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'BUREAUCRATIC' SET SYSTEMS, AND THEIR ROLE IN PHYLOGENETICS

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ABSTRACT. We say that a collection C of subsets of X is *bureaucratic* if every maximal hierarchy on X contained in C is also maximum. We characterise bureaucratic set systems and show how they arise in phylogenetics. This framework has several useful algorithmic consequences: we generalize some earlier results and derive a polynomial-time algorithm for a parsimony problem arising in phylogenetic networks.

1. BUREAUCRATIC SETS AND THEIR CHARACTERIZATION

We first recall some standard phylogenetic terminology (for more details, the reader can consult [6]). Recall that a *hierarchy* \mathcal{H} on a finite set X is a collection of sets with the property that the intersection of any two sets is either empty or equal to one of the two sets; we also assume that $X \in \mathcal{H}$.

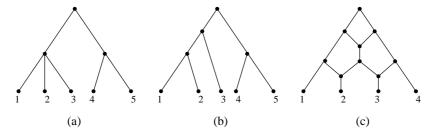


FIGURE 1. (a): A rooted tree T with leaf set $X = \{1, 2, 3, 4, 5\}$, and with cluster set c(T) being equal to the hierarchy \mathcal{H} consisting of the sets $\{1, 2, 3\}, \{4, 5\}$ and the trivial clusters. (b): A binary tree T with a cluster set consisting of $\mathcal{H} \cup \{\{1, 2\}\}$. (c): A binary and planar phylogenetic network \mathcal{N} over $X = \{1, 2, 3, 4\}$ with a soft-wired cluster set $sw(\mathcal{N})$ consisting of $\{1, 2\}, \{2, 3\}, \{3, 4\}, \{1, 2, 3\}, \{2, 3, 4\}$ and the trivial clusters.

A hierarchy is maximum if $|\mathcal{H}| = 2|X| - 1$, which is the largest possible cardinality. In this case \mathcal{H} corresponds to the set of clusters c(T) of some rooted binary tree T with leaf set X (a *cluster* of T is the set of leaves that are separated from the root of the tree by any vertex). A maximum hierarchy necessarily contains $\{x\}$ for each $x \in X$, as well as X itself; we will refer to these |X| + 1 sets as the *trivial clusters* of X. More generally, any hierarchy containing all the trivial clusters corresponds to the clusters c(T) of a rooted tree T with leaf set X (examples of these concepts are illustrated in Fig. 1(a),(b)). Note that a hierarchy \mathcal{H} is maximum if and only if (i) \mathcal{H} contains all the trivial clusters, and (ii) each set $C \in \mathcal{H}$ of size greater than 1 can be written as a disjoint union $C = A \sqcup B$, for two (disjoint) sets $A, B \in \mathcal{H}$.

We now introduce a new notion.

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Definition: We say that a collection C of subsets of a finite set X is a *bureaucracy* if (i) $C \neq \emptyset$ and $\emptyset \notin C$, and (ii) every hierarchy $\mathcal{H} \subseteq C$ can be extended to a maximum hierarchy \mathcal{H}' such that $\mathcal{H} \subseteq \mathcal{H}' \subseteq C$. In this case, we say that the collection is *bureaucratic*.

Simple examples of bureaucracies include two extreme cases: the set of clusters of a binary tree, and the set $\mathcal{P}(X)$ of all non-empty subsets of X. Notice that $\{\{a\}, \{b\}, \{c\}, \{a, b\}, \{a, b, c\}\}$ and $\{\{a\}, \{b\}, \{c\}, \{b, c\}, \{a, b, c\}\}$ are both bureaucratic subsets of $X = \{a, b, c\}$ but their intersection, $\{\{a\}, \{b\}, \{c\}, \{a, b, c\}\}$, is not. In particular, for an arbitrary subset Y of X (e.g. $Y = \{\{a\}, \{b\}, \{c\}, \{a, b, c\}\}$), there may not be a unique minimal bureaucratic subset of X containing Y.

In the next section we describe a more extensive list of examples, but first we describe some properties and provide a characterization of bureaucracies. In the following lemma, given two sets A and B from C we say that B covers A if $A \subsetneq B$ and there is no set $C \in C$ with $A \subsetneq C \subsetneq B$.

Lemma 1. If C is bureaucratic then:

- (i) For any pair $A, B \in \mathcal{C}$, if B covers A then $B A \in \mathcal{C}$.
- (ii) For any $C \in \mathcal{C}$ with |C| > 1, we can write $C = A \sqcup B$ for (disjoint) sets $A, B \in \mathcal{C}$.

Proof. For Part (i), suppose that $A, B \in C$ and that B covers A. Let $\mathcal{H} = \{A, B\}$. Then \mathcal{H} is a hierarchy that is contained within C and so there exists a maximum hierarchy $\mathcal{H}' \subseteq C$ that contains \mathcal{H} . Note that A must be a maximal sub-cluster of B in \mathcal{H}' (as otherwise B does not cover A) which requires that B - A is a cluster of \mathcal{H}' and thereby an element of C.

For Part (ii), observe that the set $\mathcal{H} = \{C\}$ is a hierarchy, and the assumption that \mathcal{C} is bureaucratic ensures the existence of a maximum hierarchy $\mathcal{H}' \subseteq \mathcal{C}$ containing \mathcal{H} , and so \mathcal{H}' contains the required sets A, B.

Note that the conditions described in Parts (i) and (ii) of Lemma 1, while they are necessary for C to be a bureaucracy, are not sufficient. For example, let $X = \{1, 2, 3, 4, 5, 6\}$ and let C be the union of

$$\{\{1,2\},\{3,4\},\{5,6\},\{1,2,3\},\{4,5,6\},\{3,4,5\},\{1,2,6\},\{1,5,6\},\{2,3,4\}\}$$

with the set of the seven trivial clusters. Then C satisfies Parts (i) and (ii) of Lemma 1, yet C is not bureaucratic since $\mathcal{H} = \{\{1,2\},\{3,4\},\{5,6\}\}$ does not extend to a maximum hierarchy on X using just elements from C.

Theorem 2. A collection C of subsets of X is bureaucratic if and only if it satisfies the following two properties:

- (P1) C contains all trivial clusters of X.
- (P2) If $\{C_1, C_2, \ldots, C_k\} \subseteq C$ are disjoint and have union $\cup_i C_i$ in C then there are distinct i, j such that $C_i \cup C_j \in C$.

Proof. First suppose that \mathcal{C} is bureaucratic. Then \mathcal{C} contains a maximal hierarchy; in particular, it contains all the trivial clusters, and so (P1) holds. For (P2), suppose that \mathcal{C}' is a collection of $k \geq 3$ disjoint subsets of X, each an element of \mathcal{C} , and $\bigcup \mathcal{C}' \in \mathcal{C}$. Then $\mathcal{H} = \mathcal{C}' \cup \{\bigcup \mathcal{C}'\}$ is a hierarchy. Let $\mathcal{H}' \subseteq \mathcal{C}$ be a maximal hierarchy on X that contains \mathcal{H} (this exists, since \mathcal{C} is bureaucratic) and let C be a minimal subset of X in \mathcal{H}' that contains the union of at least two elements of \mathcal{C}' . Since \mathcal{H}' is a binary hierarchy, and $\bigcup \mathcal{C}' \in \mathcal{H}', C$ is precisely the union of exactly two elements of \mathcal{C}' ; since $C \in \mathcal{H}' \subseteq \mathcal{C}$, this establishes (P2).

Conversely, suppose that a collection \mathcal{C} of subsets of X satisfies (P1) and (P2), and that $\mathcal{H} \subseteq \mathcal{C}$ is a maximal hierarchy which is contained within \mathcal{C} . Suppose that \mathcal{H} is not maximum (we will derive a contradiction). Then \mathcal{H} contains a set C that is the disjoint union of $k \geq 3$ maximal proper subsets A_1, \ldots, A_k , each belonging to \mathcal{H} (and thereby \mathcal{C}). Applying (P2) to

 $\mathcal{C}' = \{A_1, \ldots, A_k\}$, there exists two sets, say A_i, A_j for which $A_i \cup A_j \in \mathcal{C}$. So, if we let $\mathcal{H}' = \mathcal{H} \cup \{A_i \cup A_j\}$, then we obtain a larger hierarchy containing \mathcal{H} that is still contained within \mathcal{C} , which is a contradiction. This completes the proof.

2. Examples of bureaucracies

We have mentioned two extreme cases of bureaucracies, namely the set of clusters of a binary X-tree and the full power set $\mathcal{P}(X)$. Here are some further examples.

(1) The set of intervals of $[n] = \{1, 2, ..., n\}$ is a bureaucracy, where an *interval* is a set $[i, j] = \{k : i \le k \le j\}, 1 \le i \le j \le n.$

Proof. Let C be the set of intervals of [n]. Then C contains the trivial clusters. Also, a disjoint collection $I_1, \ldots, I_k, k > 2$ of intervals has union an interval if and only if every element of [n] between min $\bigcup I_j$ and max $\bigcup I_j$ lies in (exactly) one interval, in which case the union of any pair of consecutive intervals is an interval, so (P2) holds. By Theorem 2, C is bureaucratic.

Similarly, if we order the elements of X in any fashion, we can define the set of *intervals* on X for that ordering by this construction (associating x_i with i), and can thus obtain a bureaucracy.

A natural question at this point is the following: Does the extension of intervals in a 1-dimensional lattice (Example 1) to rectangles in a 2-dimensional lattice also necessarily lead to bureaucracies? The answer is 'no' because condition (P2) can be violated due to the existence of subdivisions of integral sized rectangles into k > 2 disjoint squares of different integral sizes, the union of any two of which must therefore fail to be a rectangle (see e.g. [2]).

(2) Let T be a rooted tree (generally not binary) with leaf set X and let \mathcal{C} be the set of all clusters compatible with all the clusters in c(T). Then \mathcal{C} is bureaucratic.

Proof. We have $C = \{C \subseteq X : C \cap C' \in \{C, C', \emptyset\}$ for all $C' \in c(T)\}$. C is also the set of clusters that occur in at least one rooted phylogenetic X- tree that refines T, that is:

$$\mathcal{C} = \bigcup_{T': c(T) \subseteq c(T')} c(T')$$

Suppose that $\mathcal{H} \subseteq \mathcal{C}$ is a hierarchy on X. Then $\mathcal{H} \cup c(T)$ is also a hierarchy on X since every element of \mathcal{H} is compatible with every element of c(T). Let \mathcal{H}' be any maximal hierarchy on X containing \mathcal{H} . Then since $c(T) \subseteq \mathcal{H}'$, we have $\mathcal{H}' \subseteq \mathcal{C}$, and so, by definition, \mathcal{C} is a bureaucracy.

(3) Let C be a collection of subsets of X that includes the trivial clusters and which satisfies the condition:

(1)

$$A, B \in \mathcal{C} \text{ and } A \cap B \neq \emptyset \Rightarrow A \cup B \in \mathcal{C}.$$

Then \mathcal{C} is bureaucratic if and only if \mathcal{C} satisfies the covering condition in Lemma 1(i).

Condition (1) is a weakening of the condition required for a 'patchwork' set system on X due to Andreas Dress and Sebastian Böcker (see e.g. [6], where the covering condition of Lemma 1(i) leads to an 'ample patchwork').

Proof. The 'only if' part follows from Lemma 1(i). Conversely, suppose that (1) holds for a set system \mathcal{C} that includes all the trivial clusters of X and that satisfies the covering condition of Lemma 1(i). Suppose that $\mathcal{H} \subseteq \mathcal{C}$ is a maximal hierarchy contained within \mathcal{C} . We show that \mathcal{H} is maximum. Suppose that this is not the case – we will derive a contradiction (by constructing a larger hierarchy \mathcal{H}' containing \mathcal{H} but still lying within

C). The assumption that \mathcal{H} is not maximum implies that there exists a set $B \in \mathcal{H}$ which is the union of three or more disjoint sets $A_1, A_2, A_3, \ldots, A_k$, where $A_i \in \mathcal{H}$ (since the rooted tree associated with \mathcal{H} has a vertex of degree $k \geq 3$). We consider two cases:

- (i) B covers none of the sets from $A_1, A_2, A_3, \ldots, A_k$.
- (ii) B covers one of the sets from $A_1, A_2, A_3, \ldots, A_k$.

We first show that Case (i) cannot arise under Condition (1). Suppose to the contrary Case (i) arises. Then for i = 1, ..., k there exists a set $C_i \in \mathcal{C}$ that contains A_i and which is covered by B. For any pair i, j with $i \neq j$, if $(B - C_i) \cap C_j = \emptyset$ then $C_j \subseteq C_i$. On the other hand, if $(B - C_i) \cap C_j \neq \emptyset$ then, by Condition (1), $(B - C_i) \cup C_j \in \mathcal{C}$, which means that $B = (B - C_i) \cup C_j$ (otherwise $(B - C_i) \cup C_j$ an element of \mathcal{C} strictly containing C_j and strictly contained by B) and so $C_i \subseteq C_j$. Thus Case (i) requires that either $C_i \subseteq C_j$ or $C_j \subseteq C_i$, which implies (again by the assumption that B covers C_i and Bcovers C_j) that $C_i = C_j$. Since this identity holds for all distinct pairs i, j it follows that C_1, C_2, \ldots, C_k are the same set C and this set contains $\bigcup_{i=1}^k A_i$ (since $A_i \subset C_i$). But then $B = \bigcup_{i=1}^k A_i \subseteq C$ which contradicts the assumption that B covers $C_1(=C)$.

Thus only Case (ii) can arise. In this case, suppose that B covers A_i . By assumption that C satisfies the covering condition described in Lemma 1(i), $B - A_i \in C$ holds, and so we can take $\mathcal{H}' = \mathcal{H} \cup \{B - A_i\}$ which provides the required contradiction.

(4) Let G = (X, E) be a connected graph. Let \mathcal{C} be the set of subsets $Y \subseteq X$ such that G[Y] is connected (where G[Y] is the subgraph formed by deleting vertices not in Y, together with their incident edges). Then \mathcal{C} is bureaucratic.

Observe that taking G to be a linear graph recovers Example (1).

Proof. First note that C satisfies (P1), since G itself is connected, as is each vertex by itself. Now suppose that $A_1, \ldots, A_k, k > 2$, are disjoint clusters in C whose union, A, is also in C. As G[A] is connected, at least two clusters A_i, A_j must contain adjacent vertices, in which case $G[A_i \cup A_j]$ is connected and $A_i \cup A_j \in C$. The result now follows by Theorem 2.

An alternative proof is to apply Example (3) and note that C satisfies Condition (1) and the covering condition of Lemma 1(i).

3. Algorithmic applications

3.1. Maximum weight hierarchies. In general, the problem of finding the largest hierarchy contained within a set of clusters is NP-hard [3]. The problem becomes trivial in a bureaucratic collection since all maximal hierarchies are maximum. Less obvious, however, is the fact that finding a hierarchy with maximum *weight* can also be solved in polynomial time.

Theorem 3. Let C be a bureaucratic collection of clusters on X and let $w : C \longrightarrow \mathbb{R}$ be a weight function on C. The problem of finding the hierarchy $\mathcal{H} \subseteq C$ such that $w(\mathcal{H}) = \sum_{A \in \mathcal{H}} w(A)$ is maximized can be solved in polynomial time.

Proof. If there are any clusters $A \in C$ with negative weight w(A) then set their weights to zero. It follows then that the weight of any maximum hierarchy $\mathcal{H} \subseteq C$ equals the weight of the maximum weight hierarchy contained within \mathcal{H} . The 'Hunting for Trees' algorithm of [1] can now be used to recover the maximum hierarchy of maximum weight. \Box

3.2. **Parsimony problems on networks.** Consider a set C of clusters on X and let $f : X \to A$ be a function that assigns each element $x \in X$ a state f(x) in a finite set A (f is referred to in phylogenetics as a (discrete) character). Suppose we have a non-negative function δ on $A \times A$

where $\delta(a, b)$ assigns a penalty score for changing state a to b for each pair $a, b \in \mathcal{A}$ (the default option is to to take $\delta(a, b) = 1$ for all $a \neq b$ and $\delta(a, a) = 0$ for all a).

Given any rooted X-tree T, with vertex set V and arc set E, let $l(f, T, \delta)$ denote the parsimony score of f on T relative to δ ; that is,

$$l(f,T,\delta) = \min_{F:V \to \mathcal{A}, F \mid X=f} \left\{ \sum_{(u,v) \in E} \delta(F(u), F(v)) \right\}.$$

In words, $l(f, T, \delta)$ is the minimum sum of δ -penalty scores that are required in order to extend f to an assignment of states to all the vertices of T. This quantity can be calculated for a given T by well-known dynamic programming techniques (see e.g. [6]). Let $l(f, \mathcal{C}, \delta)$ (respectively, $l_{\text{bin}}(f, \mathcal{C})$) denote the minimal value of $l(f, T, \delta)$ among all trees T (respectively, all *binary* trees) that have their clusters in \mathcal{C} . Then we have the following general result.

Theorem 4. Suppose that C is contained within a bureaucratic collection C' of subsets of X and $f: X \to A$. There is an algorithm for computing $l(f, C, \delta)$ with running time polynomial in n = |X|, |A| and |C'|. Moreover, the algorithm can be extended to construct a rooted phylogenetic X-tree having all its clusters in C and with parsimony score equal to $l(f, C, \delta)$ in polynomial time.

Proof. For any subset Y of X, let

$$\delta_Y(a,b) = \begin{cases} \delta(a,b), & \text{if } Y \in \mathcal{C}; \\ 0, & \text{if } Y \notin \mathcal{C} \text{ and } a = b; \\ \infty, & \text{otherwise;} \end{cases}$$

and for any rooted phylogenetic X-tree T, let

$$l'(f,T,\delta) := \min_{F:V \to \mathcal{A}, F|X=f} \left\{ \sum_{(u,v) \in E} \delta_{c(v)}(F(u),F(v)) \right\},\$$

where c(v) is the cluster of T associated with v.

Let $l'(f, \mathcal{C}', \delta)$ (respectively, $l'_{\text{bin}}(f, \mathcal{C}', \delta)$) be the minimal value of $l'(f, T, \delta)$ over all trees (respectively, all binary trees) with clusters in \mathcal{C}' . By the definition of δ_Y , we have:

(2)
$$l(f, \mathcal{C}, \delta) = l'(f, \mathcal{C}', \delta).$$

and by the assumption that \mathcal{C}' is bureaucratic we have:

(3)
$$l'(f, \mathcal{C}', \delta) = l'_{\text{bin}}(f, \mathcal{C}', \delta).$$

We now describe how $l'_{\rm bin}(f, \mathcal{C}', \delta)$ can be efficiently calculated by dynamic programming.

For an element $a \in \mathcal{A}$ and $Y \in \mathcal{C}'$, let L'(Y, a) be the minimum value of $l'(f|Y, T, \delta)$ across all binary trees T having leaf set Y and clusters in \mathcal{C}' , in which the root is assigned state a.

For |Y| = 1, say $Y = \{y\}$, we have

$$L'(Y,a) = \begin{cases} 0, & \text{if } f(y) = a; \\ \infty, & \text{otherwise} \end{cases}$$

and for |Y| > 1, we have

(4)
$$L'(Y,a) = \min_{Y_1,Y_2 \in \mathcal{C}', a_1, a_2 \in \mathcal{A}} \left\{ L'(Y_1,a_1) + \delta_{Y_1}(a,a_1) + L'(Y_2,a_2) + \delta_{Y_2}(a,a_2) : Y_1 \sqcup Y_2 = Y \right\}.$$

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Now,

$$l'_{\rm bin}(f, \mathcal{C}'\delta) = \min_{a \in \mathcal{A}} L'(X, a).$$

Notice that when one evaluates L'(X, a) using the above recursion (Eqn. (4)), it is sufficient to compute L'(Y, a) for just the sets $Y \in \mathcal{C}'$ rather than all subsets of X.

Thus, in view of Eqns. (2) and (3), one can compute $l(f, \mathcal{C}, \delta)$ in time polynomial in $n = |X|, |\mathcal{A}|$ and $|\mathcal{C}'|$. Moreover, by suitable book-keeping along the way, one can construct a rooted binary phylogenetic X-tree with clusters in \mathcal{C}' and with a parsimony score equal to $l_{\text{bin}}(f, \mathcal{C}', \delta)$; by collapsing all edges of this tree that have a δ -score equal to 0 we obtain a rooted phylogenetic X-tree with clusters in \mathcal{C} and with parsimony score equal to $l_{\text{bin}}(f, \mathcal{C}', \delta)$;

We note that this result has been described in the particular case when C is the bureaucracy described in example (2) above, and where f maps to a set A with only two elements [5]. We provide a second application, to phylogenetic networks, based on Example (1) above, of intervals as bureaucratic set systems.

Let \mathcal{N} be a rooted binary phylogenetic network on X. We say that \mathcal{N} is *planar* if it can be drawn in the plane so that all the leaves and the root all lie on the outer face. Let $sw(\mathcal{N})$ denote the set of 'soft-wired' clusters in \mathcal{N} (the union of the cluster sets of all trees embedded in \mathcal{N} ; see e.g. [4]). A simple example is shown in Fig. 1(c).

Corollary 5. Suppose that \mathcal{N} is a binary and planar phylogenetic network on X, and $f : X \to \mathcal{A}$. There is an algorithm for computing $l(f, sw(\mathcal{N}))$ with running time polynomial time in n.

Proof. Let x_1, \ldots, x_n be the ordering of X given by their positions around the outer face in a planar embedding of \mathcal{N} , where x_1 and x_n come immediately after and before the root. Then any tree T embedded in \mathcal{N} can be ordered so that the leaves are in order x_1, \ldots, x_n , implying that the clusters of T are all of the form $\{x_i, x_{i+1}, \ldots, x_j\}$ for some $1 \leq i \leq j \leq n$. It follows that the set $sw(\mathcal{N})$ is contained in the set of intervals of $X = \{x_1, \ldots, x_n\}$ (Example 1, above). The corollary now follows from Theorem 4.

We end this paper by posing a computational problem.

Question. Is there an algorithm for deciding whether or not C is bureaucratic that runs in time polynomial in |C| and |X|?

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