ACCELERATED BLOCK-COORDINATE RELAXATION FOR REGULARIZED OPTIMIZATION*

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Abstract. We discuss minimization of a smooth function to which is added a regularization function that induces structure in the solution. A block-coordinate relaxation approach with proximal linearized subproblems yields convergence to stationary points, while identification of the optimal manifold (under a nondegeneracy condition) allows acceleration techniques to be applied on a reduced space. The work is motivated by experience with an algorithm for regularized logistic regression, and computational results for the algorithm on problems of this type are presented.

Key words. regularized optimization, block coordinate relaxation, active manifold identification

AMS subject classifications. 49K40, 49M27, 90C31

1. Introduction. We discuss an algorithm for solving the problem

(1.1)
$$\min_{x \in \mathbb{R}^n} \phi_{\tau}(x) := f(x) + \tau P(x),$$

where f is smooth (at least locally Lipschitz continuously differentiable in the region of interest) and $\tau > 0$ is a parameter. The regularization function P has the following separable structure:

(1.2)
$$P(x) = \sum_{q \in Q} P_q(x_{[q]}),$$

where each P_q is a closed, proper, extended-valued, convex function, [q] denotes a subset of $\{1, 2, ..., n\}$, and $\{x_{[q]} | q \in Q\}$ is a partition of the components of x. Not all components of x need be involved in the regularization function; we may have $P_q \equiv 0$ for some q.

Problems of the form (1.1) are appearing in many applications. The following (overlapping) problems have been particularly well studied in recent times.

- Compressed sensing, where in the ℓ_2 - ℓ_1 formulation, $f(x) = (1/2)\|Ax y\|_2^2$ for some $A \in \mathbb{R}^{m \times n}$ with $m \ll n$ and special properties such as restricted isometry, and $P(x) = \|x\|_1$.
- Regularized logistic regression, where f is a log-likelihood function obtained from labeled training data and the regularizer P(x) is either $||x||_1$ [21, 19, 20] (possibly modified by omission of one or more terms from the norm) or else a group- ℓ_2 regularizer [16].
- Regularized least squares, where again f is a linear least-squares function while P could be $\|\cdot\|_1$ (leading to the LASSO estimator [22]), a group- ℓ_2 regularizer (with $P_q(z) = \|z\|_2$ in the notation above; see [33, 6]), or a group ℓ_{∞} regularizer (with $P_q(z) = \|z\|_{\infty}$ [28]). The group regularizers allow variables to be partitioned into subsets of closely related effects, where each subset is selected or deselected as a group.

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Other works [11, 12, 32] consider algorithms for both logistic and least-squares loss functions jointly.

In the examples above, P is nonsmooth, but such is not always the case. For example, in one formulation of the matrix completion problem of estimating a low-rank matrix $X \in \mathbb{R}^{m \times p}$ such that $\mathcal{A}(X) \approx b$, for noisy observations $b \in \mathbb{R}^l$ and a given linear operator $\mathcal{A} : \mathbb{R}^{m \times p} \to \mathbb{R}^l$, we can explicitly model X as a product of factors L and R^T (for $L \in \mathbb{R}^{m \times r}$ and $R \in \mathbb{R}^{p \times r}$) and solve the following problem:

$$\min_{L,R} \frac{1}{2} \|\mathcal{A}(LR^T) - b\|_2^2 + \tau(\|L\|_F^2 + \|R\|_F^2).$$

(This formulation is an obvious consequence of [18, Subsection 5.3].)

In this paper we examine a block coordinate proximal linearization algorithm for solving (1.1), in which at the current iterate x we select a subset $Q' \subset Q$ and solve the following subproblem for some $\mu \geq \mu_{\min} > 0$:

(1.3)
$$\min_{d} \sum_{q \in Q'} \nabla_{[q]} f(x)^{T} d_{[q]} + \frac{\mu}{2} |d|^{2} + \tau \sum_{q \in Q'} P_{q}(x_{[q]} + d_{[q]}),$$

where $\nabla_{[q]}f$ denotes the gradient subvector corresponding to the components of x that belong to the partition [q], and here and throughout $|\cdot|$ denotes the Euclidean norm. We refer to Q' as the relaxation set at x. Clearly, the solution of (1.3) has $d_{[q]} = 0$ for all $q \notin Q'$. Existence and uniqueness of a solution to (1.3) is immediate for $\mu > 0$, given our assumptions on the functions P_q , $q \in Q$. The optimality conditions are

$$(1.4) \qquad \qquad 0 \in \nabla_{[q]} f(x) + \mu d_{[q]} + \tau \partial P_q(x_{[q]} + d_{[q]}), \qquad \text{for all } q \in Q'.$$

If the solution of (1.3) produces a "sufficient decrease" in the objective ϕ_{τ} , the step is accepted. Otherwise μ is increased and (1.3) is re-solved, with the same relaxation set Q'; this process is repeated until a valid step is found. At iteration k, we denote this step by d^k and refer to it as a prox-descent step. We then optionally compute an enhanced step \tilde{d}^k that is required to improve on d^k and to satisfy its own sufficient decrease conditions.

Denoting the relaxation set Q' at iteration k by Q_k , we require the following "generalized Gauss-Seidel" condition to be satisfied (see [27]): For some integer $T \geq 1$ and all $k \geq T - 1$, we have

$$(1.5) Q_k \cup Q_{k-1} \cup \cdots \cup Q_{k-T+1} = Q.$$

This condition ensures that every component of x is "touched" by the relaxation scheme at least once every T iterations.

Effectiveness of the algorithm depends strongly on whether the subproblems (1.3) can be formulated and solved efficiently. In the applications mentioned above, such is the case. When $P_q(z) = \|z\|_1$, the solution can be obtained by the "soft thresholding" operator at a cost that is linear in the total number of components in $d_{[q]}$, $q \in Q'$. The costs are similar when $P_q(z) = \|z\|_2$ or $P_q(z) = \|z\|_2^2$.

The basic approach has been well studied in the case of $Q_k = Q$ for all k; see for example the SpaRSA approach for compressed sensing [31] and the ProxDescent framework of [15]. The block coordinate technique often gives better practical performance when Q_k encompasses only a small fraction of the components of x and where the cost of computing the corresponding partial gradient is small compared to the cost of the full gradient. For the regularized logistic regression problem of [21], for example, the cost of evaluating the partial gradient is approximately linear in the number of components of the gradient required. We note that "Gauss-Southwell" rules for choosing Q_k (see [27]) are less appealing than (1.5) because they appear to require knowledge of the full gradient.

1.1. Related Work. We discuss here some recent work on related algorithms and applications. Other related work can be found in the bibliographies of the papers mentioned here.

The SpaRSA approach for compressed sensing [31] solves subproblems of the form (1.3) in which f is a linear least-squares objective, $P(x) = ||x||_1$, and Q' = Q. (In many applications of compressed sensing, there is little to be saved by a partial gradient evaluation.) SpaRSA has no "enhanced" step analogous to \tilde{d}^k in Algorithm 1. In a more general setting, Lewis and Wright [15] describe an algorithm for (1.1) in which P is allowed to be non-separable and prox-regular (rather than separable and convex, as here). The subproblems have the form (1.3) but again are solved on the full space, and enhanced steps are not considered in any detail. (Global convergence results are proved and there is a discussion of manifold identification in a limited context.)

Another related line of work begins with the paper of Tseng and Yun [27], which considers the same problem (1.1) as this paper and solves block-relaxation subproblems like (1.3), but with a more general scaling in the quadratic term. A line search is performed along the direction d^k . (The algorithm described in the current paper is simpler in that it uses the quadratic term in (1.3) to modify both the direction and length of the step.) Enhanced steps are not considered explicitly in [27], though second-order information could eventually be used in the quadratic term to enhance the final convergence rate. Although the lack of a line search makes our global convergence analysis below quite different, we make use of several technical results from [27].

In later work [25], Tseng and Yun described a block relaxation approach for minimization of a smooth function subject to linear constraints (but without the separable regularization term of (1.1)). We note that this problem is not unrelated to (1.1); we can always enforce bound constraints, for example, by defining a separable P(x) that takes on the value 0 when x satisfies its bounds and ∞ otherwise. Special attention is paid to the quadratic programming formulation of support vector machines. The next paper [26] considers (1.1) with the addition of linear equality constraints, and describes a similar method. An application to bi-level optimization is described. One of Tseng's final papers [23] mentions the problem (1.1) again and outlines the algorithms presented in the earlier works, leaving open the question of whether accelerated first-order methods can be applied in a block relaxation context.

The current paper was motivated by the need to provide theoretical support for the algorithm described in Shi et al. [21] for ℓ_1 -regularized logistic regression. In the event, significant modifications were needed to make the method fit the framework of the present paper. We describe this application in detail in Section 5, and give computational results obtained with an implementation of the algorithm presented here.

There is a recent and extensive literature on least-squares and logistic regression problems with nonsmooth regularizers. We mention a few such contributions here, with a focus on methods that are suitable for large problems.

Shevade and Keerthi [19] present a relaxation algorithm for ℓ_1 -regularized logistic regression which selects one component at a time for relaxation — the one that

violates the optimality conditions maximally. Friedman, Hastie, and Tibshirani [6] discuss a coordinate descent method for the ℓ_1 -regularized least-squares loss (with an additional penalty term involving $||x||_2^2$ – the "elastic net" formulation). They describe a cyclic coordinate relaxation method with exact line search along each direction. For logistic-regression loss, they propose a sequential-quadratic-programming outer loop, solving the quadratic subproblem with the method for least-squares loss. Koh, Kim, and Boyd [13] reformulate ℓ_1 -regularized logistic regression as a linearly constrained smooth optimization problem, and apply an interior-point method that uses conjugate gradients to compute the steps. The method of Shi et al. [20] for ℓ_1 -regularized logistic regression computes steps as in (1.3), but for the full set of components and for a fixed (large) value of μ_k . An Armijo line search is added, as is a continuation strategy in the parameter τ (discussed further in Section 5). When the correct nonzero set appears to have been identified, the algorithm uses to second-order steps like those in [13]. Yuan et al. [32] present an extensive and useful survey of various methods for ℓ_1 -regularized regression, using least-squares, logistic loss functions, and various extensions. Computational comparisons between different approaches are reported in detail.

An early reference to group- ℓ_2 is the thesis of Bakin [1]. Yuan and Lin [33] discuss group- ℓ_2 regularizer with least-squares loss function. An extension of LARS [4] is proposed to solve it, but no convergence analysis is presented. Kim, Kim, and Kim [12] describe a gradient projection approach for the formulation in which regularization is imposed as a constraint of the form $P(x) \leq T$, rather than included in the objective, showing that the projection can be performed efficiently when P is the group- ℓ_2 regularizer. Meier, van de Geer, and Bühlmann [16] consider logistic regression with a group- ℓ_2 regularizer, applying variants of coordinate descent and the method from [24] to a problem in DNA splice site detection.

Turlach, Venables, and Wright [28] describe an application and computational results for an interior-point method for a least-squares objective with a group- ℓ_{∞} regularizer, and give a statistical analysis for a special case involving orthonormal coefficient matrices.

1.2. Outline. We outline briefly the remainder of the paper. Section 2 reviews the relevant optimality and nondegeneracy conditions, discusses manifolds and their characterization, and defines partial smoothness. The relationship of second-order optimality conditions to strong local minimizers is explored in Subsection 2.3; this topic is useful when we introduce the reduced-Newton acceleration scheme in Subsection 3.3.

The proximal block coordinate relaxation algorithm is introduced and analyzed in Section 3. Global convergence results are obtained in Subsection 3.1, and identification of the (assumed) partly smooth manifold on which the limit point lies is analyzed in Subsection 3.2. The reduced-Newton acceleration scheme is described and analyzed in Subsection 3.3.

Section 4 outlines how the algorithm could be applied to several nonsmooth regularization functions that have been proposed in the recent literature. In Section 5, we describe an application to ℓ_1 -regularized logistic regression, giving details on the implementation and presenting computational results on three test problems with somewhat different properties. These tests suggest that there is much to be gained, computationally speaking, by using block-coordinate relaxation rather than a standard first-order approach that evaluates a full gradient vector. The code and test data used in Section 4 is available at http://www.cs.wisc.edu/~swright/LPS/, to allow

independent reproduction of the tables in this paper (up to the effects of randomness in the algorithm, which are significant).

2. Optimality and Nondegeneracy Conditions. In this section, discuss properties of the objective function ϕ_{τ} in the neighborhood of a solution x^* . We start by discussing criticality conditions, then in Subsection 2.2 we discuss manifolds and their characterization and define the partially smooth manifolds of Lewis [14]. Finally, we discuss second-order conditions and show how the notion of a strong local minimizer x^* of ϕ_{τ} is tied to the second-order sufficient conditions of the restriction of this function to the partly smooth manifold containing x^* .

Provided that ∇f is locally Lipschitz at a point x, ϕ_{τ} is prox-regular at x. In fact, we can find $\sigma > 0$ such that for all for all x' and x'' close to x, we have

(2.1)
$$\phi_{\tau}(x'') \ge \phi_{\tau}(x') + g^{T}(x'' - x') - \sigma |x'' - x'|^{2}$$
, for each $g \in \partial \phi_{\tau}(x')$.

(Note that here, in contrast to general prox-regular functions, σ is independent of g; it can simply be chosen as the local Lipschitz constant for ∇f at x.)

2.1. Criticality and Optimality. We say that z^* is a *strong local minimizer* of a function $h: \mathbb{R}^r \to \bar{\mathbb{R}}$ with modulus c > 0 if

(2.2)
$$h(z) \ge h(z^*) + c|z - z^*|^2 + o(|z - z^*|^2) \quad \text{for all } z \text{ near } z^*.$$

The criticality condition for h is $0 \in \partial h(z^*)$, and the nondegeneracy condition is $0 \in \operatorname{ri} \partial h(z^*)$. For the particular function ϕ_{τ} of (1.1), criticality of x^* can be characterized by separating the general condition according to the index partition $\{[q] \mid q \in Q\}$ as follows:

(2.3)
$$0 \in \nabla_{[q]} f(x^*) + \tau \partial P_q(x_{[q]}^*), \quad \text{for all } q \in Q,$$

while nondegeneracy at x^* can be written in a similar partitioned form:

$$(2.4) 0 \in \operatorname{ri} \left[\nabla_{[q]} f(x^*) + \tau \partial P_q(x^*_{[q]}) \right], \text{ for all } q \in Q.$$

2.2. Manifolds and Partial Smoothness. We start our discussion of manifolds by repeating some definitions from Hare and Lewis [8, Definition 2.3] and Lewis and Wright [15, Definition 1.2]. We also use some notation and terminology regarding manifolds from Vaisman [29].

A set $\mathcal{M} \subset \mathbb{R}^m$ is a manifold about $\bar{z} \in \mathbb{R}^m$ if it can be described locally by a collection of \mathcal{C}^p functions $(p \geq 2)$ with linearly independent gradients. That is, there exists a map $F: \mathbb{R}^m \to \mathbb{R}^k$ that is \mathcal{C}^p around \bar{z} with $\nabla F(\bar{z})^T \in \mathbb{R}^{k \times m}$ surjective and such that points z near \bar{z} lie in \mathcal{M} if and only if F(z) = 0. The normal space to \mathcal{M} at \bar{z} , denoted as usual by $N_{\mathcal{M}}(\bar{z})$, is then just the range of $\nabla F(\bar{z})$, while the tangent space to \mathcal{M} at \bar{z} is the null space of $\nabla F(\bar{z})^T$

It is convenient here and later to assume that $\nabla F(\bar{z})$ is a matrix with orthonormal columns. This assumption can be made without loss of generality, by performing a QR factorization of $\nabla F(\bar{z})$ (with Q being $m \times k$ orthonormal and R being $k \times k$ upper triangular) and replacing $\nabla F(z)$ by $\nabla F(z)R^{-1}$.

We state an elementary technical result on manifold parametrization, which is essentially proved in [29, Sections 1.4-1.5]. A simple proof appear for completeness in Appendix A.

LEMMA 2.1. Let the manifold $\mathcal{M} \subset \mathbb{R}^m$ containing \bar{z} be characterized by a C^p function $F : \mathbb{R}^m \to \mathbb{R}^k$ with the properties described above, where $p \geq 2$. Then there is

a point $\bar{y} \in \mathbb{R}^{m-k}$ and a C^p function G mapping some neighborhood of \bar{y} to \mathbb{R}^m such that $G(y) \in \mathcal{M}$ for all y near \bar{y} . Moreover, $G(y) - \bar{z} = Y(y - \bar{y}) + O(|y - \bar{y}|^2)$, where $Y \in \mathbb{R}^{m \times (m-k)}$ is an orthonormal matrix whose columns span the tangent space to \mathcal{M} at \bar{z} .

The proof constructs G using the implicit function theorem and sets $\bar{y} = 0$. In practice, we can often identify a suitable G by making use of the structure of P (as demonstrated later) but we do not know (or need to know) \bar{y} until the solution of the problem is known. Hence, it is useful to state and use the results in this section without assuming $\bar{y} = 0$.

It follows immediately from Lemma 2.1 that $\nabla G(\bar{y})^T = Y$.

The next technical result shows how perturbations from a point at which h is partly smooth can be decomposed according to the manifold characterization above. A proof appears in the Appendix.

LEMMA 2.2. Let the manifold $\mathcal{M} \subset \mathbb{R}^m$ be characterized in a neighborhood of $\bar{z} \in \mathcal{M}$ by C^p mappings $F : \mathbb{R}^m \to \mathbb{R}^k$ and $G : \mathbb{R}^{m-k} \to \mathbb{R}^m$ and the point \bar{y} described above. Then for all z near \bar{z} , there are unique vectors $y \in \mathbb{R}^{m-k}$ and $v \in \mathbb{R}^k$ with $|(y - \bar{y}, v)| = O(|z - \bar{z}|)$ such that $z = G(y) + \nabla F(\bar{z})v$.

Partial smoothness can now be defined as follows [14, Section 2].

DEFINITION 2.3. A function $h: \mathbb{R}^m \to \bar{\mathcal{R}}$ is partly smooth at a point $\bar{z} \in \mathbb{R}^m$ relative to a set $\mathcal{M} \subset \mathbb{R}^m$ containing \bar{z} if \mathcal{M} is a manifold about \bar{z} and the following properties hold:

- (i) (Smoothness) The restricted function $h \mid_{\mathcal{M}} is C^2$ near \bar{z} ;
- (ii) (Regularity) h is subdifferentially regular at all points $z \in \mathcal{M}$ near \bar{z} , with $\partial h(z) \neq \emptyset$;
- (iii) (Sharpness) The affine span of $\partial h(\bar{z})$ is a translate of $N_{\mathcal{M}}(\bar{z})$;
- (iv) (Sub-continuity) The set-valued mapping $\partial h : \mathcal{M} \rightrightarrows \mathbb{R}^m$ is continuous at \bar{z} . We refer to \mathcal{M} as the active manifold.

Since f is smooth, it does not complicate the definition of active manifolds for ϕ_{τ} at x^* ; we need examine only the function P. Additionally, the structure (1.2) of P ensures that we can express the active manifold as a Cartesian product over the block components. That is, we can say that P (and hence ϕ_{τ}) is partly smooth at x^* with active manifold \mathcal{M} if and only if each $P_{[q]}$ is partly smooth at $x^*_{[q]}$ with active manifold \mathcal{M}_q , where $\mathcal{M} = \otimes_{q \in Q} \mathcal{M}_q$. (For a proof of this claim, see [14, Proposition 4.5].)

Following [14, Definition 5.6], we say that x^* is a *strong critical point* of ϕ_{τ} relative to the active manifold \mathcal{M} , where ϕ_{τ} is partly smooth with respect to \mathcal{M} at a point x^* , if

- (i) x^* is a strong local minimizer of $\phi_{\tau}|_{\mathcal{M}}$ with some modulus c>0, and
- (ii) the nondegeneracy condition (2.4) holds.
- **2.3.** Second-Order Conditions. We discuss in this section second-order conditions that ensure at least quadratic increase in the objective ϕ_{τ} as we move away from a solution x^* . These conditions motivate the Newton-based acceleration techniques of Subsection 3.3.

The first result relates the strong local minimizer property for $\phi_{\tau}|_{\mathcal{M}}$ at x^* to the second-order sufficient conditions for an explicit representation of this function along this manifold.

THEOREM 2.4. Suppose that ϕ_{τ} is partly smooth at $x^* \in \mathbb{R}^n$ relative to an active manifold $\mathcal{M} \subset \mathbb{R}^n$. Suppose that \mathcal{M} is characterized by C^2 mappings $F: \mathbb{R}^n \to \mathbb{R}^k$ and $G: \mathbb{R}^{n-k} \to \mathbb{R}^n$ and a point $y^* \in \mathbb{R}^{n-k}$, such that F(x) = 0 for all $x \in \mathcal{M}$ near x^* , $\nabla F(x^*)$ is orthonormal, $G(y) \in \mathcal{M}$ for all y near y^* , and

 $G(y) = x^* + Y(y - y^*) + O(|y - y^*|^2)$ for some matrix Y such that $|\nabla F(x^*)| Y$ is orthogonal. Then $\phi_{\tau}|_{\mathcal{M}}$ has a strong local minimizer at x^* with modulus c>0 if and only if the function defined by

$$(2.5) \psi_{\tau}(y) = \phi_{\tau}(G(y))$$

is C^2 with $\nabla \psi_{\tau}(y^*) = 0$ and $\nabla^2 \psi_{\tau}(y^*)$ positive definite, with minimum eigenvalue at

Proof. By Definition 2.3(i), we can define a neighborhood U of x^* and a C^2 mapping $\rho: U \to \bar{\mathbb{R}}$ that agrees with ϕ_{τ} on $\mathcal{M} \cap U$. Then from (2.5), we have $\psi_{\tau} = \rho \circ G$, which is a composition of two C^2 functions and is therefore itself C^2 on a neighborhood of 0. Note too that

$$|G(y) - x^*| = |Y(y - y^*) + O(|y - y^*|^2)| = |y - y^*| + O(|y - y^*|^2).$$

Since x^* is a local minimizer of $\phi_{\tau}|_{\mathcal{M}}$, we have that $\psi_{\tau}(y) - \psi_{\tau}(y^*) = \phi_{\tau}(G(y)) - \phi_{\tau}(g(y))$ $\phi_{\tau}(x^*) \geq 0$ for all y sufficiently close to y^* , from which it follows that $\nabla \psi_{\tau}(y^*) = 0$. Thus we have

$$\psi_{\tau}(y) - \psi_{\tau}(y^*) = \frac{1}{2} (y - y^*)^T \nabla^2 \psi_{\tau}(y^*) (y - y^*) + o(|y - y^*|^2).$$

Meanwhile, if $\phi_{\tau}|_{\mathcal{M}}$ has a strong local minimizer with modulus c, we have

$$\psi_{\tau}(y) - \psi_{\tau}(y^*) = \phi_{\tau}(G(y)) - \phi_{\tau}(x^*)$$

$$\geq c|G(y) - x^*|^2 + o(|G(y) - x^*|^2) = c|y - y^*|^2 + o(|y - y^*|^2).$$

The forward implication follows by combining these inequalities. For the reverse implication, we have similarly that

$$\phi_{\tau}(G(y)) - \phi_{\tau}(x^{*}) = \psi_{\tau}(y) - \psi_{\tau}(y^{*})$$

$$> c|y - y^{*}|^{2} + o(|y - y^{*}|^{2}) = c|G(y) - x^{*}|^{2} + o(|G(y) - x^{*}|^{2}),$$

giving the result. \square

We now show that strong critical points are in fact strong local minimizers for ϕ_{τ} . The argument is similar to that of Wright [30, Theorem 3.2 (i)] in a different setting, but is somewhat more general. It allows nonconvexity in the smooth part of ϕ_{τ} (namely, f). We note that the result is not true for general prox-regular functions, as the example of [14, Section 7] attests.

THEOREM 2.5. Suppose that ϕ_{τ} is partly smooth at x^* relative to \mathcal{M} , that f is Lipschitz continuously differentiable at x^* , and that x^* is a strong critical point. Then x^* is in fact a strong local minimizer.

Proof. Let the mappings F and G, the matrix Y, and the point $y^* \in \mathbb{R}^{n-k}$ be defined as in Theorem 2.4, noting that $\nabla G(y^*)^T = Y$. From Lemma 2.2, for all x near x^* , we can find unique $y \in \mathbb{R}^{n-k}$ and $v \in \mathbb{R}^k$ with $|(y-y^*,v)| = O(|x-x^*|)$ such that $x = G(y) + \nabla F(x^*)v$. We thus have

$$(2.6) \quad \phi_{\tau}(x) - \phi_{\tau}(x^*) = \left[\phi_{\tau}(G(y) + \nabla F(x^*)v) - \phi_{\tau}(G(y))\right] + \left[\phi_{\tau}(G(y)) - \phi_{\tau}(x^*)\right].$$

For the last bracketed term, we have from the strong local minimizer condition that there is c > 0 such that

(2.7)
$$\phi_{\tau}(G(y)) - \phi_{\tau}(x^*) \ge c|G(y) - x^*|^2$$

Algorithm 1 Proximal Block Coordinate Relaxation

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Input: \mu_{\text{top}} > \mu_{\text{min}} > 0, T > 1, \tau > 0, \eta > 1, \beta \ge 1, \gamma \in (0, .5), \mathbf{tol} > 0; for k = 0, 1, 2, \ldots do

Choose Q_k \subset Q such that (1.5) is satisfied;

Choose \mu_k \in [\mu_{\min}, \mu_{\text{top}}];

Solve (1.3) for d^k;

while \phi_{\tau}(x^k + d^k) > \phi_{\tau}(x^k) - |d^k|^3 do

Set \mu_k \leftarrow \eta \mu_k;

Solve (1.3) for d^k;

end while

{Try to improve on prox-descent step}

Find \tilde{d}^k with \phi_{\tau}(x^k + \tilde{d}^k) \le \phi_{\tau}(x^k + d^k) and \phi_{\tau}(x^k + \tilde{d}^k) \le \phi_{\tau}(x^k) - \gamma |\tilde{d}^k|^3;

Set x^{k+1} \leftarrow x^k + \tilde{d}^k;
end for
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for all small y. For the first bracketed term, note first that from Lemma A.1, there is $\epsilon > 0$ such that $\sup_{g \in \partial \phi_{\tau}(x^*)} g^T d \ge \epsilon |d|$ for all $d \in N_{\mathcal{M}}(x^*) = \operatorname{range} \nabla F(x^*)$. Second, from Definition 2.3 (iv), we have by choosing the neighborhood of x^* sufficiently small that for all $g \in \partial \phi_{\tau}(x^*)$, there is $\hat{g} \in \partial \phi_{\tau}(G(y))$ such that $|\hat{g} - g| \le \epsilon/2$. Third, recall that by Lipschitz continuity of ∇f at x^* , there is $\sigma > 0$ such that (2.1) holds in a neighborhood of x^* . Using all these facts, we have for all small $y - y^*$ and v that

$$\begin{split} \phi_{\tau}(G(y) + \nabla F(x^*)v) - \phi_{\tau}(G(y)) \\ &\geq \sup_{\hat{g} \in \partial \phi_{\tau}(G(y))} \hat{g}^T \nabla F(x^*)v - \sigma |\nabla F(x^*)v|^2 \\ &\geq \sup_{g \in \partial \phi_{\tau}(x^*)} g^T \nabla F(x^*)v - (\epsilon/2)|\nabla F(x^*)v| - \sigma |\nabla F(x^*)v|^2 \\ &> \epsilon |\nabla F(x^*)v| - (\epsilon/2)|\nabla F(x^*)v| - \sigma |\nabla F(x^*)v|^2. \end{split}$$

By combining with (2.7) and using (2.6), we have

$$\phi_{\tau}(x) - \phi_{\tau}(x^*) \ge (\epsilon/2)|\nabla F(x^*)v| - \sigma|\nabla F(x^*)v|^2 + c|G(y) - x^*|^2.$$

By choosing the neighborhood of x^* small enough, we can ensure that $|\nabla F(x^*)v| < \epsilon/(4\sigma)$ and therefore

$$\begin{split} \phi_{\tau}(x) - \phi_{\tau}(x^{*}) &\geq \sigma |\nabla F(x^{*})v|^{2} + c|G(y) - x^{*}|^{2} \\ &\geq \min(\sigma, c) \left[|\nabla F(x^{*})v|^{2} + |G(y) - x^{*}|^{2} \right] \\ &\geq \frac{1}{2} \min(\sigma, c) \left[|\nabla F(x^{*})v| + |G(y) - x^{*}| \right]^{2} \\ &\geq \frac{1}{2} \min(\sigma, c) |x - x^{*}|^{2}, \end{split}$$

as required. \square

3. Proximal Block Coordinate Relaxation. Algorithm 1 is the basic framework we consider in this paper. It is quite general, in that the sequence of relaxation sets need only satisfy (1.5), there are few restrictions on the choice of the initial μ_k at each iteration, and the successful proximal step d^k can be replaced by any other step \tilde{d}^k that improves the value of ϕ_{τ} and satisfies another modest decrease condition.

Subsection 3.1 proves global convergence for this framework, while Subsection 3.2 describes identification properties for the active manifold. A reduced-Newton acceleration scheme is described in Subsection 3.3, along with local convergence results.

The "sufficient decrease" criteria are key to the algorithm. From current iterate x, the prox-descent step d is required to satisfy

(3.1)
$$\phi_{\tau}(x) - \phi_{\tau}(x+d) \ge |d|^3,$$

while the step \tilde{d} actually taken must satisfy both

(3.2)
$$\phi_{\tau}(x) - \phi_{\tau}(x + \tilde{d}) \ge \gamma |\tilde{d}|^3,$$

for a given parameter $\gamma \in (0, .5)$, and

$$\phi_{\tau}(x+\tilde{d}) \le \phi_{\tau}(x+d).$$

(The choice $\tilde{d} = d$ is obviously one option that satisfies both (3.2) and (3.3).)

Note that if the solution of the subproblem (1.3) is d = 0 for the first value tried (indicating that the optimality condition (2.3) is satisfied in the components of Q_k), the acceptance condition is satisfied and μ_k is not increased. This is a reasonable outcome, as the algorithm detects correctly that, to first order, no further progress can be made in this relaxation set.

We note that value of μ_k at iteration k, for relaxation set Q_k , may have little relevance for iteration k+1, where the relaxation set Q_{k+1} may be quite different. Algorithm 1 does not assume any "memory" in the choice of damping values. In our implementations, however, we have found that an effective initial choice of μ_{k+1} is some multiple (for example, .8) of the final value of μ_k from the previous iteration.

3.1. Global Convergence. We show here that accumulation points of Algorithm 1 are stationary. We start with a simple result about the dependence of d on μ in (1.3).

LEMMA 3.1. Suppose P is finite at a point $x \in \mathbb{R}^n$ and denote the (unique) solution of (1.3) for any $\mu > 0$ and fixed relaxation set Q' by $d(\mu)$. We have that $|d(\mu)|$ is a decreasing function of μ and that $d(\mu) \to 0$ as $\mu \uparrow \infty$.

Proof. We give an elementary proof and assume for simplicity that Q' = Q. Supposing that $\tilde{\mu} > \mu > 0$, we have directly from (1.3) that

$$\nabla f(x)^T d(\tilde{\mu}) + \frac{\tilde{\mu}}{2} |d(\tilde{\mu})|^2 + \tau P(x + d(\tilde{\mu})) \le \nabla f(x)^T d(\mu) + \frac{\tilde{\mu}}{2} |d(\mu)|^2 + \tau P(x + d(\mu)),$$
$$\nabla f(x)^T d(\mu) + \frac{\mu}{2} |d(\mu)|^2 + \tau P(x + d(\mu)) \le \nabla f(x)^T d(\tilde{\mu}) + \frac{\mu}{2} |d(\tilde{\mu})|^2 + \tau P(x + d(\tilde{\mu})).$$

By adding these inequalities and rearranging, we obtain

$$\frac{1}{2}(\tilde{\mu} - \mu)|d(\tilde{\mu})|^2 \le \frac{1}{2}(\tilde{\mu} - \mu)|d(\mu)|^2,$$

which by $\tilde{\mu} - \mu > 0$ implies the first result.

Suppose now that $d(\mu) \not\to 0$ as $\mu \uparrow \infty$. By a compactness argument we can find an increasing, unbounded sequence μ_j , $j = 1, 2, \ldots$ and a limit point $\hat{d} \neq 0$ such that $d(\mu_j) \to \hat{d}$. Note that 0 is a feasible point for (1.3), for each j, so we have

$$\nabla f(x)^T d(\mu_j) + \frac{\mu_j}{2} |d(\mu_j)|^2 + \tau P(x + d(\mu_j)) \le \tau P(x).$$

By rearrangement we have

$$|d(\mu_j)|^2 \le \frac{2}{\mu_j} \left[\tau P(x) - \tau P(x + d(\mu_j)) - \nabla f(x)^T d(\mu_j) \right].$$

By taking limits as $j \to \infty$, the right-hand side approaches 0 while the left-hand side approaches $|\hat{d}|^2$, a contradiction. \Box

We now show that the algorithm is well defined (in the sense that each inner loop eventually terminates) in the neighborhood of any point at which ∇f is locally Lipschitz.

LEMMA 3.2. Suppose that ∇f is locally Lipschitz in a neighborhood of a point \bar{x} . Then there are positive constants ρ and $\hat{\mu}$ such that the solution d of (1.3) evaluated at any x with $|x - \bar{x}| \leq \rho$ and any μ with $\mu \geq \hat{\mu}$ satisfies the sufficient decrease condition (3.1).

Proof. Choose ρ small enough that for some L>0 we have that

$$(3.4) |x - \bar{x}| \le \rho \text{ and } |d| \le \rho \implies |\nabla f(x+d) - \nabla f(x)| \le L|d|.$$

Now suppose for contradiction that for some x with $|x - \bar{x}| \le \rho$, there is a sequence $\mu_j \uparrow \infty$ such that for d^j that solves (1.3) with $\mu = \mu_j$ and $Q' = Q_j \subset Q$, we have

(3.5)
$$\phi_{\tau}(x) - \phi_{\tau}(x + d^{j}) < |d^{j}|^{3}.$$

By taking a subsequence if necessary, we can assume that $Q_j \equiv \bar{Q} \subset Q$. Since $d^j \to 0$ from Lemma 3.1, we can assume further that $|d^j| \leq \rho$ for all j. By optimality conditions (1.4) for (1.3), we have

$$-\frac{1}{\tau} \left[\nabla_{[q]} f(x) + \mu_j d_{[q]}^j \right] \in \partial P_q(x_{[q]} + d_{[q]}^j), \quad \text{for all } q \in \bar{Q},$$

and therefore

$$(3.6) P_q(x_{[q]}) - P_q(x_{[q]} + d_{[q]}^j) \ge \frac{1}{\tau} (d_{[q]}^j)^T \left[\nabla_{[q]} f(x) + \mu_j d_{[q]}^j \right], \text{for all } q \in \bar{Q}.$$

Thus we have for all j that

$$\begin{split} \phi_{\tau}(x+d^{j}) - \phi_{\tau}(x) \\ &= (d^{j})^{T} \nabla f(x) + (d^{j})^{T} \left[\nabla f(x+t_{j}d^{j}) - \nabla f(x) \right] \\ &+ \tau (P(x+d^{j}) - P(x)) \qquad \text{for some } t_{j} \in (0,1) \text{ (Taylor)} \\ &\leq (d^{j})^{T} \nabla f(x) + L |d^{j}|^{2} - \sum_{q \in \bar{Q}} (d^{j}_{[q]})^{T} \left[\nabla_{[q]} f(x) + \mu_{j} d^{j}_{[q]} \right] \text{ from } (3.4) \text{ and } (3.6) \\ &= -\mu_{j} |d^{j}|^{2} + L |d^{j}|^{2}. \end{split}$$

Hence for all j sufficiently large, using again that $d^j \to 0$ and $\mu_j \uparrow \infty$, we have

$$\phi_{\tau}(x) - \phi_{\tau}(x + d^{j}) \ge (\mu_{j} - L)|d^{j}|^{2} > |d^{j}|^{3},$$

contradicting (3.5) and proving the result. \square

It follows immediately that when ∇f is locally Lipschitz in a neighborhood of an iterate x^k of Algorithm 1, the inner loop eventually terminates with a value of μ_k that satisfies the sufficient decrease condition.

We next prove a result about criticality of accumulation points.

Theorem 3.3. Suppose that Algorithm 1 generates an infinite sequence and that x^* is an accumulation point of this sequence at which ∇f is locally Lipschitz continuous. Then x^* is a critical point.

Proof. Denote by K the subsequence such that $\lim_{k \in K} x^k = x^*$. Since $\{\phi_{\tau}(x^k)\}$ is decreasing and bounded below, the sequence converges and in fact $\phi_{\tau}(x^k) \downarrow \phi_{\tau}(x^*)$. From (3.1), we have

$$\phi_{\tau}(x^k) - \phi_{\tau}(x^{k+1}) \ge \gamma |\tilde{d}^k|^3, \quad \text{for } k = 0, 1, 2, \dots,$$

so that $\tilde{d}^k \to 0$ for the full sequence. Since $\lim_{k \in \mathcal{K}} |x^k - x^*| = 0$, we have for all $j = 1, \ldots, T$ (where T is the cycle length from (1.5)) that

$$0 \le \lim_{k \in \mathcal{K}} |x^{k-j} - x^*| \le \lim_{k \in \mathcal{K}} |x^k - x^*| + \sum_{l=1}^j |\tilde{d}^{k-l}| = 0,$$

and hence $\lim_{k \in \mathcal{K}} x^{k-j} = x^*$ for all $j = 0, 1, \dots, T$.

By local Lipschitz continuity, we can define positive constants L>0 and $\rho>0$ such that $|\nabla f(x+d)-\nabla f(x)|\leq L|d|$ for all x,d with $|x-x^*|\leq \rho$ and $|d|\leq \rho$. As in Lemma 3.2, we can identify $\hat{\mu}>0$ such that the sufficient decrease condition (3.1) is satisfied along with $|d|\leq \rho$, when $|x-x^*|\leq \rho$ and d is obtained from (1.3) for $\mu\geq \hat{\mu}$, for any $Q'\subset Q$. After eliminating from the subsequence \mathcal{K} all indices k such that $k\leq T$, and all indices k such that $|x^{k-j}-x^*|>\rho$ for some $j=0,1,\ldots,T$, we still have an infinite subsequence by the argument above. The mechanism of the algorithm ensures that $\mu_{k-j}\leq \max(\eta\hat{\mu},\mu_{\mathrm{top}})$ for all $k\in\mathcal{K}$ and all $j=0,1,\ldots,T$. In particular, we have $\mu_{k-j}d^{k-j}\to 0$ where the limit is taken over all elements $k\in\mathcal{K}$ and $j=0,1,\ldots,T$.

We now choose any $q \in Q$ and note from (1.5) that $q \in Q_{k-j}$ for some $j = 0, 1, \ldots, T-1$ and for every $k \in \mathcal{K}$. Let $j_k = k-j$ for some such j. We have from subproblem optimality (1.4) that

$$0 \in \nabla_{[q]} f(x^{j_k}) + \mu_{j_k} d_{[q]}^{j_k} + \tau \partial P_q(x_{[q]}^{j_k} + d_{[q]}^{j_k}), \quad \text{for all } k \in \mathcal{K}.$$

By taking limits of this expression as $k \in \mathcal{K}$ approaches ∞ , noting from the previous paragraph that $\lim_{k \in \mathcal{K}} \mu_{j_k} d^{j_k} = 0$, and using outer semicontinuity of ∂P_q , we have

$$0 \in \nabla_{[q]} f(x^*) + \tau \partial P_q(x_{[q]}^*).$$

Since q is any element of Q, we conclude that the criticality condition (2.3) holds at x^* , completing the proof. \square

3.2. Identification. In this section, we prove results about identification of the active manifold by iterates of the algorithm. We assume throughout that the active manifold at the limit point x^* is partly smooth and that the nondegeneracy condition (2.4) is satisfied. A characterization of identification from Hare and Lewis [8] is key to the analysis. This result has recently been applied to algorithms that take prox-descent steps in Hare [9] (for smooth constrained optimization) and Lewis and Wright [15] and Hare [10] (for regularized optimization). The novelty in the analysis of this section is largely in the handling of the block-coordinate steps rather than full prox-descent steps involving all the coordinates at once.

The first result shows that the prox-descent step from (1.3) yields identification from any point x sufficiently close to a nondegenerate critical point x^* , provided that

the relaxation set Q' encompasses all components q for which $x_{[q]}$ does not lie on the correct manifold.

THEOREM 3.4. Let the nondegenerate criticality condition (2.4) be satisfied at x^* and suppose that ∇f is locally Lipschitz there. Suppose that each P_q is partly smooth at $x^*_{[q]}$, with active manifold \mathcal{M}_q , for all $q \in Q$. Then there is a $\bar{\delta} > 0$ such that for any x with $|x - x^*| < \bar{\delta}$, one step of Algorithm 1 starting from x with relaxation set Q(x) chosen such that $q \in Q(x)$ whenever $x_{[q]} \notin \mathcal{M}_q$ results in a step d for which $x + d \in \mathcal{M}$.

Proof. Suppose for contradiction that there are sequences $x^l \to x^*$ and $Q(x^l) \subset Q$ with $q \in Q(x^l)$ whenever $x^l_{[q]} \notin \mathcal{M}_q$, yet one iteration of Algorithm 1 yields a step d^l such that $x^l + d^l \notin \mathcal{M}$. We can assume without loss of generality that $Q(x^l) \equiv Q'$ for some $Q' \subset Q$.

By the local Lipschitz property of ∇f , we can use Lemma 3.2 and Theorem 3.3 to deduce existence of $\hat{\mu}$ such that the sufficient decrease condition (3.1) is satisfied for all $\mu \geq \hat{\mu}$ and all l sufficiently large. Hence, the mechanism of the algorithm will choose μ_l with $\mu_{\min} \leq \mu_l \leq \max(\eta \hat{\mu}, \mu_{\text{top}})$, and set d^l to the solution of (1.3) for $x = x^l$ and $\mu = \mu_l$. Moreover, we can apply the result [27, Lemma 4] (concerning continuity of the solution of (1.3) with respect to the linear term $\nabla f(x)$) together with the fact that d = 0 solves (1.3) for any $\mu > 0$ when $x = x^*$ to deduce that

$$(3.7) |d^{l}| \le \mu_{l}^{-1} |\nabla f(x^{l}) - \nabla f(x^{*})| \le \mu_{\min}^{-1} O(|x^{l} - x^{*}|) \to 0.$$

It follows that $\mu_l d^l \to 0$.

We have for $q \in Q'$ that

$$\begin{split} & \left[\nabla f(x^l + d^l) + \tau \partial P(x^l + d^l) \right]_{[q]} \\ = & \nabla_{[q]} f(x^l + d^l) + \tau \partial P_q(x^l_{[q]} + d^l_{[q]}) \\ = & \left[\nabla_{[q]} f(x^l) + \mu_l d^l_{[q]} + \tau \partial P_q(x^l_{[q]} + d^l_{[q]}) \right] + O(|d^l|) - \mu_l d^l_{[q]}, \end{split}$$

and so from subproblem optimality (1.4) we have

(3.8)
$$\operatorname{dist}\left(0, \left[\nabla f(x^l + d^l) + \tau \partial P(x^l + d^l)\right]_{[q]}\right) \\ \leq O(|d^l|) + \mu_l |d^l| \to 0, \quad \text{for all } q \in Q'.$$

For $q \notin Q'$, we have $x_{[q]}^l \in \mathcal{M}_q$ and $d_{[q]}^l = 0$ and so

$$\begin{split} & \left[\nabla f(x^l + d^l) + \tau \partial P(x^l + d^l) \right]_{[q]} \\ = & \nabla_{[q]} f(x^l + d^l) + \tau \partial P_q(x^l_{[q]}) \\ = & \nabla_{[q]} f(x^*) + \tau \partial P_q(x^*_{[q]}) + O(|x^l - x^*|) + O(|d^l|) + o(1) \\ = & O(|x^l - x^*|) + O(|d^l|) + o(1), \end{split}$$

where the second equality follows from the Lipschitz property of ∇f , the limit $x^l \to x^*$, and the fact (Definition 2.3(iv)) that ∂P_q is continuous along \mathcal{M}_q . It follows that

(3.9)
$$\operatorname{dist}\left(0, \left[\nabla f(x^l + d^l) + \tau \partial P(x^l + d^l)\right]_{[q]}\right) \to 0, \quad \text{for all } q \notin Q'.$$

By combining (3.8) and (3.9), we obtain

$$\operatorname{dist}\left(0,\nabla f(x^l+d^l)+\tau\partial P(x^l+d^l)\right)\to 0,$$

implying from [8, Theorem 5.3] that $x^l + d^l \in \mathcal{M}$ for all l sufficiently large, giving the desired contradiction. \square

In the next result we consider the more general case in which the choice of relaxation sets satisfies only the generalized Gauss-Seidel condition (1.5). Our goal is to obtain nevertheless a result like Theorem 3.4, that does not require an a priori assumption that the iterates converge to the stationary point in question. Obviously, we cannot hope to identify the correct manifold until all the components have had their turn for inclusion in Q_k , which because of (1.5), happens at least once in each cycle of T iterations. We also need to assume that the steps \tilde{d}^k actually taken do not move away from the manifold identified by the prox-descent steps d^k .

Theorem 3.5. Let the nondegenerate criticality condition (2.4) be satisfied at x^* and suppose that ∇f is locally Lipschitz there. Suppose that each P_q is partly smooth at $x_{[q]}^*$, with active manifold \mathcal{M}_q , for all $q \in Q$. Then there is a $\bar{\delta} > 0$ with the following property. If Algorithm 1 is started from any initial point x^0 such that $|x^0 - x^*| < \bar{\delta}$ and $\phi_{\tau}(x^0) - \phi_{\tau}(x^*) \leq \bar{\delta}$, and provided that $\phi_{\tau}(x^k) \geq \phi_{\tau}(x^*)$ and $x^k + \tilde{d}^k$ lies on the same manifold as $x^k + d^k$ for all $k = 0, 1, 2, \ldots, T-1$, then the Tth iterate x^T lies on the manifold $\mathcal{M} := \otimes_{q \in O} \mathcal{M}_q$.

Proof. We have from the assumptions that $\phi_{\tau}(x^*) + \bar{\delta} \geq \phi_{\tau}(x^0) \geq \phi_{\tau}(x^k) \geq \phi_{\tau}(x^*)$, so from (3.1) and (3.2), we have that $|d^k|$ and $|\tilde{d}^k|$ are both bounded by a multiple of $\bar{\delta}^{1/3}$ for all $k = 0, 1, \ldots, T - 1$.

For remainder of our argument, suppose for contradiction that there is a sequence $\{x^{l,0}\}_{l=1,2,\dots}$ with $|x^{l,0}-x^*|\leq l^{-1}$ and $\phi_\tau(x^{l,0})-\phi_\tau(x^*)\leq l^{-1}$ such that when we perform T steps of Algorithm 1 starting from $x^{l,0}$ under the conditions above, the Tth iterate has $x^{l,T}\notin\mathcal{M}.$ From the previous paragraph, the steps satisfy $|d^{l,k}|=O(l^{-1/3})$ and $|\tilde{d}^{l,k}|=O(l^{-1/3})$ for all l and all $k=0,1,2,\dots,T-1,$ and thus $|x^{l,k}-x^*|=O(l^{-1/3})$ for all l and all $k=0,1,2,\dots,T.$

Choosing any $q \in Q$, we denote by k_l the largest iteration index in $0, 1, \ldots, T-1$ for which $q \in Q_{k_l}$. (Note that (1.5) guarantees existence of k_l .) Similarly to the proof of Theorem 3.4, we use Lipschitz continuity of ∇f at x^* along with the reasoning in the proofs of Lemma 3.2 and Theorem 3.3 to deduce that the damping parameter μ_{l,k_l} used at each of these steps is uniformly bounded over l. We now have

$$\begin{split} & \left[\nabla f(x^{l,T}) + \tau \partial P(x^{l,T}) \right]_{[q]} \\ = & \nabla_{[q]} f\left(x^{l,k_l} + \sum_{k=k_l}^{T-1} \tilde{d}^{l,k} \right) + \tau \partial P_q \left(x_{[q]}^{l,k_l} + \sum_{k=k_l}^{T-1} \tilde{d}^{l,k}_{[q]} \right) \\ = & \nabla_{[q]} f\left(x^{l,k_l} + d^{l,k_l} \right) + \tau \partial P_q \left(x_{[q]}^{l,k_l} + d^{l,k_l}_{[q]} \right) + O(|d^{l,k_l}|) + \sum_{k=k_l}^{T-1} O(|\tilde{d}^{l,k}|) + o(1) \\ = & \left[\nabla_{[q]} f(x^{l,k_l}) + \mu_{l,k_l} d^{l,k_l}_{[q]} + \tau \partial P_q (x_{[q]}^{l,k_l} + d^{l,k_l}_{[q]}) \right] \\ & + O(|d^{l,k_l}|) + \sum_{k=k_l}^{T-1} O(|\tilde{d}^{l,k}|) - \mu_{l,k_l} d^{l,k_l}_{[q]} + o(1), \end{split}$$

where the second equality follows from Definition 2.3(iv) (continuity of ∂P_q along the manifold identified by $x^{l,k_l}+d^{l,k_l}$) and the fact that each subsequent iterate $x_{[q]}^{l,k}$, $k=k_l+1,\ldots,T$ lies on the manifold identified by $x^{l,k_l}+d^{l,k_l}$. Using subproblem

optimality (1.4) and our estimates of $|d^{l,k_l}|$, $|\tilde{d}^{l,k_l}|$, and μ_{l,k_l} , we have that

$$\operatorname{dist}\left(0, \left[\nabla f(x^{l,T}) + \tau \partial P(x^{l,T})\right]_{[q]}\right) \to 0.$$

Since this estimate can be derived for all $q \in Q$, we have that

$$\operatorname{dist}\left(0, \nabla f(x^{l,T}) + \tau \partial P(x^{l,T})\right) \to 0,$$

implying from [8, Theorem 5.3] that $x^{l,T} \in \mathcal{M}$ for all l sufficiently large, giving the desired contradiction. \square

We note that when each P_q is everywhere finite valued, the function P is Lipschitz on R^n , and in this case we can dispense with the assumption that $\phi_{\tau}(x^0) - \phi_{\tau}(x^*) \leq \bar{\delta}$ in Theorem 3.5.

3.3. Reduced-Newton Acceleration. We now describe a variant of Algorithm 1 in which the step \tilde{d}^k is obtained from a reduced-Newton step on the current estimate of the optimal manifold \mathcal{M} . At iteration k, the procedure is as follows: Compute d^k satisfying (3.1) and find a manifold \mathcal{M}^k containing $x^k + d^k$ that is partly smooth at $x^k + d^k$. (If no such manifold can be conveniently identified, set $\tilde{d}^k = d^k$ and skip the acceleration step.) Now identify a mapping G^k that parametrizes the manifold \mathcal{M}^k , in the sense of Lemma 2.1, and a point y^k such that $G^k(y^k) = x^k + d^k$ and $G^k(y) \in \mathcal{M}^k$ for all y in a neighborhood of y^k . Next, define $\psi^k_{\tau}(y) := \phi_{\tau}(G^k(y))$, and compute a Newton step w^k for ψ^k_{τ} from y^k . Finally, define the step to be taken as $\tilde{d}^k := G(y^k + w^k) - x^k$, if this step satisfies the acceptance conditions (3.2) and (3.3), and if $x^k + \tilde{d}^k$ lies on the same manifold \mathcal{M}^k as $x^k + d^k$. Otherwise, set $\tilde{d}^k = d^k$.

We now prove a superlinear convergence for this procedure, building on the identification result of Theorem 3.5, the properties of manifolds and their parametrizations introduced in Subsection 2.2, and the standard properties of Newton's method.

THEOREM 3.6. Suppose that x^* is a strong critical point of ϕ_{τ} , where f is C^2 at x^* and each P_q is partly smooth at $x^*_{[q]}$ with respect to an active manifold \mathcal{M}_q . Let $\{x^k\}$ be the sequence generated by the algorithm, with the acceleration procedure described above, and assume that $x^k \to x^*$. Then $x^k \in \mathcal{M} := \bigotimes_{q \in Q} \mathcal{M}_q$ for all k sufficiently large, and the convergence of $\{x^k\}$ to x^* is Q-quadratic.

Proof. We can use Theorem 3.5 to deduce that $x^k + d^k \in \mathcal{M}$ for all k sufficiently large, so the acceleration procedure ensures that in fact $x^{k+1} = x^k + \tilde{d}^k \in \mathcal{M}$ for all k sufficiently large. Hence we can assume that $\mathcal{M}^k \equiv \mathcal{M}$ and $G^k \equiv G$ in the description of the acceleration procedure.

In the remainder of the proof, we identify a radius $\delta > 0$ such that the step \tilde{d}^k obtained by the acceleration procedure is accepted for all k large enough that $|x^k - x^*| < \delta$. For clarity, in the analysis below, we drop the superscript "k" and replace "k + 1" by "+".

Since the assumptions of Theorems 2.4 and 2.5 are satisfied, we have that x^* is a strong local minimizer for some modulus of convexity c > 0. By constructing the parametrization G of \mathcal{M} as described above, and defining ψ_{τ} as in (2.5), we have that $\nabla^2 \psi_{\tau}(\bar{y})$ is positive definite with smallest eigenvalue at least 2c at the solution \bar{y} for which $G(\bar{y}) = x^*$, while $\nabla \psi_{\tau}(\bar{y}) = 0$.

By applying [27, Lemma 4] as in (3.7), we have for $|x - x^*| \le \delta$ (by decreasing δ if necessary) that the solution d of (1.3) for $\mu \ge \mu_{\min}$ satisfies

$$(3.10) |d| \le \mu^{-1} |\nabla f(x) - \nabla f(x^*)| \le c_2 |x - x^*| \le c_2 \delta,$$

for some constant $c_2 > 0$. Hence, we have

$$(3.11) |x+d-x^*| \le (1+c_2)\delta.$$

Consider now the reduced Newton step from x + d. From Lemma 2.1, we have

$$(3.12) x + d - x^* = G(y) - x^* = Y(y - \bar{y}) + O(|y - \bar{y}|^2),$$

for an orthonormal matrix Y, so that by reducing δ further as needed, we have

(3.13)
$$\frac{1}{2}|y-\bar{y}| \le |x+d-x^*| \le 2|y-\bar{y}|.$$

Using this estimate together with (3.11), we see that $|y - \bar{y}| = O(\delta)$, so by reducing δ again if necessary and defining ψ_{τ} as in (2.5), the Newton step w from y is well defined, and we have

(3.14)
$$w = -[\nabla^2 \psi_{\tau}(y)]^{-1} \nabla \psi_{\tau}(y).$$

Moreover, standard analysis of Newton's method yields that

$$(3.15) |y + w - \bar{y}| \le c_3 |y - \bar{y}|^2$$

for some $c_3 > 0$. We have in particular that

(3.16)
$$\frac{1}{2}|y-\bar{y}| \le |w| \le 2|y-\bar{y}|.$$

Defining $\tilde{d} = G(y+w) - x$, we have from Lemma 2.1 that

$$(3.17) x + \tilde{d} - x^* = G(y+w) - x^* = Y(y+w-\bar{y}) + O(|y+w-\bar{y}|^2),$$

for the same orthonormal matrix Y as in (3.12), so by decreasing δ further if necessary, we have

(3.18)
$$\frac{1}{2}|y+w-\bar{y}| \le |x+\tilde{d}-x^*| \le 2|y+w-\bar{y}|.$$

By comparing (3.12) with (3.17), we obtain

(3.19)
$$\tilde{d} - d = Yw + O(|y - \bar{y}|^2) + O(|y + w - \bar{y}|^2),$$

so from (3.16), we have

(3.20)
$$\tilde{d} - d = Yw + O(|w|^2) = Yw + O(|y - \bar{y}|^2).$$

By the usual argument, we thus have

(3.21)
$$\frac{1}{2}|d - \tilde{d}| \le |w| \le 2|d - \tilde{d}|.$$

Denoting the next iterate by x^+ , defined by $x^+ := x + \tilde{d}$, we have

$$|x^{+} - x^{*}| \leq 2|y + w - \bar{y}| \qquad \text{from (3.18)}$$

$$\leq 2c_{3}|y - \bar{y}|^{2} \qquad \text{from (3.15)}$$

$$\leq 8c_{3}|x + d - x^{*}|^{2} \qquad \text{from (3.13)}$$

$$\leq 8c_{3}(1 + c_{2})^{2}|x - x^{*}|^{2} \qquad \text{from (3.11)}$$

$$\leq 8c_{3}(1 + c_{2})^{2}\delta|x - x^{*}| \qquad \text{since } |x - x^{*}| < \delta.$$

By decreasing δ again if necessary, we have that $|x^+ - x^*| \leq 0.5|x - x^*|$, so all the estimates obtained above and below for x (and its corresponding steps d and \tilde{d}) continue to apply at x^+ and indeed at all subsequent iterates. Note too that for this choice of δ , we have

$$|\tilde{d}| \le |x^+ - x^*| + |x - x^*| \le 1.5|x - x^*| \le 1.5\delta.$$

We conclude by showing that \tilde{d} satisfies the acceptance conditions (3.2) and (3.3). We have from standard Newton analysis, and using (3.21), that

$$\phi_{\tau}(x+\tilde{d}) = \psi_{\tau}(y+w) \le \psi_{\tau}(y) - c_4|w|^2$$

$$= \phi_{\tau}(x+d) - c_4|w|^2 \le \phi_{\tau}(x+d) - \frac{1}{4}c_4|d-\tilde{d}|^2,$$
(3.24)

for some $c_4 > 0$, so that (3.3) holds. Since d satisfies (3.1), we have

$$\phi_{\tau}(x) - \phi_{\tau}(x + \tilde{d}) \ge [\phi_{\tau}(x) - \phi_{\tau}(x + d)] + [\phi_{\tau}(x + d) - \phi_{\tau}(x + \tilde{d})]$$

$$\ge |d|^3 + \frac{1}{4}c_4|\tilde{d} - d|^2.$$
(3.25)

We consider two cases. First, when $|\tilde{d} - d| \le .2|\tilde{d}|$, we have $|d| \ge |\tilde{d}| - |d - \tilde{d}| \ge .8|\tilde{d}|$, so from (3.25) it follows that

$$\phi_{\tau}(x) - \phi_{\tau}(x + \tilde{d}) \ge |d|^3 \ge (.8)^3 |\tilde{d}|^3 \ge \gamma |\tilde{d}|^3$$

(since $\gamma \in (0,.5)$), so that (3.2) holds. Second, when $|\tilde{d} - d| > .2|\tilde{d}|$, we have immediately from (3.25) that

$$\phi_{\tau}(x) - \phi_{\tau}(x + \tilde{d}) \ge \frac{1}{4}c_4|\tilde{d} - d|^2 \ge .01c_4|\tilde{d}|^2$$

By using (3.23) and reducing δ if necessary (to ensure that $|\tilde{d}| \leq .01c_4/\gamma$), we have that (3.2) holds in this case too.

We conclude that it is possible to choose $\delta > 0$ such that if $|x^k - x^*| \le \delta$ for any iterate x^k generated by Algorithm 1, and using the acceleration procedure outlined above, the enhanced step \tilde{d}^l is accepted at all iterates $l \ge k$. Because of (3.22), the subsequent iterates converge Q-quadratically to x^* , as claimed. \square

4. Applications. We discuss here implementation of the approaches of Section 3 to several particular cases of regularization function P in (1.1).

We start with the case of ℓ_1 regularized optimization, in which f is smooth and $P(x) = ||x||_1$. In the notation of (1.2), we have $Q = \{1, 2, ..., n\}$, [q] = q for q = 1, 2, ..., n, and $P_q(x_{[q]}) = |x_q|$. Each subproblem (1.3) then becomes

$$\min_{d} \sum_{q \in Q'} \nabla_{q} f(x) d_{q} + \frac{\mu}{2} \sum_{q \in Q'} d_{q}^{2} + \tau \sum_{q \in Q'} |x_{q} + d_{q}|.$$

It is well known that the solution d can be evaluated in O(|Q'|) operations via the "shrinkage operator." After rearrangement and a change of variables, we can write this problem equivalently as

$$\min_{z} \frac{1}{2} |z - g|^2 + \frac{\tau}{\mu} ||z||_1,$$

for $z_q := x_q + d_q$ and $g_q := x_q - (1/\mu)\nabla_q f(x)$ $(q \in Q')$, whose explicit solution is

$$z_q = \operatorname{sign}(g_q) \max(|g_q| - \tau/\mu, 0), \qquad q \in Q'.$$

For each vector x and each component q, there are three appropriate choices of component manifold \mathcal{M}_q : $\alpha < 0$, $\alpha > 0$, and $\alpha = 0$ for scalar α , depending on whether x_q is negative, positive, or zero, respectively. The estimate \mathcal{M} for the active manifold at iterate x+d is the Cartesian product of these component manifolds. We derive an explicit representation along the lines of Lemma 2.1 as follows. Define the sets $Q_0 := \{i: x_i + d_i = 0\}, \ Q_- := \{i: x_i + d_i < 0\}, \ \text{and} \ Q_+ := \{i: x_i + d_i > 0\} \ \text{and}$ the matrix E whose columns are the columns of the $n \times n$ identity that correspond to indices in Q_0 , while Y is its complement. The mappings F and G described in Lemma 2.1 are thus

$$F(x) = E^T x, \qquad G(y) = Yy,$$

where the components of y are indexed not sequentially but rather with the indices i from Q_- and Q_+ .

The optimality condition (2.3) for x^* is thus

$$(4.1) \qquad \nabla f(x^*) + \tau v = 0,$$

where

(4.2)
$$v_i \begin{cases} = -1 & \text{if } x_i^* < 0 \\ = 1 & \text{if } x_i^* > 0 \\ \in [-1, 1] & \text{if } x_i^* = 0. \end{cases}$$

The nondegeneracy condition (2.4) is the same, except that we require v_i to be in the open interval (-1,1) when $x_i^* = 0$.

For this case, the function $\psi_{\tau}(y)$ defined in (2.5) is thus

$$\psi_{\tau}(y) = f(Yy) - \tau \sum_{i \in Q} y_i + \tau \sum_{i \in Q} y_i,$$

which is evidently as smooth as f. The Newton step for ψ_{τ} is easily calculated if $Y^T \nabla f$ and $Y^T (\nabla^2 f) Y$ are known. If $|Q_-| + |Q_+| \ll n$, it may be much less expensive to evaluate these quantities (or approximations to them) than to evaluate the full gradient and Hessian of f, as we discuss further in Section 5.

Consider next the case in which P is a group- ℓ_2 regularizer:

$$P(x) = \sum_{q \in Q} |x_{[q]}|,$$

where here each $x_{[q]}$ may be a subvector rather than a single component. The subproblem (1.3) is again separable in the subvectors $d_{[q]}$; we solve

$$\min_{d_{[q]}} \nabla_{[q]} f(x)^T d_{[q]} + \frac{\mu}{2} |d_{[q]}|^2 + P_q(x_{[q]} + d_{[q]}), \qquad q \in Q'.$$

A closed-form solution is again available; see for example [31, Section II.D]. When [q] contains at least two components, the most natural possibilities for the partial

manifold \mathcal{M}_q identified at $x_{[q]}+d_{[q]}$ are the two cases $x_{[q]}+d_{[q]}=0$ and $x_{[q]}+d_{[q]}\neq 0$. The reduced function ψ_{τ} is thus obtained by zeroing out the components [q] in the argument of f for which $x_{[q]}+d_{[q]}=0$, and omitting these same terms from the summation $\sum_{q\in Q'}\|x_{[q]}\|_2$. Note that both $\nabla\psi_{\tau}$ and $\nabla^2\psi_{\tau}$ will have contributions from the regularization terms q for which $x_{[q]}+d_{[q]}\neq 0$.

Finally, we mention the group- ℓ_{∞} case in which $P_q(x_{[q]}) = ||x_{[q]}||_{\infty}$. Here again, the subproblem (1.3) can be solved in time linear in the number of components; see [31, Section II.D] and [3]. The estimate of active manifold \mathcal{M}_q at a point $x_{[q]} \neq 0$ is

$$\mathcal{M}_q = \{x_{[q]} + z : z_i = t \operatorname{sign}(x_{[q]})_i \text{ for all } i \text{ with } |(x_{[q]})_i| = ||x_{[q]}||_{\infty} \text{ and some } t \in \mathbb{R}\},$$

that is, the manifold is (locally) the set of vectors whose components that achieve the absolute maximum are the same as in $x_{[q]}$. It is easy to find linear mappings F and G corresponding to such manifolds, and the restriction of ϕ_{τ} to \mathcal{M} is as smooth as f, in a neighborhood of x. From the subgradient of $||u||_{\infty}$ at a point $u \neq 0$ defined by

$$\partial \|u\|_{\infty} = \begin{cases} [-1,0] & \text{if } u_i = -\|u\|_{\infty}, \\ [0,1] & \text{if } u_i = \|u\|_{\infty}, \\ 0 & \text{otherwise,} \end{cases}$$

we see that $\partial P_q(x_{[q]}+z)$ is in fact constant for all $x_{[q]}+z\in\mathcal{M}_q$ in a neighborhood of $x_{[q]}$. (When $x_{[q]}=0$, we have simply $\mathcal{M}_q=0\in\mathbb{R}^{|[q]|}$ and $\partial P_q(0)=[-1,1]^{|[q]|}$.)

- 5. Computational Example. For illustrative purposes, we present some results for the framework above on ℓ_1 -regularized logistic regression. Optimized implementations and exhaustive testing of the various algorithmic options on a variety of realistic data sets will be the subject of another study. In this section, we describe the application and our algorithmic choices in enough detail to show why it is a good fit for the framework of this paper. We give some numerical results that show the effect of various algorithmic options in particular, that block coordinate relaxation and reduced Newton-like steps can greatly improve performance.
- **5.1.** ℓ_1 -Regularized Logistic Regression. The application can be described thus. Suppose we are given a "training set" of m feature vectors $x_i \in \mathbb{R}^n$, i = 1, 2, ..., m and corresponding binary labels $b_i \in \{-1, +1\}$, i = 1, 2, ..., m. Our goal is to learn a regression function $p : \mathbb{R}^n \to [0, 1]$ that predicts the chance of a given feature vector x having label +1. (It follows that 1 p(x) is the chance of x having label -1.) We parametrize p by a vector $z \in \mathbb{R}^n$, and assume that it has the following form:

(5.1)
$$p(x;z) = \frac{1}{1 + e^{z^T x}}.$$

Note that $1 - p(x; z) = 1/(1 + e^{-z^T x})$. We use the training set to find an appropriate value for z, ideally one for which $p(x_i; z)$ is close to 1 when $b_i = +1$ and close to zero when $b_i = -1$.

The log-likelihood function for the observed data is

(5.2)
$$\mathcal{L}(z) := \sum_{i:b_i = +1} \log p(x_i; z) + \sum_{i:b_i = -1} \log(1 - p(x_i; z))$$
$$= \sum_{i:b_i = -1} z^T x_i - \sum_{i=1}^m \log(1 + e^{z^T x_i}).$$

In logistic regression, z is chosen to maximize $\mathcal{L}(z)$. We can obtain a sparse z (one with few nonzeros, their locations highlighting the most significant components of the feature vector) by incorporating a multiple of $||z||_1$ in the objective. The function to be minimized is thus

(5.3)
$$\phi_{\tau}(z) = -\frac{1}{m}\mathcal{L}(z) + \tau ||z||_{1}.$$

(In our experiment below, we include an "intercept" in the regression by appending 1 to each feature vector but not including the corresponding additional component of z in the regularization term. For simplicity of exposition, however, we base our description on formulation (5.3).)

We now outline the cost of evaluating the function \mathcal{L} and its gradient and Hessian. To evaluate \mathcal{L} , we need to compute $z^T x_i$, i = 1, 2, ..., m. Using X to denote the $m \times n$ matrix whose rows are x_i^T , we see that the matrix-vector product Xz is required, where z is usually a vector of few nonzeros. If we assume no sparsity of the vectors x_i , the cost would be approximately m times the number of nonzeros in z. An additional O(m) exponentiations, logarithms, and basic arithmetic operations are required.

For the gradient, we have

(5.4)
$$\nabla \mathcal{L}(z) = -X^T w, \text{ where } w_i = \begin{cases} -(1 + e^{z^T x_i})^{-1}, & \text{if } b_i = -1, \\ (1 + e^{-z^T x_i})^{-1}, & \text{if } b_i = +1. \end{cases}$$

Since the evaluation of Xz has already been performed as part of the function evaluation, the additional costs here are (i) computation of w (O(m) operations); and (ii) computation of $(X^Tw)_j$ for the desired components $j \in \mathcal{G} \subset \{1, 2, ..., n\}$ of the gradient. For most data sets, (i) is dominated by (ii), and the cost of evaluating a partial gradient for indices in the set \mathcal{G} is approximately the fraction $|\mathcal{G}|/n$ of the cost of a full gradient.

The Hessian of \mathcal{L} is

(5.5)
$$\nabla^2 \mathcal{L}(z) = -X^T \operatorname{diag}(u) X$$
, where $u_i = \frac{e^{z^T x_i}}{(1 + e^{z^T x_i})^2}$, $i = 1, 2, \dots, m$.

The cost of computing u is just O(m), as Xz is known from the function evaluation. Hence the main cost of evaluating a principal submatrix $[\nabla^2 \mathcal{L}(z)]_{\mathcal{CC}}$ of the Hessian, corresponding to the subset of variables $\mathcal{C} \subset \{1, 2, \ldots, n\}$ used in the acceleration step, is essentially the cost of a weighted matrix multiplication of the column submatrix $X_{\mathcal{C}}$ by its transpose. To reduce cost further, we can use sampling of rows of X to obtain an approximation to $[\nabla^2 \mathcal{L}(z)]_{\mathcal{CC}}$, as in Byrd et al. [2]. After selecting the subset $\mathcal{S} \subset \{1, 2, \ldots, m\}$ at random, the approximation is obtained by performing a weighted matrix-matrix multiplication of $X_{\mathcal{SC}}$ and its transpose.

5.2. Implementation. We now discuss several aspects of the implementation. For selection of the relaxation set Q_k , we try two alternatives. In the first scheme, we set Q_k to be some fixed fraction (an algorithmic parameter), randomly chosen with equal probability, of the indices in $\{1, 2, ..., n\}$. We refer to this as the "unbiased" scheme. In the second, "biased" scheme, we include in Q_k all components of z that are nonzero at the current z_k , and add some fixed fraction of the other components, randomly chosen. In neither scheme do we check explicitly that the condition (1.5) is satisfied, though our random selection strategy makes it highly unlikely that any index will be overlooked indefinitely.

For computation of the accelerated step \tilde{d}^k , we use essentially the reduced Newton scheme described in Section 3.3. Optionally, we use a sampled approximation to the reduced Hessian, as described above. Since the reduced Hessian is ill-conditioned in many instances, we also add a damping term $\lambda_k I$ to the reduced Hessian, choosing λ_k to be 10 times the norm of the smallest vector in the subdifferential of ϕ_τ taken over the subset of components at which this vector was most recently computed. Finally, after computing the reduced (approximate) Newton step \tilde{d}^k , we scale it by a line search parameter α_k , setting α_k to be the largest positive value for which none of the components of $x^k + \alpha_k \tilde{d}^k$ have different signs from the components of $x^k + d^k$. If this α_k is too small (below 10^{-2} in our implementation), we conclude that the truncation is too severe for the reduced Newton step to have much value, so we discard it without evaluating the function at this point. In the formula (3.2), we set the parameter γ to 10^{-3} , so that the modified step \tilde{d}^k almost always satisfies this condition whenever (3.3) holds.

Testing for termination occurs when the smallest vector in the subdifferential of ϕ_{τ} over the current relaxation set falls below a specified threshold (in our case, 10^{-6}). When this occurs, we evaluate the subdifferential over *all* components and check whether it satisfies the same criterion, terminating the algorithm if it does so and continuing to iterate otherwise.

As we noted earlier, Algorithm 1 places few restrictions on the choice of μ_k . In our implementations, we used a scheme rooted in the Levenberg-Marquardt method for nonlinear least squares. The initial choice of μ_k at each iteration is $\max(\mu_{\min}, 0.8\mu_{k-1})$, where μ_{k-1} is the final value of this parameter from the previous step (after any increases that are required to satisfy the sufficient decrease condition). We set the parameter η (the factor by which μ_k is increased at inner iterations) to be 2, while μ_{\min} is set somewhat arbitrarily to 10^{-3} . We do not set μ_{top} or check for it explicitly.

Finally, we note that a heuristic to perform continuation in the regularization parameter τ is essential to efficient performance, for problems with mild regularization (that is, those for which the number of nonzero components in z is relatively large). Specifically, we initially solve (5.3) for a large value of τ , then decrease τ by equal factors until the target value is attained, taking the starting point at each value of τ to be the solution calculated for the previous value of τ . The "large value" used to initialize τ is 0.95 times $(1/m)\|\nabla \mathcal{L}(0)\|_{\infty}$. (If $\tau \geq (1/m)\|\nabla \mathcal{L}(0)\|_{\infty}$, the minimizer of (5.3) is z=0.) Apart from its advantages of efficiency, continuation is useful from the application point of view, as an appropriate value of τ is usually not known a priori. It is useful to inspect the solutions for a range of values and to use statistical procedures or domain knowledge to select the ones most appropriate. The use of continuation heuristics is common in compressed sensing (see, for example, [7, 5, 31]), but there have been few attempts to provide theoretical support.

5.3. Results. The algorithm was implemented in Matlab, by modifying an earlier version of the LPS code at http://www.cs.wisc.edu/~swright/LPS/. Computational results were obtained on a four-core 64-bit Linux system with 2.66 GHz Intel Xeon processors and 8 GB main memory.

In reporting the results, we show the total number of function evaluations and the total CPU time summed over all the cores in the system (which may of course exceed wall-clock time). We also show an "equivalent" number of full gradient evaluations, calculated by summing the total number of gradient components evaluated during the run and dividing by n. (This statistic captures fairly the effect that evaluation of, say 10% of the elements of the gradient requires 10% of the effort of a full gradient.)

Table 5.1

Performance of the method described in Section 5, showing number of function evaluations (\mathbf{nf}) , number of equivalent gradient evaluations (\mathbf{ng}) , and CPU time (seconds) on the bigdata2 set $(n=20000,\ m=4000)$.

		unbiased Q_k		biased Q_k			
$ \mathcal{G} /n$	$ \mathcal{S} /m$	nf	ng	CPU	nf	ng	CPU
1	1	256	175.1	258.5			
1	.2	247	164.1	223.0			
1	.05	241	146.1	199.0	no	t applica	able
1	.01	503	312.3	427.2			
1	none	2756	2745.0	3805.			
.2	1	183	32.6	60.2	205	34.5	69.0
.2	.2	217	39.2	75.1	268	44.7	90.7
.2	.05	268	43.8	86.3	272	43.8	89.3
.2	.01	764	124.5	256.8	523	72.9	153.8
.2	none	2899	644.2	1311.	2245	459.7	1016.
.05	1	173	22.1	38.0	256	23.5	44.5
.05	.2	225	24.4	43.2	310	25.1	48.8
.05	.05	509	37.8	95.3	347	26.2	50.9
.05	.01	809	51.7	114.0	1092	44.7	124.2
.05	none	3227	348.1	709.8	2310	130.2	390.0
.01	1	146	19.6	29.3	252	20.4	34.0
.01	.2	184	21.9	32.9	256	19.4	32.9
.01	.05	206	23.0	35.9	325	20.8	38.2
.01	.01	753	65.3	120.4	1949	28.1	112.6
.01	none	4454	420.7	755.1	2219	37.8	169.3

As mentioned above, termination occurs for each value of τ when the norm of the smallest subgradient vector falls below 10^{-6} . A total of 10 continuation steps are used in all cases.

We constructed test data sets like those of [21], as follows. Given dimensions m and n, each feature vector $x_i \in \mathbb{R}^n$ is completely dense, with elements chosen randomly to be +1 or 0 with equal probability. A "true" coefficient vector \bar{z} is selected, and an intercept of -3 is introduced, so that the "true" odds function is $p(x;\bar{z}) = (1 + \exp(x^T\bar{z} - 3))^{-1}$. The label is chosen to be $b_i = +1$ with probability $p(x_i,\bar{z})$, and 0 otherwise.

In our first data set bigdata2.mat, there are n=20000 features and m=4000 training points. The target coefficient vector \bar{z} is selected to have 10 nonzero components, each chosen from N(0,1). The second data set bigdata11.mat selects \bar{z} in the same way but has markedly different dimensions: n=1000 and m=100000. In the third data set bigdata13.mat, we have n=1000 and m=50000, but \bar{z} has 100 nonzeros with values 10^{ξ} , where ξ is chosen from N(0,1), independently for each nonzero component. In all data sets, the target value of τ is set to .05 of the "maximum" value of $(1/m)\|\nabla\mathcal{L}(0)\|_{\infty}$. For the training sets bigdata2.mat and bigdata11.mat, the solution for this value has 28 and 9 nonzeros, respectively — similar to the 10 nonzeros in target vector \bar{z} . For bigdata13.mat, the solution has 53 nonzeros, which would be sufficient to capture the most significant components from the 100 nonzeros in the \bar{z} for this data set.

Tables 5.1, 5.3, and 5.5 show results for bigdata2.mat, bigdata11.mat, and

Table 5.2 Profile of a single run of the code on the bigdata2 set. The run corresponds to the third-last line in Table 5.1 (for unbiased Q_k).

τ	nonzeros	iterations	nf	ng	CPU
1.77e-01	1	10	20	1.1	1.74
1.32e-01	1	2	3	1.0	1.41
9.83e-02	1	2	3	1.0	1.13
7.32e-02	1	2	4	1.0	1.37
5.45e-02	1	2	3	1.0	1.48
4.06e-02	3	8	15	2.1	2.59
3.03e-02	6	10	20	2.1	2.83
2.25e-02	7	18	25	3.1	5.20
1.68e-02	8	9	17	2.1	3.71
1.25e-02	8	10	19	3.1	4.47
9.32e-03	28	43	77	5.4	9.93
total			206	23.0	35.9

bigdata13.mat, respectively, for different choices of the parameters governing the size of the partial gradient set \mathcal{G} , the density of Hessian sampling $|\mathcal{S}|/m$, and the two different strategies for choice of the relaxation set Q_k . Results for the variants that use no reduced Newton acceleration (that is, set $\tilde{d}^k = d^k$ for all k) are also shown in Tables 5.1, 5.3, and 5.5, on the lines with the entry "none" in the column headed $|\mathcal{S}|/m$. Note that when the full gradient is evaluated $(|\mathcal{G}|/n=1)$ there is no distinction between the "biased" and "unbiased" sampling strategies, since $Q_k \equiv \{1, 2, \ldots, n\}$. Hence, the top right box of each table is not filled.

Tables 5.2, 5.4, and 5.6 show a profile for a particular run of the code for a single set of parameter choices. We note that all variants produced the same solutions (in terms of the final number of nonzeros, for each value of τ). These tables show how the work was distributed between the sequence of τ values used in the continuation heuristic for one of the better parameter combinations for each data set.

We can make several general observations about the performance reported in Tables 5.1, 5.3, and 5.5.

- 1. The use of reduced Newton acceleration vastly improves performance over the method that uses only first-order information. In many cases, the first-order method is an order of magnitude or more slower than the best method that uses reduced-Newton acceleration. The difference in performance would only grow if we were to use convergence tolerances tighter than the 10⁻⁶ used in these tests, though tighter tolerances would probably not be needed in most applications. In a few cases, however, the first-order method is not much worse than the reduced-Newton variants, for example in the bottom right of Table 5.1, where we evaluate only 1% of the gradient and use the "biased" scheme for selecting the relaxation set.
- 2. There is a large performance benefit for all data sets from using partial gradient evaluations. For all sets, the best results were generally obtained when only 1% of gradient components were evaluated the smallest value tried for this parameter. (Note that for the "biased" choice of Q_k , the number of components evaluated is actually slightly larger than the given parameter, as we add to Q_k all indices j for which the current solution estimate is nonzero.)

Table 5.3

Performance of the method described in Section 5, showing number of function evaluations (nf), number of equivalent gradient evaluations (ng), and CPU time (seconds) on the bigdata11 set (n = 1000, m = 100000).

		unbiased Q_k		biased Q_k			
$ \mathcal{G} /n$	$ \mathcal{S} /m$	nf	ng	CPU	nf	ng	CPU
1	1	274	209.4	561.2			
1	.2	274	209.4	528.3			
1	.05	274	209.4	527.4	no	t applic	able
1	.01	272	204.5	499.5			
1	none	773	762.0	1429.			
.2	1	149	37.1	204.1	234	57.9	320.1
.2	.2	172	40.7	153.4	232	53.4	208.8
.2	.05	165	40.5	137.8	204	48.6	168.5
.2	.01	177	40.0	129.7	246	63.6	207.3
.2	-	1596	401.8	1031.3	720	173.1	475.9
.05	1	195	27.0	122.8	216	24.0	95.1
.05	.2	197	26.8	114.1	193	21.4	82.0
.05	.05	190	24.7	94.0	205	21.8	80.5
.05	.01	212	26.5	105.1	206	20.9	77.4
.05	-	2925	370.8	1176.	684	51.7	226.5
.01	1	181	20.2	90.0	196	17.7	68.2
.01	.2	166	19.9	71.6	197	18.8	66.0
.01	.05	163	19.8	66.5	204	18.8	67.4
.01	.01	162	20.7	67.7	224	19.1	71.4
.01	-	3388	408.7	1193.8	765	26.0	159.8

- 3. The most obvious variant of the algorithm full gradient evaluation, no reduced-Newton acceleration gives for all three data sets quite poor results. This underlies the importance of partial gradient evaluation and second-order acceleration in producing good performance.
- 4. There is sometimes a slight benefit from using sampled approximation of the reduced Hessian, as opposed to full evaluation using all training data, but it is not particularly significant. Possibly this is because the reduced Hessians required by this algorithm are not large (because the final active sets contain only a small fraction of nonzeros), so Hessian evaluation consumes only a small part of the overall run time.
- 5. There is no consistent benefit to be gained from using the "biased" technique for choosing Q_k .

The experience reported above suggests that there are benefits to using partial gradient information and reduced Newton acceleration on large problems. However, we repeat that our results are mainly illustrative in nature. Conclusions may be quite different on problems in which the final number of nonzero elements is relatively larger, or when the number of training examples m is huge, or when the data matrix X has different properties from the dense random matrix used here.

5.4. Reproducibility. In the interests of reproducibility, we have placed the code at http://www.cs.wisc.edu/~swright/LPS/ (see version 2.0 of LPS), along with code and instructions for reproducing the data in the tables of this paper. Be-

Table 5.4

Profile of a single run of the code on the **bigdata11** set. The run corresponds to the third-last line in Table 5.3 (for unbiased Q_k).

τ	nonzeros	iterations	nf	ng	CPU
7.63e-02	1	45	60	3.1	22.69
5.69e-02	1	2	4	1.0	1.77
4.24e-02	1	2	3	1.0	1.88
3.16e-02	1	2	3	1.0	1.78
2.35e-02	1	2	3	1.0	2.08
1.75e-02	2	7	12	2.1	5.01
1.30e-02	3	9	17	2.1	6.41
9.72e-03	3	8	14	2.1	5.63
7.24e-03	5	8	14	2.1	6.09
5.39e-03	9	11	21	2.2	7.39
4.02e-03	9	6	12	2.1	5.75
total			163	19.8	66.5

cause of the random nature of the algorithm (both in the selection of gradient components and in the selection of training points to use in the Hessian estimate), results will usually differ from run to run.

We include in the distribution the data sets number of smaller test problems, mostly following those reported in [20], along with code to run these problems.

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Appendix A. Manifold Characterization: Proofs.

Proof. (Lemma 2.1) We prove the result constructively via the implicit function theorem; see for example [17, Theorem A.2]. We set $\bar{y}=0$ for convenience. Assuming WLOG that $\nabla F(\bar{z})$ is orthonormal and defining Y as in the statement of the theorem, we observe that the $m \times m$ matrix $\begin{bmatrix} \nabla F(\bar{z}) & Y \end{bmatrix}$ is nonsingular, in fact orthogonal. We now consider the map $\Phi: \mathbb{R}^m \times \mathbb{R}^{m-k} \to \mathbb{R}^m$ defined as follows:

$$\Phi(z,y) = \begin{bmatrix} F(z) \\ Y^T(z-\bar{z}) - y \end{bmatrix}.$$

Note first that $\Phi(\bar{z},0)=0$. Second, we have

$$\nabla_z \Phi(z,y) = \begin{bmatrix} \nabla F(z) & Y \end{bmatrix},$$

which is nonsingular at the point $(z, y) = (\bar{z}, 0)$, as noted above. Third, Φ is p times continuously differentiable in a neighborhood of $(\bar{z}, 0)$, by the assumed properties of F. Thus, by applying the implicit function theorem, we have that z is implicitly a C^p function of y. We identify G(y) with z to obtain the main result.

For the final statements, note from the implicit function theorem that

$$\nabla G(y) = -\nabla_y \Phi(z,y) [\nabla_z \Phi(z,y)]^{-1} = \begin{bmatrix} 0 & I \end{bmatrix} \begin{bmatrix} \nabla F(z) & Y \end{bmatrix}^{-1},$$

Table 5.5

Performance of the method described in Section 5, showing number of function evaluations (nf), number of equivalent gradient evaluations (ng), and CPU time (seconds) on the bigdata13 set $(n=1000,\ m=5000)$.

		unbiased Q_k		biased Q_k			
$ \mathcal{G} /n$	$ \mathcal{S} /m$	nf	ng	CPU	nf	ng	CPU
1	1	204	130.5	168.9			
1	.2	240	156.0	191.5			
1	.05	299	206.2	249.9	no	t applica	able
1	.01	225	137.7	155.4			
1	none	6622	6611.	6561.			
.2	1	184	32.8	74.7	231	42.2	97.9
.2	.2	210	36.9	72.6	232	42.8	87.8
.2	.05	227	40.0	75.3	252	43.8	90.8
.2	.01	293	51.4	106.1	276	47.3	91.2
.2	-	5015	1073.	1927.	6046	1420.	2550.
.05	1	178	22.8	63.5	285	30.7	94.3
.05	.2	249	25.4	64.4	316	32.9	83.3
.05	.05	289	29.6	69.0	384	34.8	90.1
.05	.01	307	31.4	73.4	424	38.0	99.8
.05	-		fail		5983	541.7	1534.
.01	1	149	21.0	51.5	260	23.4	74.4
.01	.2	242	25.5	68.2	266	25.7	63.0
.01	.05	148	21.3	39.2	322	25.0	67.6
.01	.01	207	24.5	50.5	387	30.3	83.5
.01	-		fail		6017	294.6	1161.

and thus at y = 0, using $\begin{bmatrix} \nabla F(\bar{z}) & Y \end{bmatrix}^{-1} = \begin{bmatrix} \nabla F(\bar{z}) & Y \end{bmatrix}^T$, we have $\nabla G(0) = Y^T$. Thus, by Taylor's theorem, we have

$$G(y) - \bar{z} = G(y) - G(0) = Yy + O(|y|^2).$$

Proof. (Lemma 2.2) Assume for contradiction that there are sequences $z^r \to \bar{z}$, $(y^r, v^r) = O(|z^r - \bar{z}|)$ and $(\hat{y}^r, \hat{v}^r) = O(|z^r - \bar{z}|)$ such that

$$z^{r} = G(y^{r}) + \nabla F(\bar{z})v^{r} = G(\hat{y}^{r}) + \nabla F(\bar{z})\hat{v}^{r},$$

and $(y^r, v^r) \neq (\hat{y}^r, \hat{v}^r)$ for all r. By taking differences, and using the properties of G from Lemma 2.1, we have

$$G(y^{r}) - G(\hat{y}^{r}) + \nabla F(\bar{z})(v^{r} - \hat{v}^{r}) = 0$$
(A.1)
$$\Rightarrow Y(y^{r} - \hat{y}^{r}) + o(|y^{r} - \hat{y}^{r}|) + \nabla F(\bar{z})(v^{r} - \hat{v}^{r}) = 0,$$

where $\left[\nabla F(\bar{z}) \quad Y\right]$ is orthogonal. We cannot have $v^r - \hat{v}^r = o(|y^r - \hat{y}^r|)$, since (A.1) would then imply that $y^r - \hat{y}^r = o(|y^r - \hat{y}^r|)$, so that $y^r = \hat{y}^r$ for all r sufficiently large and so also $v^r = \hat{v}^r$ for all r sufficiently large, a contradiction. Neither can we have $y^r - \hat{y}^r = o(|v^r - \hat{v}^r|)$, since it then follows from (A.1) that $v^r - \hat{v}^r = o(|v^r - \hat{v}^r|)$, so that $v^r = \hat{v}^r$ for all r sufficiently large, so also $y^r = \hat{y}^r$ for all r sufficiently large, another contradiction. Hence, the ratio $|v^r - \hat{v}^r|/|y^r - \hat{y}^r|$ is bounded above and

Table 5.6

Profile of a single run of the code on the **bigdata13** set. The run corresponds to the third-last line in Table 5.5 (for unbiased Q_k).

τ	nonzeros	iterations	nf	ng	CPU
1.79e-01	1	10	19	1.1	2.36
1.33e-01	1	2	3	1.0	1.15
9.94e-02	1	2	3	1.0	1.01
7.41e-02	1	2	3	1.0	1.01
5.52e-02	1	2	3	1.0	0.80
4.11e-02	1	2	3	1.0	1.00
3.06e-02	3	7	12	2.1	2.87
2.28e-02	15	10	16	2.2	3.47
1.70e-02	23	15	23	2.4	7.19
1.27e-02	42	13	25	4.6	7.71
9.43e-03	53	23	38	3.9	10.60
total			148	21.3	39.2

below by positive constants for all r sufficiently large, so we can assume WLOG that $(v^r - \hat{v}^r)/|y^r - \hat{y}^r| \to \tilde{v} \neq 0$. By taking a further subsequence if necessary, we have $(y^r - \hat{y}^r)/|y^r - \hat{y}^r| \to \tilde{y}$ with $|\tilde{y}| = 1$. Dividing (A.1) by $|y^r - \hat{y}^r|$ and taking limits, we thus have $Y\tilde{y} + \nabla F(\bar{z})\tilde{v} = 0$, which implies $\tilde{y} = 0$ and $\tilde{v} = 0$, giving the desired contradiction. \Box

Finally, we include the following result for completeness.

LEMMA A.1. Suppose we have a function $h: \mathbb{R}^m \to \bar{\mathbb{R}}$, a point \bar{z} , and a manifold \mathcal{M} with $\bar{z} \in \mathcal{M} \subset \mathbb{R}^m$ such that h is partly smooth at \bar{z} with respect to \mathcal{M} . Suppose in addition that the nondegenerate criticality condition $0 \in \text{ri } \partial h(\bar{z})$ holds. Then there is $\epsilon > 0$ such that for all $d \in N_{\mathcal{M}}(\bar{z})$, we have

$$\sup_{g \in \partial h(\bar{z})} g^T d \ge \epsilon |d|.$$

Proof. Since aff $\partial h(\bar{z}) = N_{\mathcal{M}}(\bar{z})$ and $0 \in \text{ri}\,\partial h(\bar{z})$, there is $\epsilon > 0$ such that $g \in \partial h(\bar{z})$ for all $g \in N_{\mathcal{M}}(\bar{z})$ with $|g| \leq \epsilon$. Thus for any $d \in N_{\mathcal{M}}(\bar{z})$, we have $\epsilon d/|d| \in \partial h(\bar{z})$, and the result follows immediately. \square

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