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OPTIMAL APPROXIMATION OF SPARSE HESSIANS AND
ITS EQUIVALENCE TO A GRAPH COLORING PROBLEM

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OPTIMAL APPROXIMATION OF SPARSE HESSIANS AND ITS EQUIVALENCE TO A GRAPH COLORING PROBLEM

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ABSTRACT

We consider the problem of approximating the Hessian matrix of a smooth non-linear function using a minimum number of gradient evaluations, particularly in the case that the Hessian has a known, fixed sparsity pattern. We study the class of Direct Methods for this problem, and propose two new ways of classifying Direct Methods. Examples are given that show the relationships among optimal methods from each class. The problem of finding a non-overlapping direct cover is shown to be equivalent to a generalized graph coloring problem — the distance-2 graph coloring problem. A theorem is proved showing that the general distance- k graph coloring problem is NP-Complete for all fixed $k \geq 2$, and hence that the optimal non-overlapping direct cover problem is also NP-Complete. Some worst-case bounds on the performance of a simple coloring heuristic are given. An appendix proves a well known folklore result, which implies as a corollary that another class of methods, the Elimination Methods, includes optimal polynomially-bounded algorithms.

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1. Introduction

The problem of interest is the approximation of the Hessian matrix of a smooth nonlinear function $F : \mathbb{R}^n \rightarrow \mathbb{R}$. In many circumstances, it is difficult or even impossible to evaluate the Hessian of F from its exact representation. Under these conditions, an approximation to the Hessian can be computed using finite differences of the gradient. When the Hessian is a dense matrix, this approximation is usually obtained by differencing the gradient along the coordinate vectors, and hence requires n evaluations of the gradient (which is the minimum possible number; see Appendix 1). However, if the Hessian has a fixed sparsity pattern at every point (i.e., certain elements are known to be zero), the Hessian may be approximated with a smaller number of gradient evaluations by differencing along specially selected sets of vectors.

For example, consider the following sparsity pattern, in which 0 stands for a known zero and 1 stands for a possible non-zero of the Hessian:

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 1 & 1 \end{pmatrix}.$$

If the gradient is differenced along the directions $(1, 1, 0)^T$ and $(0, 0, 1)^T$, the Hessian may be approximated with only two additional gradient evaluations.

When n is large and the proportion of zero elements is high, the number of gradient evaluations needed to approximate the Hessian may be only a small fraction of n . This result is particularly useful in numerical optimization algorithms.

Let $g(x)$ denote the gradient of F , and $H(x)$ denote the Hessian. Assume that $g(x^0)$ is known, and that we wish to approximate $H(x^0)$ by evaluating $g(x^0 + hd^l)$, $l = 1, \dots, k$, for some step size h and a set of k difference vectors $\{d^l\}$. For each l and sufficiently small h , we obtain n approximate linear equations

$$hH(x^0)d^l \approx g(x^0 + hd^l) - g(x^0), \quad (1)$$

so that there are a total of nk equations. Note that many of the components of d^l and $H(x^0)$ are usually zero.

Schemes for evaluating a Hessian approximation have been divided into three categories, depending on the complexity of the subsystem of (1) that must be solved for the unknown elements of the Hessian (see e.g., Coleman and Moré (1981)). **Direct Methods** correspond to a diagonal subsystem; **Substitution Methods** correspond to a triangular subsystem; and **Elimination Methods** correspond simply to a nonsingular subsystem. There is a tradeoff here; as we move from Direct Methods to Elimination Methods, we are less restricted and thus expect fewer evaluations to be required, but we lose ease of approximation and possibly numerical stability.

Once a class of methods has been selected, the problem is to choose a specific method that minimizes k for a given sparsity pattern, without requiring too much effort to determine the vectors $\{d^l\}$. This paper is concerned primarily with a partial solution to this problem for direct methods. (The solution for elimination methods is well known, but seems never to have been published. Appendix 1 gives a proof of the theorem behind the solution in this case.) Section 2 gives a new classification for direct methods, Section 3 reduces one of these classes to a graph coloring problem and shows that problem to be NP-complete, Section 4 gives some heuristic results for the same class, and Section 5 points out possible future avenues of research.

2. Classifying Direct Methods

Let H denote the Hessian of F at the point x^0 . Any element of H that is not known to be zero is called an unknown. An illuminating interpretation of a direct method is to regard the non-zero components of a given d^l as specifying a subset S_l of the columns of H ; S_l is called the l^{th} group of columns; by a slight abuse of notation, a column index j is said to belong to S_l when its column does. When two columns belonging to S_l both have an unknown in row i , there is said to be an overlap in S_l in row i .

By definition of a direct method, the family of subsets $\{S_l\}$ must satisfy the Direct Cover Property (DC):

(DC) For each unknown h_{ij} , there must be at least one S_l containing column j such that column j is the only column in S_l that has an unknown in row i .

Any family of subsets of columns satisfying (DC) is called a direct cover for H , and naturally gives a scheme for approximating H . That is, if e_i is the i^{th} unit vector, differencing along

$$d^l = \sum_{j \in S_l} e_j, \quad l = 1, \dots, k$$

is the scheme associated with the family $\{S_l\}$. The problem of interest is thus that of finding a minimum cardinality direct cover for a given H (an optimal direct cover).

Since it is difficult to find a general optimal direct cover, the problem is often approached heuristically by restricting the acceptable direct covers and attempting to choose an optimal or near-optimal direct cover from the restricted set. We suggest a new classification scheme for types of permitted direct covers. From most to least restrictive, the categories are:

(1) Non-Overlap Direct Covers (NDC): No overlap may occur within any group of columns, i.e. every group has at most one unknown in each row. The best-

known heuristic, the CPR method, belongs to this class (see Curtis, Powell and Reid (1974)).

(2) **Sequentially Overlapping Direct Covers (SeqDC)**: A less restricted class may be defined by observing that overlap within a group of an ordered direct cover does not violate the direct cover property if the values of overlapping unknowns can be resolved using preceding groups. In a SeqDC, columns in group l are allowed to overlap in row m only if column m belongs to some group k such that $k < l$. This definition implies that (DC) is satisfied: Consider an unknown h_{ij} and let $k = \min\{l \mid \text{either } i \text{ or } j \text{ belongs to group } l\}$ (k is called the **minimum index group** of h_{ij}); note that h_{ij} cannot overlap with any other unknown in its row in group l . Powell and Toint (1979) propose a heuristic of this class.

(3) **Simultaneously Overlapping Direct Covers (SimDC)**: This is the most general class of direct covers. Any kind of overlap is allowed, as long as (DC) is not violated. In particular, an unknown may overlap in its row even in its minimum index group as long as the overlap is resolved in some succeeding group. Thapa's "New Direct Method" (1980) falls in this class, though he adds several other restrictions.

Note that $\text{NDC} \subset \text{SeqDC} \subset \text{SimDC}$; these inclusions are strict, as the following examples show. Consider

$$\begin{pmatrix} 1 & 1 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 1 & 1 \end{pmatrix}.$$

Since every column overlaps with every other column, an NDC must use at least five groups (and of course, five suffice). But $\{\{3\}, \{2, 4\}, \{1\}, \{5\}\}$ is a SeqDC of cardinality $4 < 5$. Now consider (from Powell and Toint (1979))

$$\begin{pmatrix} 1 & 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 & 1 & 0 \\ 1 & 1 & 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 \end{pmatrix}.$$

It is easy to see that any SeqDC requires at least four groups, but $\{\{1, 5\}, \{2, 6\}, \{3, 4\}\}$ is a SimDC of size only three.

The above discussion glossed over whether a column can belong to more than one group. This consideration leads to an independent classification scheme for direct covers into:

(1) **Partitioned Direct Covers (prefix P)**: These require the direct cover to be a partition of $\{1, 2, \dots, n\}$, i.e., every column must belong to exactly one group.

(2) **General Direct Covers** (prefix G): These allow either columns that belong to no group, or columns that belong to more than one group.

All heuristics proposed so far known to this author restrict themselves to partitioned direct covers. When h_{ii} is an unknown, column i must belong to at least one group, for otherwise h_{ii} would not be determined. Since h_{ii} is an unknown for all i in most unconstrained problems, it seems natural to restrict our attention to direct covers in which each column belongs to at least one group. However, sometimes the optimal direct cover is larger under this restriction. For example, consider an NDC for

$$\begin{pmatrix} 0 & 1 & 1 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}.$$

Since all three pairs of columns overlap, a PNDC must use three groups; however, $\{\{2\}, \{3\}\}$ is a valid GNDC of smaller size. But such problems rarely occur in unconstrained problems, and we shall henceforth consider only direct covers in which every column belongs to at least one group.

From the remark in the definition of SeqDC that the definition of a SeqDC implies (DC), it is easy to see that in *any* GSeqDC, we can delete a column from all groups in which it appears except for its minimum index group, without violating (DC) (*i.e.*, since any h_{ij} is always determined directly by some column in that column's minimum index group, any later occurrences of that column are superfluous). Thus in the SeqDC case, and so also in the NDC case, it suffices to consider only partitioned direct covers.

But, unfortunately, PSimDC's are *not* optimal in the class of GSimDC. Consider

$$\begin{pmatrix} 1 & 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 1 \end{pmatrix}. \quad (2)$$

Laborious calculations verify that any PSimDC must have more than four groups. However, $\{\{1, 2\}, \{1, 3\}, \{4, 6\}, \{5, 7\}\}$ is a GSimDC of size four where column 1 appears in two different groups. (The matrix (2) is the smallest possible such example in terms of number of columns.)

3. An Equivalent Graph Coloring Problem; NP-Completeness

We show that the problem of finding an optimal NDC (which can be assumed to be partitioned) is equivalent to a graph coloring problem, which is then shown

to be NP-Complete. Our notation and terminology for graphs follow that of Bondy and Murty (1976). Our way of writing a sparsity pattern as a $(0,1)$ -matrix, call it S , could just as well be interpreted as the vertex-vertex incidence matrix of an undirected graph. That is, the symmetry of the sparsity pattern is reflected in the undirectedness of the graph. A partition of the columns of the sparsity pattern naturally induces a partition of the vertices of the associated graph; the vertex partition can be considered to be some sort of coloring on the graph.

Two columns in the same group, *i.e.* two vertices of the same color, cannot "overlap". Column i overlaps column j if $s_{ki} = s_{kj} = 1$ for some row k , *i.e.*, if vertex i and vertex j are both adjacent to vertex k . Thus the restriction on our graph coloring is that no two vertices of the same color can have a common neighbor. If distance from vertex i to vertex j in the graph is measured by "minimum number of edges in any path between i and j ", then we require that any two vertices of the same color must be more than two units apart. In the usual Graph Coloring Problem, we require that any two vertices of the same color be more than one unit apart. This leads to defining a proper distance- k coloring of a graph G to be a partition of the vertices of G into classes (colors) so that any two vertices of the same color are more than k units apart. Then we want to solve the

Distance- k Graph Coloring Problem (D k GCP) on a graph G : Find a proper distance- k coloring of G in the minimum possible number of colors.

Then the usual Graph Coloring Problem (GCP) is D1GCP, and the optimal NDC problem is equivalent to D2GCP. We shall use this equivalence to show that the optimal NDC problem is NP-Complete by showing that D2GCP is NP-Complete; in fact, we shall show the stronger result that D k GCP is NP-Complete for any fixed $k \geq 2$.

First we review the definition of NP-Completeness (see Garey and Johnson (1979)). The fundamental NP-Complete problem is the Satisfiability Problem (SAT), which we use in a slightly simpler, but equivalent form:

3-Satisfiability (3SAT): Given a set of atoms u_1, u_2, \dots, u_n , we get the set of literals $L = \{u_1, \bar{u}_1, u_2, \bar{u}_2, \dots, u_n, \bar{u}_n\}$. Let $C = \{C_1, C_2, \dots, C_m\}$ be a set of 3-clauses drawn from L , that is, each $C_s \subset L$, and $|C_s| = 3$. Is there a truth assignment $T : \{u_1, \dots, u_n\} \rightarrow \{\text{true}, \text{false}\}$ such that each C_s contains at least one u_i with $T(u_i) = \text{true}$ or at least one \bar{u}_i with $T(u_i) = \text{false}$?

The set of clauses is really an abstraction of a logical formula; imagine the clauses as parenthesized subformulae whose literals are connected by 'or', with all the clauses connected with 'and'. Then a satisfying truth assignment makes the whole formula true. 3SAT has been shown to be "at least as hard as" a whole

class of hard problems. Thus, if 3SAT can be encoded into any other problem X , then X inherits the "at least as hard as" property and is called NP-Complete.

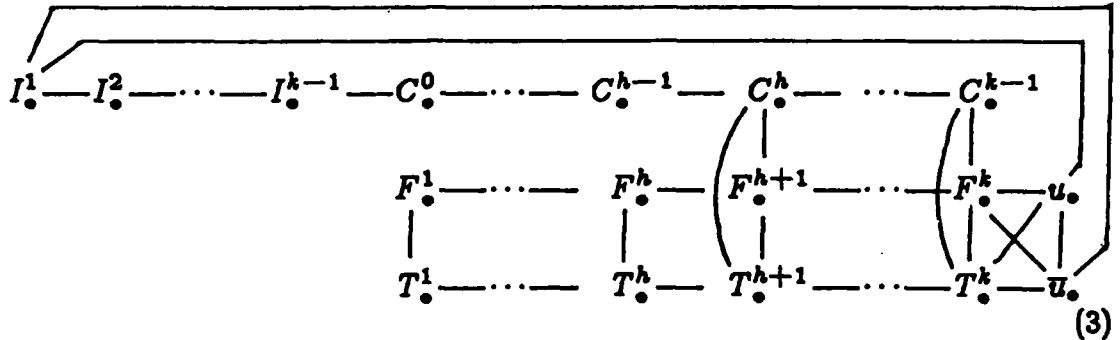
In order to encode 3SAT into D_kGCP , D_kGCP must be recast as a decision problem. As is standard with optimization problems, we re-phrase D_kGCP to "Is there a distance- k coloring that uses p or fewer colors?" Our encoding is a generalization of the one found in Karp's original proof (1972) of the NP-Completeness of GCP. The theorem about the encoding requires the exclusion of the case in which a clause contains both an atom and its negation. But such clauses are always trivially satisfied, so we henceforth understand "3SAT" to mean "3-Satisfiability without trivial clauses".

Given a 3SAT problem P , we construct from it a decision problem on a graph $G_k(P)$. If P has atoms u_1, u_2, \dots, u_n and clauses C_1, C_2, \dots, C_m , let $h = \lceil k/2 \rceil$ and $p = 2nk + m(k-1)$. Let V and E denote the vertices and edges of $G_k(P)$, and define them by

$$V = \begin{cases} \left. \begin{array}{l} \{u_i, \bar{u}_i\} \\ \{F_i^r, T_i^r, \quad r = 1, \dots, k\} \end{array} \right\} & i = 1, \dots, n \quad \text{literal vertices, false ver-} \\ & \text{tices, true vertices} \\ \left. \begin{array}{l} \{C_s^r, \quad r = 0, \dots, k-1\} \\ \{I_s^r, \quad r = 1, \dots, k-1\} \end{array} \right\} & s = 1, \dots, m \quad \text{clause vertices, intermediate} \\ & \text{vertices} \end{cases}$$

$$E = \begin{cases} \left. \begin{array}{l} \{u_i, \bar{u}_i\} \quad \text{all } i \\ \{F_i^r, F_i^{r+1}\} \\ \{T_i^r, T_i^{r+1}\} \\ \{F_i^r, T_j^r\} \\ \{F_i^r, F_j^r\} \\ \{T_i^r, T_j^r\} \end{array} \right\} & \text{all } r, \text{ all } i \neq j \quad \text{all } F\text{'s, } T\text{'s different colors} \\ \left. \begin{array}{l} \{I_s^r, I_s^{r+1}\} \quad \text{all } r \\ \{I_s^{k-1}, C_s^0\} \\ \{I_s^1, u_i\} \quad \text{if } u_i \in C_s \\ \{I_s^1, \bar{u}_i\} \quad \text{if } \bar{u}_i \in C_s \end{array} \right\} & \text{all } s \quad \begin{array}{l} C_s^0 \text{ different color than its} \\ \text{literals} \end{array} \\ \left. \begin{array}{l} \{u_i, F_j^h\} \\ \{u_i, T_j^h\} \\ \{u_i, F_j^h\} \\ \{u_i, T_j^h\} \end{array} \right\} & \text{all } i \neq j \quad \begin{array}{l} u_i, \bar{u}_i \text{ can only be } F_i^1 \text{ or} \\ T_i^1 \end{array} \\ \left. \begin{array}{l} \{C_s^r, C_t^r\} \quad r \geq h \\ \{C_s^r, F_i^{r+1}\} \quad r \geq h \\ \{C_s^r, T_i^{r+1}\} \quad r \geq h \\ \{C_s^r, C_s^{r+1}\} \quad r \geq 0 \end{array} \right\} & \text{all } s \neq t, \text{ all } i \quad \begin{array}{l} C_i^r, r > 0, \text{ different from} \\ \text{each other and } F\text{'s and} \\ T\text{'s} \end{array} \\ \left. \begin{array}{l} \{C_s^{h-1}, F_i^h\} \quad u_i, \bar{u}_i \notin C_s \\ \{C_s^{h-1}, T_i^h\} \quad \text{all } i \end{array} \right\} & \text{all } s, k \text{ odd} \\ \left. \begin{array}{l} \{C_s^h, F_i^h\} \quad u_i, \bar{u}_i \notin C_s \\ \{C_s^h, T_i^h\} \quad \text{all } i \end{array} \right\} & \text{all } s, k \text{ even} \quad \begin{array}{l} C_s^0 \text{ can only be } F^1 \text{ colors} \\ \text{of its literals} \end{array} \end{cases}$$

Note that we consider $G_k(P)$ only for $k \geq 2$, implying that $h + 1 \leq k$, so $h + 1$ makes sense as a superscript for the F 's and the T 's. The global structure of $G_k(P)$ looks like:



We need three propositions about the structure of a proper distance- k coloring of $G_k(P)$.

Proposition 1. The vertices F_i^r , T_i^r , and C_s^r , $i = 1, \dots, n$, $s = 1, \dots, m$, $r = 1, \dots, k$ must all have different colors, thus using up all p colors.

Proof. Consider the length k paths

$$\left. \begin{matrix} F_i^1 \\ T_i^1 \end{matrix} \right\} \text{---} \left\{ \begin{matrix} F_j^1 \text{---} F_j^2 \text{---} \dots \text{---} F_j^k \\ T_j^1 \text{---} T_j^2 \text{---} \dots \text{---} T_j^k \end{matrix} \right.$$

which demonstrate that all F 's and T 's must be different colors. Now consider the length $k - 1$ paths

$$C_s^1 \text{---} C_s^2 \text{---} \dots \text{---} C_s^h \text{---} \left\{ \begin{matrix} F_i^{h+1} \text{---} F_i^{h+2} \text{---} \dots \text{---} F_i^k \\ T_i^{h+1} \text{---} T_i^{h+2} \text{---} \dots \text{---} T_i^k \end{matrix} \right. \quad (4)$$

which show that no C_s^q , $0 < q \leq h$ can be any F_i^r or T_i^r color, $r > h$. The length at most $k - 1$ paths

$$C_s^{k-1} \text{---} C_s^{k-2} \text{---} \dots \text{---} C_s^h \text{---} \left\{ \begin{matrix} F_i^{h+1} \text{---} F_i^{h+2} \text{---} \dots \text{---} F_i^k \\ T_i^{h+1} \text{---} T_i^{h+2} \text{---} \dots \text{---} T_i^k \end{matrix} \right.$$

show that no C_s^q , $h \leq q < k$ can be any F_i^r or T_i^r color, $r > h$. Let l be an index such that $u_l \notin C_s$ and $\bar{u}_l \notin C_s$, and consider the length $k - 1$ paths

$$C_s^1 \text{---} \dots \text{---} C_s^{h-1} \text{---} \left\{ \begin{matrix} T_i^h \text{---} T_i^{h-1} \text{---} \dots \text{---} T_i^1 & k \text{ odd} \\ C_s^h \text{---} T_i^h \text{---} \dots \text{---} T_i^1 & k \text{ even} \end{matrix} \right. \quad (5)$$

which show that no C_s^q , $0 < q < h$ can be any T_i^r color, $r \leq h$. The length k paths

$$C_s^1 \text{---} C_s^2 \text{---} \dots \text{---} C_s^{h-1} \text{---} \left\{ \begin{matrix} F_i^h \text{---} F_i^h \text{---} F_i^{h-1} \text{---} \dots \text{---} F_i^1 & k \text{ odd} \\ C_s^h \text{---} F_i^h \text{---} F_i^h \text{---} \dots \text{---} F_i^1 & k \text{ even} \end{matrix} \right. \quad (6)$$

show that no C_s^q , $0 < q < h$ can be any F_i^r color, $r \leq h$. The length k paths

$$C_s^{k-1} \text{---} C_s^{k-2} \text{---} \dots \text{---} C_s^h \text{---} \begin{cases} F_i^{h+1} \text{---} F_i^h \text{---} \dots \text{---} F_i^1 \\ T_i^{h+1} \text{---} T_i^h \text{---} \dots \text{---} T_i^1 \end{cases}$$

show that no C_s^q , $h \leq q < k$, can be any F_i^r or T_i^r color, $r \leq h$. The length $k-1$ paths

$$C_s^1 \text{---} C_s^2 \text{---} \dots \text{---} C_s^{h-1} \text{---} \begin{cases} T_i^h \text{---} C_s^{h-1} \text{---} C_s^{h-2} \text{---} \dots \text{---} C_s^1 & k \text{ odd} \\ C_s^h \text{---} C_s^h \text{---} C_s^{h-1} \text{---} \dots \text{---} C_s^1 & k \text{ even} \end{cases} \quad (7)$$

show that no C_s^q can be the same color as any C_t^r , $0 < q, r < h$. Finally, the length $k-1$ path

$$C_s^1 \text{---} C_s^2 \text{---} \dots \text{---} C_s^h \text{---} C_t^h \text{---} C_t^{h+1} \text{---} \dots \text{---} C_t^{k-1} \quad (8)$$

shows that no C_s^q can be the same color as any C_t^r , $h \leq q, r < k$. \square

Since F_i^r , T_i^r and C_s^q , $q > 0$, use up all the colors, we subsequently refer to the colors by these vertex names.

Proposition 2. Vertices u_i and \bar{u}_i must be colored F_i^1 and T_i^1 in some order, $i = 1, \dots, n$.

Proof. Let $j \neq i$ and consider the length k paths

$$\left. \begin{matrix} u_i \\ \bar{u}_i \end{matrix} \right\} \text{---} \begin{cases} F_j^k \text{---} \begin{cases} F_i^k \text{---} F_i^{k-1} \text{---} \dots \text{---} F_i^2 \\ F_j^{k-1} \text{---} F_j^{k-2} \text{---} \dots \text{---} F_j^1 \end{cases} \\ T_j^k \text{---} \begin{cases} T_i^k \text{---} T_i^{k-1} \text{---} \dots \text{---} T_i^2 \\ T_j^{k-1} \text{---} T_j^{k-2} \text{---} \dots \text{---} T_j^1 \\ C_s^{k-1} \text{---} C_s^{k-2} \text{---} \dots \text{---} C_s^1 \end{cases} \end{cases} \quad (9)$$

which show that u_i and \bar{u}_i cannot be any color other than F_i^1 and T_i^1 . Also, u_i and \bar{u}_i certainly cannot be the same color. \square

Thus a proper distance- k coloring of $G_k(P)$ induces a truth assignment on the literals.

Proposition 3. If the literals in clause C_s have indices a , b , and c , then C_s^0 must be colored F_a^1 , F_b^1 , or F_c^1 , $s = 1, \dots, m$.

Proof. We can add C_s^0 to the beginning of the paths in (4), (5), (6), (7) and (8), thus excluding all colors except F_i^1 from C_s^0 . If l is an index such that $u_l \notin C_s$, $\bar{u}_l \notin C_s$, then we can drop the edge $F_l^h \text{---} F_l^h$ from (6) and add C_s^0 to the beginning to show that C_s^0 cannot be any F_l^1 color either. \square

Now we are ready to state and prove the NP-Completeness theorem, which then immediately implies that finding an optimal NDC is NP-Complete. This theorem is a symmetric version of a result in Section 3 of Coleman and Moré (1981).

Theorem 1. For fixed $k \geq 2$, $DkGCP$ is NP-Complete.

Proof. Since the size of $G_k(P)$ is a polynomial in m and n , it is clear that the above reduction of 3SAT to $DkGCP$ can be carried out in polynomial time. We must show that there is a satisfying truth assignment for the 3SAT problem P if and only if the graph $G_k(P)$ has a proper distance- k coloring in p or fewer colors.

First suppose that $G_k(P)$ is properly distance- k colored. If l_a, l_b , and l_c are the literals contained in C_s , then the length k path

$$C_s^0 - I_s^{k-1} - I_s^{k-2} - \dots - I_s^1 - l_i$$

shows that C_s^0 cannot be the same color as any of l_a, l_b , or l_c . But C_s^0 must be colored F_a^1, F_b^1 , or F_c^1 by Proposition 3. By Proposition 2, each l_i is colored either F_i^1 or T_i^1 , so each clause must contain at least one true literal under the truth assignment induced by the proper coloring, i.e., the clauses are satisfiable.

Now we need only show that $G_k(P)$ can always be colored in p or fewer colors if P is satisfiable. Let τ be some satisfying truth assignment for C_1, C_2, \dots, C_m . First color the F_r^1 's, T_r^1 's and C_r^0 's, $r > 0$, as decreed by Proposition 1. Color u_i with T_i^1 if $\tau(u_i) = \text{true}$, color u_i with F_i^1 otherwise; color \bar{u}_i with the complementary color. Each C_s has at least one true literal, say l_a . Color C_s^0 with color F_a^1 . Finally, color I_s^r with C_{s+1}^r , $r = 1, \dots, k-1$, where the subscript on C_s^r is interpreted modulo m .

We now show that this coloring is proper. The colors F_r^1, T_r^1 , $1 < r \leq k$, each appear on only one vertex and so are proper. Color C_{s+1}^r appears on exactly two vertices, itself and I_s^r . A shortest possible path between these vertices in $G_k(P)$ is

$$I_s^r - I_s^{r-1} - \dots - I_s^1 - u_i - T_j^k - C_{s+1}^{k-1} - C_{s+1}^{k-2} - \dots - C_{s+1}^r$$

and is of length $k+1$. This is a shortest path because at least k edges must be used to get from layer I_s^r to layer C_{s+1}^r , and one extra edge must be used to get from an F or a T to a C . Also, any alternative path between these vertices that goes through a C_s^0 has at least $k+2h$ edges because of the difference in subscripts, and because the C_s^r 's do not interconnect for $r < h$; thus color C_s^r is proper. Color T_i^1 also appears on exactly two vertices, itself and one of u_i or \bar{u}_i . A shortest possible path between these vertices is the third one in (9) with T_i^1 added at the end. For $j \neq i$, at least k edges must be used to get from the u_i .

layer to the T_i^1 layer, and an extra edge is necessary to go from an i vertex to a j vertex. Any other path between these vertices through the I 's uses at least $k + 2h - 1$ edges (see (3)), so T_i^1 is proper. Finally, F_i^1 can appear in three places: on itself, on u_i or \bar{u}_i , and on any number of C_s^0 's whose clauses contain neither u_i nor \bar{u}_i . As with u_i or \bar{u}_i and T_i^1 above, u_i or \bar{u}_i and F_i^1 do not cause a conflict. Some shortest possible paths between F_i^1 and any C_s^0 are those in (6) with C_s^0 added to the beginning. Again, at least k edges are necessary to go from the C_s^0 layer to the F_i^1 layer, and an extra edge is necessary to go from an l vertex to an i vertex. In (3) we see that any other path between these vertices through the I 's uses at least $2k$ edges, so no C_s^0, F_i^1 pair causes a conflict. Between a u_i or \bar{u}_i and a C_s^0 , some shortest possible paths are

$$\left. \begin{array}{l} u_i \\ \bar{u}_i \end{array} \right\} \begin{array}{l} \text{---} \left\{ \begin{array}{l} I_i^1 \text{---} I_s^2 \text{---} \dots \text{---} I_s^{k-1} \text{---} C_s^0 \\ T_j^k \text{---} C_s^{k-1} \text{---} \dots \text{---} C_s^1 \text{---} C_s^0 \end{array} \right. \end{array}$$

of lengths k and $k + 1$ respectively. The first cannot exist because of the truth assignment and because there are no trivial clauses. Once again, the second must use k edges going from layer u_s to layer C_s^0 , and an extra edge going from an F or a T to a C , so no u_i or \bar{u}_i, C_s^0 pair conflicts. Finally, a shortest possible path between C_s^0 and C_i^0 is (7) with C_s^0 added to the beginning and C_i^0 added to the end, of length $k + 1$. In (3) we see that any other path between these vertices through the I 's uses at least $2k$ edges, so no F_i^1 color conflicts. Thus the coloring is proper, and the theorem is proved. \square

4. Heuristics for Finding Non-Overlapping Direct Covers

Theorem 1 is, unfortunately, a negative result, since it implies that finding an optimal NDC is very hard. On a more positive note, much work has been done on finding near-optimal, polynomial-time, heuristic algorithms for NP-Complete problems (see Garey and Johnson (1979), chapter 6).

In the present case, the most obvious heuristic approach is to reduce D2GCP to GCP and then apply known heuristic results on GCP to the reduced graph. Given a graph $G = (V, E)$, define $D_2(G)$ (the distance-2 completion of G) to be the graph on the same vertex set V , and with edges $E = \{\{i, j\} \mid i \text{ and } j \text{ are distance 2 or less apart in } G\}$. Then it is easy to verify that a coloring of V is a proper distance-2 coloring of G if and only if it is a proper (distance-1) coloring of $D_2(G)$ (note that this reduction also implies that D1GCP is NP-Complete).

If there were a "good" heuristic for GCP, then we could compose it with $D_2(\bullet)$ to obtain a "good" heuristic for D2GCP. Coleman and Moré (1981), Section 4, gives a good overview of the present state of the art in GCP heuristics, which is *not* "good". In fact, if $c^H(G)$ denotes the number of colors used by the best heuristic on graph G , and $\chi(G)$ denotes the optimal number of colors necessary

for G (its chromatic number), then in the worst case

$$\max_{G \text{ on } n \text{ vertices}} \frac{c^H(G)}{\chi(G)} = O\left(\frac{n}{\log n}\right) \quad (10)$$

(this best heuristic and the bound (10) are due to Johnson (1974)). Two facts mitigate the unpleasantness of (10). First, the range of $D_2(\bullet)$ does not include all graphs, and hence a better bound than (10) can be obtained for D2GCP. Second, average-case results have been obtained for GCP heuristics that are considerably better than (10).

To improve on (10) for D2GCP, consider the specific heuristic called the distance-2 sequential algorithm (D2SA). Define $\mathcal{N}(i) = \{j \neq i \mid j \text{ is distance } \leq 2 \text{ from } i\}$, the distance-2 neighborhood of a vertex i in a graph. Thus, if i has color c in a proper distance-2 coloring, no $j \in \mathcal{N}(i)$ can be color c . Then D2SA assigns color

$$\min\{c \geq 1 \mid \text{no } j \in \mathcal{N}(i), j < i, \text{ is colored } c\}$$

to vertex i , $i = 1, \dots, |V|$. That is, D2SA assigns vertex i the smallest color not conflicting with those already assigned. (This is just the distance-2 version of the best known GCP heuristic, the sequential algorithm, which is called the CPR method in its applications to approximating sparse Jacobians (see Curtis, Powell and Reid (1974)).) Let $c^S(G)$ denote the number of colors used by D2SA when applied to G .

In order to obtain bounds on $c^S(G)$, we require two definitions. The maximum degree of G , $\Delta(G)$, is defined as

$$\Delta(G) = \max_i |\{j \mid \{i, j\} \in E(G)\}|.$$

The distance-2 chromatic number of G , $\chi_2(G)$ is defined as the optimal number of colors in a proper distance-2 coloring of G , i.e.

$$\chi_2(G) = \min\{k \mid G \text{ has a proper distance-2 coloring with } k \text{ colors}\}.$$

The following theorem bounds $\chi_2(G)$ and $c^S(G)$ in terms of $\Delta(G)$, and a corollary improves (10) for D2SA:

Theorem 2. Let $d = \Delta(G)$. Then

$$d + 1 \leq \chi_2(G) \leq c^S(G) \leq d^2 + 1 \quad (11)$$

for all graphs G .

Proof. Let i be a vertex incident to exactly d edges, and note that i and its d nearest neighbors must all be different colors in a proper distance-2 coloring; this proves the lower bound in (11). The second inequality in (11) is trivial.

To prove the upper bound in (11), note that for any vertex i , $|N(i)| \leq d + d(d-1) = d^2$. Suppose that D2SA assigns color l to vertex i ; by definition of D2SA, this can happen only if at least one vertex of each color $1, \dots, l-1$ is in $N(i)$. Thus, if i were assigned color $l > d^2 + 1$, then $|N(i)| \geq d^2 + 1$ (a contradiction). (This proof is essentially a constructive proof of Corollary 8.2.1 of Bondy and Murty (1976).) \square

Corollary 1. For all $n \geq 1$,

$$\max_{G \text{ on } n \text{ vertices}} \frac{c^S(G)}{\chi_2(G)} \leq \sqrt{n-1} + 1 = O(\sqrt{n}). \quad (12)$$

Proof. Clearly, $c^S(G) \leq n$. Let $k = \chi_2(G)$. Applying the first and third inequalities of (11), we obtain

$$c^S(G) \leq (k-1)^2 + 1. \quad (13)$$

Consider separately two cases:

Case 1: If $n \leq (k-1)^2 + 1$, this implies that $\sqrt{n-1} + 1 \leq k$ and so

$$\frac{c^S(G)}{k} \leq \frac{n}{k} \leq \frac{n}{\sqrt{n-1} + 1} = \sqrt{n-1} + 1 - 2 + \frac{2}{\sqrt{n-1} + 1} \leq \sqrt{n-1} + 1.$$

Case 2: If $n > (k-1)^2 + 1$, then $k < \sqrt{n-1} + 1$, and so

$$\frac{c^S(G)}{k} \leq \frac{(k-1)^2 + 1}{k} = k - 2 + \frac{2}{k} \leq k < \sqrt{n-1} + 1. \quad \square$$

Graphs that attain bound (13) for a certain ordering of their vertices exist for $k = 1, 2, 3, 4$. The cases $k = 1, 2$ are trivial. For $k = 3$, consider $G_3 = (V_3, E_3)$ defined by

$$V_3 = x_{ij} \quad i = 1, 2, 3, \quad j = 1, 2, 3, 4, 5,$$

$$E_3 = \{x_{ij}, x_{i+1, j+1}\} \quad \text{all } i, j \quad (\text{subscripts modulo 3 and 5}).$$

Then D2SA assigns x_{ij} color i when the vertices are ordered by i (which is optimal by (11)), and assigns x_{ij} color j when the vertices are ordered by j (which is the worst possible, by (13)). For $k = 4$, consider $G_4 = (V_4, E_4)$ defined by

$$V_4 = x_{ij} \quad i = 1, 2, 3, 4, \quad j = 1, \dots, 10,$$

$$E_4 = \left\{ \begin{array}{l} \{x_{ij}, x_{i+2, j+5}\} \quad \text{all } j \\ \{x_{ij}, x_{i+1, j+2}\} \quad \text{all odd } j \\ \{x_{ij}, x_{i+1, j+4}\} \quad \text{all even } j \end{array} \right\} \quad \text{all } i \quad (\text{subscripts modulo 4 and 10}).$$

Then D2SA applied to G_4 also colors x_{ij} with i when ordered by i , and with j when ordered by j (which are again respectively optimal and worst possible). However, this construction seems difficult to extend. Even if it can be extended, the number of vertices is given by $n = k((k - 1)^2 + 1)$ so that

$$\frac{c^S(G_k)}{k} = O(n^{1/3})$$

which is a better result than (12). Thus, while (11), (12) and (13) are better results than (10), I believe that the associated bounds are not the best possible.

For the average case, Grimmet and McDiarmid (1975) proved the following theorem:

Theorem 3. Fix n vertices, and let vertices i and j be independently connected by an edge with fixed probability p , $0 < p < 1$. Let $c^C(G)$ be the number of colors used by CPR on G , and $\chi(G)$ be the optimal number of colors (so that $c^C(G)$ and $\chi(G)$ are random variables). Then

$$\frac{c^C(G)}{\chi(G)} \leq 2 + \epsilon$$

for all $\epsilon > 0$ with probability $1 - o(1)$.

Thus, on average, CPR almost never performs more than twice as badly as the optimal strategy. This is a nice result, but for our purposes it has at least two flaws. First, sparsity patterns in practical problems are not uniformly random as Theorem 3 supposes. Second, even if they were, the density of sparsity patterns tends to be $O(1/n)$ rather than constant with increasing n , so the theorem does not apply anyway. It would be useful to determine a better random model for sparsity patterns, or at least to prove Theorem 3 under the assumption that $p = O(1/n)$.

5. Conclusions and Further Questions

As we move from Direct Methods to Elimination Methods, and from NDCs to GSimDCs within Direct Methods, we are less restricted, and so can find potentially more powerful methods. We also move from an NP-Complete problem (finding an optimal NDC) to a polynomially-bounded one (a general Elimination Method) (using Theorem 1, and Theorem 4 of the Appendix). It would be interesting to know what intermediate point divides NP-Complete methods from polynomial methods (if indeed there is a continuum at all).

In particular, it is usually easy to remove some restrictions so as to change an NDC method into a SeqDC method (see Powell and Toint (1979)), and to see

what properties a graph coloring must have to be a SeqDC. Can this be used to prove a version of Theorem 1 for SeqDCs? SimDCs are harder to deal with because of their simultaneous nature, but they can still be shown to be equivalent to a form of graph "multi-coloring". Is the corresponding Theorem 1 still true? The expectation is that these graph coloring problems are also NP-Complete, which, if true, means that we must rely on heuristic algorithms to construct SeqDCs and SimDCs. Can the bound (12) be significantly improved, or, more importantly, can a provably better heuristic be found?

Other interesting questions involve the observed performance of heuristics. Even CPR, one of the simplest possible heuristics, seems to give good results on practical problems (see Coleman and Moré (1981), tables 3, 4 and 5). Can this behavior be proved under some convincing randomness assumption, as suggested at the end of Section 4? Much work remains to be done before we know whether we are approximating sparse Hessians efficiently.

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Appendix 1. Elimination Methods

Assume that we approximate the Hessian of $F : \mathbb{R}^n \rightarrow \mathbb{R}$ using an elimination method by evaluating the gradient of F at x^0 along directions d^1, d^2, \dots, d^k . If no entry of the Hessian is known to be zero, there are $n(n+1)/2$ unknowns, namely h_{ij} for all $1 \leq i \leq j \leq n$. The following theorem is well known in the folklore, but the present author knows of no published proof:

Theorem 4. The maximum number of unknowns that can be determined from a set of gradient evaluations along any k directions, $0 \leq k \leq n$, is given by

$$r_{n,k} = n + (n-1) + \dots + (n-k+1) = \frac{k(2n-k+1)}{2}.$$

In particular, in the completely dense case, n evaluations are necessary to obtain all $n(n+1)/2$ unknowns.

Proof. Let $g(x)$ denote the gradient of F at x , and $H(x)$ denote the Hessian of F at x . Evaluating $g(x)$ along the k directions d^1, d^2, \dots, d^k produces the nk approximate linear equations

$$(d^i)^T H(x^0) \approx g(x^0 + d^i) - g(x^0), \quad i = 1, \dots, k. \quad (14)$$

We assume that H is symmetric, and so identify unknowns h_{ij} and h_{ji} in (14). The number of unknowns that can be determined from equations (14) is bounded above by the rank of the nk by $n(n+1)/2$ coefficient matrix of the h_{ij} 's when no h_{ij} is assumed to be zero. Questions of rank could be affected by dependence among the d^i ; we thus assume the Haar Condition, namely that every maximal square submatrix of the matrix whose i^{th} column is d^i is non-singular.

To describe the coefficient matrix, order the equations in (14) so that equations with left-hand side $(d^i)^T H_{\bullet,1}$, $i = 1, \dots, k$ appear first, those with left-hand side $(d^1)^T H_{\bullet,2}$, $i = 1, \dots, k$ appear next, etc., and then order the unknowns as $h_{11}, h_{21}, h_{22}, h_{31}, h_{32}, \dots, h_{nn}$. Given this ordering, call the coefficient matrix in (14) A^k ; partition A^k row-wise into n blocks of k rows each, and column-wise into n blocks, where the i^{th} column block has i columns. Let the i, j^{th} submatrix of the partition be denoted by $A_{i,j}^k$, $i, j = 1, \dots, n$. Define c^j as the k -vector of the j^{th} components of the $\{d^i\}$, i.e., $c^j = (d_j^1, d_j^2, \dots, d_j^k)^T$, $j = 1, \dots, n$. Each $A_{i,j}^k$ is completely described by

$$A_{i,j}^k = \begin{cases} 0, & \text{if } i > j; \\ (c^1, c^2, \dots, c^j), & \text{if } i = j; \\ (0, 0, \dots, c^j, \dots, 0), & \text{if } i < j. \end{cases}$$

For example, when $n = 4$, A^k has the form

$$\begin{pmatrix} h_{11} & h_{21} & h_{22} & h_{31} & h_{32} & h_{33} & h_{41} & h_{42} & h_{43} & h_{44} \\ c^1 & c^2 & & c^3 & & & c^4 & & & \\ & c^1 & c^2 & & c^3 & & & c^4 & & \\ & & & c^1 & c^2 & c^3 & & & c^4 & \\ & & & & & & c^1 & c^2 & c^3 & c^4 \end{pmatrix}, \quad (15)$$

where zero elements are not shown.

To complete the proof, it must be shown that $\text{rank}(A^k) = r_{n,k} = (n + (n - 1) + \dots + 2 + 1) - ((n - k) + (n - k - 1) + \dots + 2 + 1)$. We show first that the last $n - k$ columns of column block n , the last $(n - k - 1)$ columns of column block $n - 1$, ..., and the last column of column block $k + 1$ can be eliminated using linear combinations of the remaining columns. Note that the complementary set of columns, denoted by C , is precisely the set of columns whose non-zero entry of largest row index is c_k^j for some $j \leq k$.

Define λ^l to be the solution of the system

$$(c^1 \ c^2 \ \dots \ c^k)\lambda^l = -c^l, \quad l = k + 1, k + 2, \dots, n$$

(λ^l must be unique under the assumption of the Haar condition). The following computations show that linear combinations of the columns in C , using the λ^l 's as multipliers, can be used to eliminate the columns mentioned above; since the form of the linear combinations is complicated, the result is best understood by referring to example (15) and assuming that $k = 2$.

To eliminate the last column of column block n from A^k , we add to it λ_j^n times column j of column block n , $j = 1, \dots, k$, and $\lambda_m^n \lambda_j^n$ times column j of column block m , $m = 1, \dots, k$, $j = 1, \dots, m$. In row block n , the new last column is $c^n + \sum_{j=1}^k \lambda_j^n c^j$, which is zero by definition of the λ_j^n . (all terms from the first column block). In row blocks $k \leq i \leq n$, there is no contribution from any column block. In row blocks $i \leq k$, the sum includes $\lambda_i^n c^n$ from column block n , zero from column block m when $k < m < n$, $\lambda_i^n \lambda_k^n c^k$ from column block k , $\lambda_i^n \lambda_{k-1}^n c^{k-1}$ from column block $k-1$, ..., $\lambda_i^n (\lambda_i^n c^i + \lambda_{i-1}^n c^{i-1} + \dots + \lambda_1^n c^1)$ from column block i , and zero from column blocks m when $m < i$, for a total of $\lambda_i^n (c^n + (\lambda_1^n c^1 + \lambda_2^n c^2 + \dots + \lambda_k^n c^k))$, which is again zero. Thus the last column of column block n is dependent on the columns in C , and by symmetry so is the last column of each column block $k + 1, k + 2, \dots, n - 1$.

Now we eliminate column $n - 1$ of column block n using the columns in C . Add to it λ_j^{n-1} times column j of column block n , $j = 1, \dots, k$, λ_j^n times column

j of column block $n-1$, $j = 1, \dots, k$, and $(\lambda_m^n \lambda_j^{n-1} + \lambda_m^{n-1} \lambda_j^n)$ times column j of column block m , $m = 1, \dots, k$, $j = 1, \dots, m$. In row block n the new column $n-1$ of column block n is $c^{n-1} + \sum_{j=1}^k \lambda_j^{n-1} c^j$, which is zero by the definition of the λ_j^{n-1} (all terms from column block n). In row block $n-1$, the new column is $c^n + \sum_{j=1}^k \lambda_j^n c^j$, which is again zero (the first term from column block n , the rest from column block $n-1$). In row block $k < i < n-1$, no contribution is made by any column block. In row block $i \leq k$, the sum includes $\lambda_i^{n-1} c^n$ from column block n , $\lambda_i^n c^{n-1}$ from column block $n-1$, zero from column block m when $k < m < n-1$, $(\lambda_k^n \lambda_i^{n-1} + \lambda_k^{n-1} \lambda_i^n) c^k$ from column block k , \dots , $\lambda_i^n (\lambda_i^{n-1} c^i + \lambda_{i-1}^{n-1} c^{i-1} + \dots + \lambda_1^{n-1} c^1) + \lambda_i^{n-1} (\lambda_i^n c^i + \lambda_{i-1}^n c^{i-1} + \dots + \lambda_1^n c^1)$ from column block i , and zero from column block m when $m < i$, for a total of $\lambda_i^n (c^{n-1} + (\lambda_k^{n-1} c^k + \dots + \lambda_1^{n-1} c^1)) + \lambda_i^{n-1} (c^n + (\lambda_k^n c^k + \dots + \lambda_1^n c^1)) = 0$. Thus column $n-1$ of column block n is also dependent on the columns in C , and again by symmetry, so are all columns j in column blocks m with $k < j \leq m$.

By eliminating $1 + 2 + \dots + (n-k)$ columns we have shown that $\text{rank}(A^k) \leq r_{n,k}$. To show that $\text{rank}(A^k) = r_{n,k}$, delete the columns that were eliminated above from A^k , and delete the last $k-i$ rows from each row block i , $i < k$. Then the remaining matrix is $r_{n,k}$ by $r_{n,k}$ and is block upper triangular with square, non-singular diagonal blocks. Thus this submatrix of A^k is non-singular, so $\text{rank}(A^k) \geq r_{n,k}$, and the theorem is proved. \square

A corollary to this proof is that the minimum number of gradient evaluations necessary to approximate a Hessian (sparse or dense) can be found in time bounded by $O(n^7)$ by the following procedure:

1. Set $k = 1$.
2. Form A^k , deleting the columns corresponding to variables known to be zero.
3. Evaluate $\text{rank}(A^k) = t_k$, say. If $t_k \geq$ number of unknowns, then k is optimal; otherwise, set $k = k + 1$ and go to (2).

Step 3 can be performed at most n times, on a matrix whose number of columns is $O(n^2)$. Evaluation of rank requires $O(|\text{columns}|^3)$ operations, giving a total bound of $O(n^7)$. In practice, Theorem 4 can be used to get reasonable bounds on k , making the work more like $O(n^6)$. However, numerical difficulties may make a general elimination method untrustworthy in any case.

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SOL 81-22: OPTIMAL APPROXIMATION OF SPARSE HESSIANS AND ITS EQUIVALENCE TO A GRAPH COLORING PROBLEM, by S. Thomas McCormick

We consider the problem of approximating the Hessian matrix of a smooth non-linear function using a minimum number of gradient evaluations, particularly in the case that the Hessian has a known, fixed sparsity pattern. We study the class of Direct Methods for this problem, and propose two new ways of classifying Direct Methods. Examples are given that show the relationships among optimal methods from each class. The problem of finding a non-overlapping direct cover is shown to be equivalent to a generalized graph coloring problem -- the distance-2 graph coloring problem. A theorem is proved showing that the general distance-k graph coloring problem is NP-Complete for all fixed $k > 2$, and hence that the optimal non-overlapping direct cover problem is also NP-Complete. Some worst-case bounds on the performance of a simple coloring heuristic are given. An appendix proves a well known folklore result, which implies as a corollary that another class of methods, the Elimination Methods, includes optimal polynomially-bounded algorithms.

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