibly causal path to \mathbf{Z} . Define the distance-from- \mathbf{Z} of collider C to be the length of a shortest b-possibly causal path from C to \mathbf{Z} , and define the distance-from- \mathbf{Z} of p to be the sum of the distances from \mathbf{Z} of the colliders on p.

Lemma A.2. (Lemma A.7 in Ernest et al., 2016) Let X and Y be nodes in a maximal PDAG \mathcal{G} such that X - Yis in \mathcal{G} . Let $\mathcal{G}' = \text{ConstructMaxPDAG}(\mathcal{G}, \{X \to Y\})$. For any $Z, W \in \mathbf{V}$ if $Z \to W$ is in \mathcal{G}' and Z - W is in \mathcal{G} , then $W \in \text{De}(Y, \mathcal{G}')$.

Lemma A.3. (cf. Lemma A.8 in Ernest et al., 2016) Let X be a node in a maximal PDAG \mathcal{G} . Then there is a maximal PDAG \mathcal{G}' in $[\mathcal{G}]$ such that $X \to S$ is in \mathcal{G}' for all $S \in \operatorname{Sib}(X, \mathcal{G})$.

B PROOFS FOR SECTION 3

Proof of Lemma 3.2. Since $p^* = \langle X = V_0, \dots, V_k = Y \rangle$, $k \ge 1$ is b-non-causal in \mathcal{G} , we have $V_i \leftarrow V_j$ in \mathcal{G} for some i, j such that $0 \le i < j \le k$. Let \mathcal{D} be an arbitrary DAG in $[\mathcal{G}]$ and let p be the path corresponding to p^* in \mathcal{D} . Since $V_i \leftarrow V_j$ in \mathcal{D} , $p(V_i, V_j)$ is non-causal from V_i to V_j in \mathcal{D} . Hence, p is b-non-causal in \mathcal{D} . \Box

Proof of Lemma 3.5. One direction is trivial and we only prove that if there is no $V_i \leftarrow V_{i+1}$, for $i \in \{1, \ldots, k-1\}$ in \mathcal{G} , then p^* is b-possibly causal in \mathcal{G} . Suppose for a contradiction that p^* is b-non-causal, that is, there is an edge $V_j \leftarrow V_r$, for $1 \le j < r \le k$, where $r \ne j + 1$.

Since there is no $V_i \leftarrow V_{i+1}$ for any $i \in \{1, \ldots, k-1\}$ in $\mathcal{G}, V_i - V_{i+1}$ or $V_i \rightarrow V_{i+1}$ is in \mathcal{G} for every $i \in \{1, \ldots, k-1\}$. Let \mathcal{D} be a DAG in $[\mathcal{G}]$ that contains $V_1 \rightarrow V_2$ and let p be the path corresponding to p^* in \mathcal{D} . Since p^* is of definite status in \mathcal{G} and since no $V_i \leftarrow V_{i+1}, i \in \{1, \ldots, k-1\}$ is in \mathcal{G} , it follows that p^* contains only definite non-colliders. Then since $V_1 \rightarrow V_2$ is on p, p is a causal path in \mathcal{D} . But then $p(V_j, V_r)$ together with $V_j \leftarrow V_r$ create a directed cycle in \mathcal{D} .

Lemma 3.6 is analogous to Lemma B.1 in Zhang (2008) and the proof follows the same reasoning as well.

Proof of Lemma 3.6. The proof is by induction on the length of p. Let $p = \langle X = V_1, \ldots, V_k = Y \rangle$. Suppose that k = 3. Then either p is unshielded, or there is an edge X - Y or $X \to Y$ in \mathcal{G} ($X \leftarrow Y$ is not in \mathcal{G} since p is b-possibly causal).

For the induction step suppose that the lemma holds for paths of length n - 1 and let k = n. Then either p is unshielded, or there is a node V_i , i > 1 on p, such that $V_{i-1} - V_{i+1}$ or $V_{i-1} \rightarrow V_{i+1}$ is in \mathcal{G} ($V_{i-1} \leftarrow V_{i+1}$ is not in \mathcal{G} since p is b-possibly causal). Then p' = $p(X, V_{i-1}) \oplus \langle V_{i-1}, V_{i+1} \rangle \oplus p(V_{i+1}, Y)$ is a b-possibly causal path from X to Y of length n - 1 and p' is a subsequence of p.

The following lemma is analogous to Lemma 7.2 in Maathuis and Colombo (2015) and follows directly from our definitions of b-possibly causal paths and definite status paths.

Lemma B.1. Let $p = \langle V_1, \ldots, V_k \rangle$ be a b-possibly



Figure 1: Proof structure of Theorem 4.4.

causal definite status path in a maximal PDAG \mathcal{G} . If there is a node $i \in \{1, ..., n-1\}$ such that $V_i \to V_{i+1}$, then $p(V_i, V_k)$ is a causal path in \mathcal{G} .

C PROOFS FOR SECTION 4.1 OF THE MAIN TEXT

C.1 PROOF OF THEOREM 4.4

Figure 1 shows how all lemmas fit together to prove Theorem 4.4. Theorem 4.4 is closely related to Theorem 3.6 for CPDAGs from Perković et al. (2017). Since every CPDAG is a maximal PDAG, all the results presented here subsume the existing results for CPDAGs. Throughout, we inform the reader when our results and proofs differ from the existing ones for CPDAGs.

Proof of Theorem 4.4. This proof is basically the same as the proof of Theorem 3.6 from Perković et al. (2017), except that instead of using Lemmas 3.12, 3.13 and 3.14 from Perković et al. (2017), we need to use Lemmas C.1, C.2 and C.3. We give the entire proof for completeness.

Suppose first that \mathbf{Z} satisfies the b-adjustment criterion relative to (\mathbf{X}, \mathbf{Y}) in the maximal PDAG \mathcal{G} . We need to show that \mathbf{Z} is an adjustment set (Definition 4.1) relative to (\mathbf{X}, \mathbf{Y}) in every DAG \mathcal{D} in $[\mathcal{G}]$. By applying Lemmas C.1, C.2 and C.3 in turn, it directly follows that \mathbf{Z} satisfies the b-adjustment criterion relative to (\mathbf{X}, \mathbf{Y}) in any DAG \mathcal{D} in $[\mathcal{G}]$. Since the b-adjustment criterion reduces to the adjustment criterion (Shpitser et al., 2010; Shpitser, 2012) in DAGs and the adjustment criterion is sound for DAGs, \mathbf{Z} is an adjustment set relative to (\mathbf{X}, \mathbf{Y}) in \mathcal{D} .

To prove the other direction, suppose that \mathbf{Z} does not satisfy the b-adjustment criterion relative to (\mathbf{X}, \mathbf{Y}) in \mathcal{G} . First, suppose that \mathcal{G} violates the b-amenability condition relative to (\mathbf{X}, \mathbf{Y}) . Then by Lemma C.1, there is no adjustment set relative to (\mathbf{X}, \mathbf{Y}) in \mathcal{G} . Otherwise, suppose \mathcal{G} is b-amenable relative to (\mathbf{X}, \mathbf{Y}) . Then \mathbf{Z} violates the b-forbidden set condition or the b-blocking condition. We need to show \mathbf{Z} is not an adjustment set in at least one DAG \mathcal{D} in $[\mathcal{G}]$. Suppose \mathbf{Z} violates the forbidden set condition. Then by Lemma C.2, it follows that there exists a DAG \mathcal{D} in $[\mathcal{G}]$ such that **Z** does not satisfy the b-adjustment criterion relative to (\mathbf{X}, \mathbf{Y}) in \mathcal{D} . Since the b-adjustment criterion reduces to the adjustment criterion (Shpitser et al., 2010; Shpitser, 2012) in DAGs and the adjustment criterion is complete for DAGs, it follows that \mathbf{Z} is not an adjustment set relative to (\mathbf{X}, \mathbf{Y}) in \mathcal{D} . Otherwise, suppose Z satisfies the forbidden set condition, but violates the b-blocking condition. Then by Lemma C.3, it follows that there is a DAG \mathcal{D} in $[\mathcal{G}]$ such that Z does not satisfy the b-adjustment criterion relative to (\mathbf{X}, \mathbf{Y}) in \mathcal{D} . Since the b-adjustment criterion reduces to the adjustment criterion (Shpitser et al., 2010; Shpitser, 2012) in DAGs and the adjustment criterion is complete for DAGs, it follows that \mathbf{Z} is not an adjustment set relative to (\mathbf{X}, \mathbf{Y}) in \mathcal{D} . \square

Lemma C.1. Let \mathbf{X} and \mathbf{Y} be disjoint node sets in a maximal PDAG \mathcal{G} . If \mathcal{G} violates the b-amenability condition relative to (\mathbf{X}, \mathbf{Y}) , then there is no adjustment set relative to (\mathbf{X}, \mathbf{Y}) in \mathcal{G} .

Proof. This lemma is related to Lemma 3.12 from Perković et al. (2017). The proofs are not the same due to the differences between CPDAGs and maximal PDAGs. We will point out where the two proofs diverge.

Suppose that \mathcal{G} violates the b-amenability condition relative to (\mathbf{X}, \mathbf{Y}) . We will show that in this case one can find DAGs \mathcal{D}_1 and \mathcal{D}_2 in $[\mathcal{G}]$, such that there is no set that satisfies the b-adjustment criterion relative to (\mathbf{X}, \mathbf{Y}) in both \mathcal{D}_1 and \mathcal{D}_2 .

Since \mathcal{G} is not b-amenable relative to (\mathbf{X}, \mathbf{Y}) , there is a proper b-possibly causal path q^* from a node $X \in \mathbf{X}$ to a node $Y \in \mathbf{Y}$ that starts with a undirected edge. Let $q'^* = \langle X = V_0, V_1, \dots, V_k = Y \rangle, k \ge 1$ (where $V_1 = Y$ is allowed) be a shortest subsequence of q^* such that q'^* is also a proper b-possibly causal path that starts with a undirected edge in \mathcal{G} .

Suppose first that q'^* is of definite status in \mathcal{G} . Let \mathcal{D}_1 be a DAG in $[\mathcal{G}]$ that contains $X \to V_1$ and let \mathcal{D}_2 be a DAG in $[\mathcal{G}]$ that has no additional edges into V_1 as compared to \mathcal{G} (Lemma A.3). Then the path corresponding to q'^* in \mathcal{D}_1 is causal, whereas the path corresponding to q'^* in \mathcal{D}_2 is b-non-causal and contains no colliders. Hence, no set can satisfy both the b-forbidden set condition in \mathcal{D}_1 and the b-blocking condition in \mathcal{D}_2 relative to (\mathbf{X}, \mathbf{Y}) .

Otherwise, q'^* is not of definite status in \mathcal{G} . In the proof of Lemma 3.12 from Perković et al. (2017), the authors show that if q'^* is not of definite status, this leads to a contradiction. However, q'^* can be of non-definite status in \mathcal{G} and this is where the proofs diverge.

By Lemma 3.6, $q'^*(V_1, Y)$ must be unshielded and hence, of definite status in \mathcal{G} , since otherwise we can

choose a shorter b-possibly causal path. Since q'^* is not of definite status and $q'^*(V_1, Y)$ is of definite status, it follows that V_1 is not of definite status on q'^* . Then $\langle X, V_1, V_2 \rangle$ is a shielded triple. By choice of $q'^*, X - V_1$ is in \mathcal{G} . Additionally, since V_1 is not of definite status on $q'^*, V_1 - V_2$ must be in \mathcal{G} . This implies that $X - V_1 - V_2$ is in \mathcal{G} and $X \in \operatorname{Adj}(V_2, \mathcal{G})$. Moreover, we must have $X \to V_2$, since $X - V_2$ contradicts the choice of q'^* , and $X \leftarrow V_2$ contradicts that q'^* is b-possibly causal in \mathcal{G} .

Let \mathcal{D}_1 be a DAG in \mathcal{G} that has no additional edges into V_1 as compared to \mathcal{G} (Lemma A.3). Let q_1 be the path corresponding to q'^* in \mathcal{D}_1 . Then q_1 is of the form $X \leftarrow V_1 \rightarrow V_2 \rightarrow \cdots \rightarrow Y$ in \mathcal{D}_1 . Since $X \rightarrow V_2 \rightarrow \cdots \rightarrow Y$ is a proper causal path in $\mathcal{D}_1, \{V_2, \ldots, V_{k-1}\} \subseteq$ b-Forb $(\mathbf{X}, \mathbf{Y}, \mathcal{D}_1)$. Hence, any set that satisfies the b-blocking condition and the bforbidden set condition relative to (\mathbf{X}, \mathbf{Y}) in \mathcal{D}_1 must contain V_1 and not $\{V_2, \ldots, V_{k-1}$.

Let \mathcal{D}_2 be a DAG in \mathcal{G} that has no additional edges into V_2 as compared to \mathcal{G} (Lemma A.3). Let q_2 be the path corresponding to q'^* in \mathcal{D}_2 . Since $X \to V_2 \to V_1$ is in \mathcal{D}_2 , $X \to V_1$ is in \mathcal{D}_2 (Rule R2). Then q_2 is of the form $X \to V_1 \leftarrow V_2 \to \cdots \to Y$ in \mathcal{D}_2 . Hence, any set that satisfies the b-forbidden set condition and the b-blocking condition relative to (\mathbf{X}, \mathbf{Y}) in \mathcal{D}_1 , violates the b-blocking condition relative to (\mathbf{X}, \mathbf{Y}) in \mathcal{D}_2 .

Lemma C.2. Let \mathbf{X} and \mathbf{Y} be disjoint node sets in a maximal PDAG \mathcal{G} . If \mathcal{G} is b-amenable relative to (\mathbf{X}, \mathbf{Y}) , then the following statements are equivalent:

- (i) Z satisfies the b-forbidden set condition (see Definition 4.3) relative to (X, Y) in G.
- (ii) Z satisfies the b-forbidden set condition relative to
 (X, Y) in every DAG in [G].

Proof. This lemma is related to Lemma 3.14 from Perković et al. (2017), but instead of using Lemma A.9 and Lemma A.10 from Perković et al. (2017), we use Lemma 3.6 and Lemma B.1.

By Lemma 3.2 b-Forb $(\mathbf{X}, \mathbf{Y}, \mathcal{D}) \subseteq$ b-Forb $(\mathbf{X}, \mathbf{Y}, \mathcal{G})$ hence, (i) \Rightarrow (ii) holds. We now prove \neg (i) $\Rightarrow \neg$ (ii).

Let $V \in \mathbf{Z} \cap$ b-Forb $(\mathbf{X}, \mathbf{Y}, \mathcal{G})$. Then $V \in$ b-PossDe (W, \mathcal{G}) for some $W = V_i$ on a proper bpossibly causal path $p = \langle X = V_0, V_1, \dots, V_k =$ $Y \rangle, 1 \leq i \leq k$ from $X \in \mathbf{X}$ to $Y \in \mathbf{Y}$. Let q = p(X, W), r = p(W, Y) and let s be a b-possibly causal path from W to V, where r and s are allowed to be of zero length (if W = Y and/or W = V).

Let q', r' and s' be subsequences of q, r and s that form unshielded b-possibly causal paths, with r' and s' possibly of zero length (Lemma 3.6). Then q' must start with a directed edge, otherwise $q' \oplus r'$ would violate the bamenability condition. Hence, q' must be causal in \mathcal{G} (Lemma B.1).

Let \mathcal{D} be a DAG in $[\mathcal{G}]$ that has no additional edges into W as compared to \mathcal{G} (Lemma A.3). Then since r'and s' are unshielded and b-possibly causal, the paths corresponding to r' and s' in \mathcal{D} are causal (or of zero length). Hence, $V \in \text{b-Forb}(\mathbf{X}, \mathbf{Y}, \mathcal{D})$, so that $\mathbf{Z} \cap$ b-Forb $(\mathbf{X}, \mathbf{Y}, \mathcal{D}) \neq \emptyset$.

The final lemma needed to prove Theorem 4.4 is Lemma C.3. This lemma relies on Lemma C.6, which depends on Lemma C.4, C.5 and C.6. We first give Lemma C.3 with its proof. This is followed by Lemmas C.4, C.5 and C.6 with their proofs.

Lemma C.3. Let \mathbf{X} and \mathbf{Y} be disjoint node sets in a maximal PDAG \mathcal{G} . If \mathcal{G} is b-amenable relative to (\mathbf{X}, \mathbf{Y}) and \mathbf{Z} satisfies the b-forbidden set condition relative to (\mathbf{X}, \mathbf{Y}) in \mathcal{G} , then the following statements are equivalent:

- (i) Z satisfies the b-blocking condition (see Definition 4.3) relative to (X, Y) in G.
- (ii) **Z** satisfies the b-blocking condition relative to (\mathbf{X}, \mathbf{Y}) in every DAG in $[\mathcal{G}]$.
- (iii) **Z** satisfies the b-blocking condition relative to (\mathbf{X}, \mathbf{Y}) in a DAG \mathcal{D} in $[\mathcal{G}]$.

Proof of Lemma C.3. This lemma is related to Lemma 3.15 from Perković et al. (2017),but instead of using Lemma B.6 from Perković et al. (2017), we use Lemma C.6.

To prove \neg (i) $\Rightarrow \neg$ (iii) let p be a proper b-non-causal definite status path from **X** to **Y** that is d-connecting given **Z** in \mathcal{G} . The path corresponding to p in any DAG \mathcal{D} in [\mathcal{G}] is proper, non-causal (Lemma 3.2) and d-connecting given **Z**.

The implication \neg (iii) $\Rightarrow \neg$ (ii) trivially holds, so it is only left to prove that \neg (ii) $\Rightarrow \neg$ (i). Thus, assume there is a DAG \mathcal{D} in $[\mathcal{G}]$ such that a proper b-non-causal path from **X** to **Y** in \mathcal{D} is d-connecting given **Z**. Among the shortest proper non-causal paths from **X** to **Y** that are dconnecting given **Z** in \mathcal{D} , choose a path p with a minimal distance-from-**Z** (Definition A.1). Let p^* in \mathcal{G} be the path corresponding to p in \mathcal{D} . By Lemma C.6, p^* is a proper b-non-causal definite status path from **X** to **Y** that is d-connecting given **Z**.

Lemma C.4. Let \mathbf{X} , \mathbf{Y} and \mathbf{Z} be pairwise disjoint node sets in a maximal PDAG \mathcal{G} . Let \mathbf{Z} satisfy the bamenability condition and the b-forbidden set condition relative to (\mathbf{X}, \mathbf{Y}) in \mathcal{G} . Let \mathcal{D} be a DAG in $[\mathcal{G}]$ and let $p = \langle X = V_0, V_1, \ldots, V_k = Y \rangle, k \ge 1$, be a proper non-causal path from $X \in \mathbf{X}$ to $Y \in \mathbf{Y}$ that is d-connecting given \mathbf{Z} in \mathcal{D} . Let p^* in \mathcal{G} denote the path corresponding to p. Then:

- (i) Let $i, j \in \mathbb{N}, 0 < i < j \leq k$, such that there is an edge $\langle V_i, V_j \rangle$ in \mathcal{G} . The path $p^*(X, V_i) \oplus \langle V_i, V_j \rangle \oplus p^*(V_j, Y)$ ($p^*(V_j, Y)$ is possibly of zero length) is a proper b-non-causal path in \mathcal{G} . For j = i + 1, this implies that p^* is a proper b-non-causal path.
- (ii) If X ← V₁ and V₁ → V₂ are not in G and there is an edge ⟨X, V₂⟩ in G, then q* = ⟨X, V₂⟩ ⊕ p*(V₂, Y), (p*(V₂, Y) is possibly of zero length) is a proper b-non-causal path in G.

Proof. This lemma is related to Lemma B.3 from Perković et al. (2017). In particular, (i) in Lemma C.4 and (i) in Lemma B.3 from Perković et al. (2017) and their proofs match. The result in (ii) differs in both statement and proof from (ii)-(iii) in Lemma B.3 from Perković et al. (2017).

All paths considered are proper as they are subsequences of p^* , which corresponds to p.

(i) We use proof by contradiction. Thus, suppose that $q^* = p^*(X, V_i) \oplus \langle V_i, V_j \rangle \oplus p^*(V_j, Y)$ is bpossibly causal in \mathcal{G} . Then $\{V_1, \ldots, V_i, V_j, \ldots, V_k\} \subseteq$ b-Forb $(\mathbf{X}, \mathbf{Y}, \mathcal{G})$. Since \mathcal{G} is b-amenable relative to $(\mathbf{X}, \mathbf{Y}), q^*$ and $p^*(X, V_i)$ as well must start with $X \to$ V_1 . Then p also starts with $X \to V_1$ and since pis non-causal, there is at least one collider on p. Let $V_r, r \ge 1$, be the collider closest to X on p, then $V_r \in$ b-Forb $(\mathbf{X}, \mathbf{Y}, \mathcal{D})$. Since p is d-connecting given $\mathbf{Z}, \mathbf{Z} \cap$ $\mathrm{De}(V_r, \mathcal{D}) \neq \emptyset$. Since $\mathrm{De}(V_r, \mathcal{D}) \subseteq \mathrm{b-Forb}(\mathbf{X}, \mathbf{Y}, \mathcal{D})$ and since b-Forb $(\mathbf{X}, \mathbf{Y}, \mathcal{D}) \subseteq \mathrm{b-Forb}(\mathbf{X}, \mathbf{Y}, \mathcal{G})$, this contradicts $\mathbf{Z} \cap \mathrm{b-Forb}(\mathbf{X}, \mathbf{Y}, \mathcal{G}) = \emptyset$.

(ii) We again use proof by contradiction. Suppose neither $X \leftarrow V_1$ nor $V_1 \rightarrow V_2$ are in \mathcal{G} and q^* is a b-possibly causal path. Since \mathcal{G} is b-amenable relative to (\mathbf{X}, \mathbf{Y}) , $X \rightarrow V_2$ is in \mathcal{G} and $\{V_2, \ldots, V_k\} \subseteq$ b-Forb $(\mathbf{X}, \mathbf{Y}, \mathcal{G})$. Since $V_1 \rightarrow V_2$ is not in \mathcal{G} , either $V_1 - V_2$ or $V_1 \leftarrow V_2$ is in \mathcal{G} . Hence, $V_1 \in$ b-PossDe (V_2, \mathcal{G}) . Since b-PossDe $(V_2, \mathcal{G}) \subseteq$ b-Forb $(\mathbf{X}, \mathbf{Y}, \mathcal{G})$, it follows that $V_1 \in$ b-Forb $(\mathbf{X}, \mathbf{Y}, \mathcal{G})$.

Suppose that $V_1 \leftarrow V_2$ is in \mathcal{G} . Then $X \rightarrow V_2 \rightarrow V_1$ and rule R2 implies that $X \rightarrow V_1$ is in \mathcal{G} . Then $X \rightarrow V_1 \leftarrow V_2$, so since p is d-connecting given $\mathbf{Z}, \mathbf{Z} \cap \text{De}(V_1, \mathcal{D}) \neq \emptyset$. But $\text{De}(V_1, \mathcal{D}) \subseteq$ b-PossDe $(V_1, \mathcal{G}) \subseteq$ b-Forb $(\mathbf{X}, \mathbf{Y}, \mathcal{G})$, which contradicts that $\mathbf{Z} \cap$ b-Forb $(\mathbf{X}, \mathbf{Y}, \mathcal{G}) = \emptyset$. Otherwise, $V_1 - V_2$ is in \mathcal{G} . Additionally, $X \to V_2$ is in \mathcal{G} and $p^*(V_2, Y)$ is b-possibly causal. So since p^* is b-noncausal (from (i)), $X \leftarrow V_1$ must be in \mathcal{G} . This contradicts our assumption in (ii).

Lemma C.5. Let \mathbf{X} , \mathbf{Y} and \mathbf{Z} be pairwise disjoint node sets in a maximal PDAG \mathcal{G} . Let \mathbf{Z} satisfy the bamenability condition and the b-forbidden set condition relative to (\mathbf{X}, \mathbf{Y}) in \mathcal{G} . Let \mathcal{D} be a DAG in $[\mathcal{G}]$ and let p be a shortest proper non-causal path from \mathbf{X} to \mathbf{Y} that is d-connecting given \mathbf{Z} in \mathcal{D} . Let p^* in \mathcal{G} be corresponding path to p in \mathcal{D} . Then p^* is a proper bnon-causal definite status path in \mathcal{G} such that for every subpath $C_l \to C \leftarrow C_r$ of p^* there is no edge $\langle C_l, C_r \rangle$ in \mathcal{G} .

Proof. This lemma is related to Lemma B.4 from Perković et al. (2017). Our lemma additionally contains the result that if $\langle C_l, C, C_r \rangle$ is a subpath of p^* , then there is no edge $\langle C_l, C_r \rangle$ in \mathcal{G} . The proofs of this lemma and Lemma B.4 from Perković et al. (2017) overlap for cases (1)-(3) and then diverge after that.

Path p^* is proper and b-non-causal ((i) in Lemma C.4) in \mathcal{G} , so it is only left to prove that it is of definite status and that for any subpath $C_l \to C \leftarrow C_r$ of p^* there is no edge $\langle C_l, C_r \rangle$ in \mathcal{G} . Let $p^* = \langle X = V_0, V_1, \ldots, V_k =$ $Y \rangle, k > 1, X \in \mathbf{X}, Y \in \mathbf{Y}$. We first prove that p^* is of definite status, by contradiction.

Hence, suppose that a node on p^* is not of definite status. Let $V_i, i \ge 1$, be the node closest to X on p^* that is not of definite status. Then $\langle V_{i-1}, V_i, V_{i+1} \rangle$ is shielded in \mathcal{G} and there is an edge between V_{i-1} and V_{i+1} in \mathcal{G} . Let $q = p(X, V_{i-1}) \oplus \langle V_{i-1}, V_{i+1} \rangle \oplus p(V_{i+1}, Y)$ in \mathcal{D} . Let q^* be the path corresponding to q in \mathcal{G} . Then q^* is proper and b-non-causal (Lemma C.4) in \mathcal{G} . Hence, q is also a proper non-causal path (Lemma 3.2). Since p is a shortest proper b-non-causal path from X to Y that is d-connecting given \mathbf{Z} , it follows that q must be blocked by Z. The collider/non-collider status of all nodes, except possibly V_{i-1} and V_{i+1} , is the same on p and q. Hence, V_{i-1} or V_{i+1} block q, so $V_{i-1} \neq X$ or $V_{i+1} \neq Y$. We now discuss the different cases for the collider/noncollider status of V_{i-1} and V_{i+1} on p and q and derive a contradiction in each case.

- (1) V_{i-1} is a non-collider on p, a collider on q and $De(V_{i-1}, \mathcal{D}) \cap \mathbf{Z} = \emptyset$. Then $V_{i+1} \to V_{i-1} \to V_i$ and rule R2 implies that $V_i \leftarrow V_{i+1}$ is in \mathcal{D} . Since p is d-connecting given \mathbf{Z} , $De(V_i, \mathcal{D}) \cap \mathbf{Z} \neq \emptyset$. As $De(V_i, \mathcal{D}) \subseteq De(V_{i-1}, \mathcal{D})$, this contradicts $De(V_{k-1}, \mathcal{D}) \cap \mathbf{Z} = \emptyset$.
- (2) V_{i+1} is a non-collider on p, a collider on q and $De(V_{i+1}, D) \cap \mathbf{Z} = \emptyset$. This case is symmetric to

case (1) and the same argument leads to a contradiction.

- (3) V_{i-1} is a collider on p, a non-collider on q and $V_{i-1} \in \mathbb{Z}$. Since V_{i-1} is of definite status on p^* it follows that $V_{i-2} \rightarrow V_{i-1} \leftarrow V_i$ is in \mathcal{G} . This implies V_i is a definite non-collider on p^* , which is a contradiction.
- (4) V_{i+1} is a collider on p, a non-collider on q and V_{i+1} ∈ Z. Then V_i → V_{i+1} ← V_{i+2} and V_{i-1} ← V_{i+1} is in D. V_{i+1} is not of definite status on p*, otherwise V_i would be of definite status on p*. Thus, there is an edge ⟨V_i, V_{i+2}⟩ in G. The path r = p(X, V_i) ⊕ ⟨V_i, V_{i+2}⟩ ⊕ p(V_{i+2}, Y) is proper, bnon-causal (Lemma C.4) and shorter than p. Hence, r must be blocked by Z in D. The collider/noncollider status of all nodes except possibly V_i and V_{i+2} is the same on r and p, so either V_i or V_{i+2} must block r.

Since $V_i \to V_{i+1} \to V_{i-1}$ is in \mathcal{G} , rule R2 implies that $V_{i-1} \leftarrow V_i$ is in \mathcal{G} . Since $V_{i-1} \leftarrow V_i$ is on both r and p, V_i cannot block r. Additionally, $V_{i+1} \leftarrow$ V_{i+2} is in \mathcal{D} so V_{i+2} is a non-collider on p. Thus, V_{i+2} must be a collider on r and $\text{De}(V_{i+2}, \mathcal{D}) \cap \mathbf{Z} = \emptyset$. However, by assumption in (4), $V_{i+1} \in \mathbf{Z}$ and $V_{i+1} \in \text{De}(V_{i+2}, \mathcal{D})$.

Lastly, let $C_l \to C \leftarrow C_r$ be a subpath of p^* and suppose for a contradiction that there is an edge $\langle C_l, C_r \rangle$ in \mathcal{G} . Let $q^* = p^*(X, C_l) \oplus \langle C_l, C_r \rangle \oplus p^*(C_r, Y)$. Then q^* is proper and b-non-causal (Lemma C.4) in \mathcal{D} . Let q in \mathcal{D} be the path corresponding to q^* in \mathcal{G} . Then q is a proper non-causal path from X to Y that is shorter than p, so qmust be blocked by \mathbb{Z} . Then as above, either C_l or C_r must block q.

Since $C_l(C_r)$ is a non-collider on p, it must be a collider on q and $De(C_l, \mathcal{D}) \cap \mathbf{Z} \neq \emptyset$ ($De(C_r, \mathcal{D}) \cap \mathbf{Z} \neq \emptyset$). Since p is d-connecting given \mathbf{Z} , $De(C, \mathcal{D}) \cap \mathbf{Z} \neq \emptyset$. Additionally, $De(C_l, \mathcal{D}) \supseteq De(C, \mathcal{D})$ ($De(C_r, \mathcal{D}) \supseteq De(C, \mathcal{D})$), which contradicts $De(C_l, \mathcal{D}) \cap \mathbf{Z} \neq \emptyset$ ($De(C_r, \mathcal{D}) \cap \mathbf{Z} \neq \emptyset$).

Lemma C.6. Let \mathbf{X} , \mathbf{Y} and \mathbf{Z} be pairwise disjoint node sets in a maximal PDAG \mathcal{G} . Let \mathbf{Z} satisfy the bamenability condition and the b-forbidden set condition relative to (\mathbf{X}, \mathbf{Y}) in \mathcal{G} . Let \mathcal{D} be a DAG in $[\mathcal{G}]$ and let p be a path with minimal distance-from- \mathbf{Z} among the shortest proper non-causal paths from \mathbf{X} to \mathbf{Y} that are d-connecting given \mathbf{Z} in \mathcal{D} . Let p^* in \mathcal{G} be the path corresponding to p in \mathcal{D} . Then p^* is a proper b-non-causal definite status path from \mathbf{X} to \mathbf{Y} that is d-connecting given \mathbf{Z} in \mathcal{G} . *Proof.* This lemma is related to Lemma B.6 from Perković et al. (2017). The line of reasoning used in this first part of this proof overlaps with the proof of Lemma B.6. We will point out where the two proofs diverge.

From Lemma C.5 we know that p^* is a proper b-noncausal definite status path from **X** to **Y** in \mathcal{G} . We only need to prove that it is also d-connecting given **Z** in \mathcal{G} .

Since p is d-connecting given \mathbb{Z} in \mathcal{D} and p^* is of definite status, it follows that no definite non-collider on p^* is in \mathbb{Z} and that every collider on p^* has a possible descendant in \mathbb{Z} (Lemma C.4). Since every collider on p^* has a b-possibly causal path to \mathbb{Z} , by Lemma 3.6 there is b-possibly causal definite status path from every collider on p^* and let d^* be a shortest b-possibly causal definite status path from C to a node in \mathbb{Z} . It is only left to show that d^* is causal in \mathcal{G} , since then $C \in \operatorname{An}(\mathbb{Z}, \mathcal{G})$.

If d^* starts with a directed edge out of C, then d^* is causal in \mathcal{G} (Lemma B.1). Otherwise, $d^* = C - S \dots Z, Z \in \mathbb{Z}$ (possibly S = Z). We will prove that this leads to a contradiction. Hence, let $C_l \to C \leftarrow C_r$ be a subpath of p^* .

From this point onwards, this proof deviates somewhat from the proof of Lemma B.6 from Perković et al. (2017), due to the additional result in Lemma C.5. Since $C_l \rightarrow C - S (C_r \rightarrow C - S)$ is in \mathcal{G} , rule R1 and R2 imply that either $C_l \rightarrow S$ or $C_l - S (C_r \rightarrow S)$ or $C_r - S$) is in \mathcal{G} . Suppose that $C_l - S$ is in \mathcal{G} . Since $C_l \notin \operatorname{Adj}(C_r, \mathcal{G})$ (Lemma C.5), $C_r - S$ must be in \mathcal{G} , otherwise $C_l - S \leftarrow C_r$ violates R1 in \mathcal{G} . But then $C_l \rightarrow C \leftarrow C_r, C_l - S - C_r$ and C - S violate R3 in \mathcal{G} .

Hence, $C_l \to S$ is in \mathcal{G} . Then $C_r \to S$ must be in \mathcal{G} , otherwise $C_l \notin \operatorname{Adj}(C_r, \mathcal{G})$ and $C_l \to S - C_r$ violates R1. Now, depending on whether S is a node on p, we can derive the final contradiction.

Suppose S is not on p. Then if $S \notin \mathbf{X} \cup \mathbf{Y}$, $p(X, C_l) \oplus \langle C_l, S, C_r \rangle \oplus p(C_r, Y)$ is a proper noncausal path from **X** to **Y** in \mathcal{D} that is of the same length as p, but with a shorter distance-from-**Z** than p and d-connecting given **Z**. This contradicts our choice of p. Otherwise, suppose $S \in \mathbf{X}$. Then $\langle S, C_r \rangle \oplus$ $p(C_r, Y)$ contradicts our choice of p. Otherwise, $S \in$ **Y**. Then $S \notin$ b-Forb $(\mathbf{X}, \mathbf{Y}, \mathcal{G})$ otherwise, $Z \in$ b-Forb $(\mathbf{X}, \mathbf{Y}, \mathcal{G})$, it follows that $S \notin$ b-Forb $(\mathbf{X}, \mathbf{Y}, \mathcal{D})$, so $p(X, C_r) \oplus \langle C_l, S \rangle$ is a non-causal path from **X** to **Y** in \mathcal{D} . Then $p(X, C_r) \oplus \langle C_l, S \rangle$ contradicts our choice of p.

Otherwise, S must be on p. Hence, $S \notin \mathbf{X}$. Suppose

first that S is on $p(X, C_r)$. Let $q = p(X, S) \oplus \langle S, C_r \rangle \oplus p(C_r, Y)$. Since q is proper, non-causal and shorter than p, we only need to prove that q is d-connecting given **Z** to derive a contradiction. For this we only need to discuss the collider/non-collider status of S on q. If S is a collider on q, then q is d-connecting given **Z**. Otherwise, S is a non-collider on q. Then since $S \leftarrow C_r$ is on q, S must also be a non-collider on p. Since p is d-connecting given **Z**, $S \notin \mathbf{Z}$. Thus, q must be d-connecting given **Z** in \mathcal{G} .

Otherwise, S is on $p(C_r, Y)$. Then let $r = p(X, C_l) \oplus \langle C_l, S \rangle \oplus p(S, Y)$. Since $S \notin$ b-Forb $(\mathbf{X}, \mathbf{Y}, \mathcal{G})$ (otherwise $Z \in$ b-Forb $(\mathbf{X}, \mathbf{Y}, \mathcal{G})$) since $Z \in$ b-PossDe (S, \mathcal{G})) and since r is proper, it follows that r is a non-causal path. Hence, we only need to prove that r is d-connecting given \mathbf{Z} to derive a contradiction. For this we again only discuss the collider/non-collider status of S on q. If S is a collider on r, r is d-connecting given \mathbf{Z} . Otherwise, S is a non-collider on r. Then since $C_l \to S$ is on q, S must also be a non-collider on p. Since p is d-connecting given \mathbf{Z} of \mathcal{G} . \Box

C.2 PROOF OF THEOREM 4.6

Proof of Theorem 4.6. This theorem is related to Theorem 4.3 from Perković et al. (2017). This proof relies on similar line of reasoning however since Theorem 4.3 from Perković et al. (2017) states a somewhat different result and relies on a few lemmas for the proof, we do not make a direct comparison between the two as we did with the result presented in Section C.

We only need to prove that if there is a set that satisfies the b-adjustment criterion relative to (\mathbf{X}, \mathbf{Y}) in \mathcal{G} , then b-Adjust $(\mathbf{X}, \mathbf{Y}, \mathcal{G})$ also satisfies the b-adjustment criterion relative to (\mathbf{X}, \mathbf{Y}) in \mathcal{G} . Hence, assume that \mathbf{Z} satisfies the b-adjustment criterion relative to (\mathbf{X}, \mathbf{Y}) in \mathcal{G} and that b-Adjust $(\mathbf{X}, \mathbf{Y}, \mathcal{G})$ does not satisfy the badjustment criterion relative to (\mathbf{X}, \mathbf{Y}) in \mathcal{G} . We will show that this leads to a contradiction.

Since Z is an adjustment set relative to (X, Y) in \mathcal{G} (Theorem 4.4), \mathcal{G} is b-amenable relative to (X, Y). By construction b-Adjust (X, Y, \mathcal{G}) satisfies the b-forbidden set condition, so it must violate the b-blocking condition. Let $p = \langle X = V_0, V_1, \ldots, V_k = Y \rangle, k \ge 1, X \in X, Y \in Y$ be a shortest proper b-non-causal definite status paths from X to Y in \mathcal{G} that is d-connecting given b-Adjust (X, Y, \mathcal{G}) . Since Z blocks p, k > 1. So there is at least one non-endpoint node on p.

Since p is d-connecting given b-Adjust($\mathbf{X}, \mathbf{Y}, \mathcal{G}$) and b-Adjust($\mathbf{X}, \mathbf{Y}, \mathcal{G}$) = b-PossAn($\mathbf{X} \cup \mathbf{Y}, \mathcal{G}$) \ ($\mathbf{X} \cup \mathbf{Y} \cup$ b-Forb($\mathbf{X}, \mathbf{Y}, \mathcal{G}$)) any collider on p is in b-PossAn($\mathbf{X} \cup \mathbf{Y}, \mathcal{G}$). Additionally, no collider C on p is in b-Forb($\mathbf{X}, \mathbf{Y}, \mathcal{G}$) otherwise, $De(C, \mathcal{G}) \subseteq b$ -Forb($\mathbf{X}, \mathbf{Y}, \mathcal{G}$) and b-Forb($\mathbf{X}, \mathbf{Y}, \mathcal{G}$) \cap b-Adjust($\mathbf{X}, \mathbf{Y}, \mathcal{G}$) = \emptyset contradicts that p is dconnecting given b-Adjust($\mathbf{X}, \mathbf{Y}, \mathcal{G}$). Thus, every collider on p is in b-PossAn($\mathbf{X} \cup \mathbf{Y}, \mathcal{G}$)\ b-Forb($\mathbf{X}, \mathbf{Y}, \mathcal{G}$).

Any definite non-collider on p is a b-possible ancestor of X, Y or a collider on p. Hence, any definite non-collider on p is in b-PossAn($\mathbf{X} \cup \mathbf{Y}, \mathcal{G}$). Since p is d-connecting given b-Adjust($\mathbf{X}, \mathbf{Y}, \mathcal{G}$), no definite non-collider on p is in b-Adjust($\mathbf{X}, \mathbf{Y}, \mathcal{G}$). Then since b-Adjust($\mathbf{X}, \mathbf{Y}, \mathcal{G}$) = b-PossAn($\mathbf{X} \cup \mathbf{Y}, \mathcal{G}$) \ ($\mathbf{X} \cup$ $\mathbf{Y} \cup$ b-Forb($\mathbf{X}, \mathbf{Y}, \mathcal{G}$)), every definite non-collider on p is in $\mathbf{X} \cup \mathbf{Y} \cup$ b-Forb($\mathbf{X}, \mathbf{Y}, \mathcal{G}$). Since p is proper, no definite non-collider on p is in \mathbf{X} . Additionally, if there was a definite non-collider V on p such that $V \in \mathbf{Y} \setminus$ b-Forb($\mathbf{X}, \mathbf{Y}, \mathcal{G}$), then p(X, V) would be a shorter proper b-non-causal definite status path in \mathcal{G} that is d-connecting given b-Adjust($\mathbf{X}, \mathbf{Y}, \mathcal{G}$). Hence, any definite non-collider on p must be in b-Forb($\mathbf{X}, \mathbf{Y}, \mathcal{G}$).

Suppose that there is no collider on p. Then since \mathbb{Z} blocks p, a non-collider on p must be in \mathbb{Z} . This contradicts that \mathbb{Z} satisfies the b-forbidden set condition. Thus, there is a collider on p so let $V_{i-1} \rightarrow V_i \leftarrow V_{i+1}$ be a subpath of p. If there is a definite non-collider on p, then V_{i-1} or V_{i+1} is a non-collider on p. Suppose without loss of generality that V_{i-1} is a definite non-collider on p. Then $V_{i-1} \in \text{b-Forb}(\mathbb{X}, \mathbb{Y}, \mathcal{G})$. Since $V_{i-1} \rightarrow V_i$ is in $\mathcal{G}, V_i \in \text{b-Forb}(\mathbb{X}, \mathbb{Y}, \mathcal{G})$, which contradicts that V_i is a collider on p. Thus, there is no definite non-collider on p.

Since there is at least one collider on p and no definite non-collider is on p, it follows that p is of the form $X \to V_1 \leftarrow Y$ in \mathcal{G} . Since $V_1 \in \text{b-PossAn}(\mathbf{X} \cup \mathbf{Y}, \mathcal{G}) \setminus$ b-Forb $(\mathbf{X}, \mathbf{Y}, \mathcal{G})$, let q be a shortest b-possibly causal definite status path from V_1 to a node in $\mathbf{X} \cup \mathbf{Y}$. Then $q = \langle V_1, \ldots, V \rangle$, for some $V \in \mathbf{X} \cup \mathbf{Y}$. Then $V \in \mathbf{X}$ otherwise, $V_1 \in \text{b-Forb}(\mathbf{X}, \mathbf{Y}, \mathcal{G})$.

Thus, $r = (-p)(Y, V_1) \oplus q$ is a b-possibly causal path, so let r' be an unshielded subsequence of r that forms a b-possibly causal path from Y to \mathbf{X} in \mathcal{G} . Since (-r) is a proper path with respect to \mathbf{X} , (-r') is also a proper path with respect to \mathbf{X} . Then (-r') must be a b-non-causal path otherwise, $Y \in \text{b-Forb}(\mathbf{X}, \mathbf{Y}, \mathcal{G})$ which also implies $V_1 \in \text{b-Forb}(\mathbf{X}, \mathbf{Y}, \mathcal{G})$. Since r' is also unshielded, (-r') is a proper b-non-causal definite status path from \mathbf{X} to \mathbf{Y} in \mathcal{G} . Thus, \mathbf{Z} must block (-r'). Since r' is b-possibly causal, (-r') does not contain a collider, so a definite non-collider on (-r') must be in \mathbf{Z} . However, all definite non-colliders on (-r') are also on q, so \mathbf{Z} cannot block both (-r') and p in \mathcal{G} .

D EMPIRICAL STUDY

The following empirical study compares the runtimes of local IDA and our semi-local IDA on CPDAGs. We consider the 20 000 simulation settings described in the paper. The times are recorded in seconds on an Intel(R) Core(TM) i7-4765T CPU 2.00GHz processor running under Fedora 24 and using R version 3.4.0 and pcalg version 2.4-6.) The summary is given in Table 1.

	Median	Mean	Max
Local IDA	0.003	0.003	0.009
Semi-local IDA	0.003	0.016	4.881

Table 1: Median, mean and max computation times of local IDA and semi-local IDA.

We see that the median computation times are identical for both methods. The mean and maximum computation times, however, are larger for semi-local IDA. This indicates some outliers in the computation time of semilocal IDA. This could be explained by the presence of a small number of CPDAGs where our semi-local method is forced to orient a large subgraph of the CPDAG.

We also investigated the difference in runtimes between semi-local IDA and local IDA as a function of the number of variables (p) and the expected neighborhood size (E[N]), these results are given in Table 2 and Table 3 respectively. We see that the mean difference in runtimes increases with p, while there is not a very clear relationship with neighborhood size.

p	mean difference
20	0.009
30	0.007
40	0.010
50	0.009
60	0.016
70	0.013
80	0.014
90	0.015
100	0.021

Table 2: The mean runtime difference aggregated according to the number of variables (p).

E[N]	mean difference
3	0.016
4	0.013
5	0.013
6	0.011
7	0.009
8	0.011
9	0.015
10	0.014

Table 3: The mean runtime difference aggregated according to the expected neighborhood size (E[N]).

References

- Ernest, J., Rothenhäusler, D., and Bühlmann, P. (2016). Causal inference in partially linear structural equation models: identifiability and estimation. arXiv:1607.05980.
- Maathuis, M. H. and Colombo, D. (2015). A generalized back-door criterion. *Ann. Stat.*, 43:1060–1088.
- Perković, E., Textor, J., Kalisch, M., and Maathuis, M. H. (2017). Complete graphical characterization and construction of adjustment sets in Markov equivalence classes of ancestral graphs. *J. Mach. Learn. Res.* to appear.
- Shpitser, I. (2012). Appendum to "On the validity of covariate adjustment for estimating causal effects". Personal communication.
- Shpitser, I., VanderWeele, T., and Robins, J. M. (2010). On the validity of covariate adjustment for estimating causal effects. In *Proceedings of UAI 2010*, pages 527–536.
- Zhang, J. (2008). On the completeness of orientation rules for causal discovery in the presence of latent confounders and selection bias. *Artif. Intell.*, 172:1873– 1896.