Regularized Nonsmooth Newton Algorithms for Best Approximation with Applications *

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Abstract

We consider the problem of finding the best approximation point from a polyhedral set, and its applications, in particular to solving large-scale linear programs. The classical best approximation problem has many various solution techniques as well as applications. We study a regularized nonsmooth Newton type solution method where the Jacobian is singular; and we compare the computational performance to that of the classical projection method of Halpern-Lions-Wittmann-Bauschke (HLWB).

We observe empirically that the regularized nonsmooth method significantly outperforms the HLWB method. However, the HLWB method has a convergence guarantee while the nonsmooth method is not monotonic and does not guarantee convergence due in part to singularity of the generalized Jacobian.

Our application to solving large-scale linear programs uses a parametrized best approximation problem. This leads to a finitely converging *stepping stone external path following* algorithm. Other applications are finding triangles from branch and bound methods, and generalized constrained linear least squares. We include scaling methods and sensitivity analysis to improve the efficiency.

Keywords: best approximation, projection methods, Halpern-Lions-Wittmann-Bauschke algorithm, nonsmooth and semismooth methods, sparse large-scale linear programming, constrained linear least squares.

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*PLEASE NOTE We are including a table of contents, lists of tables, index, to help the referees. We fully intend to delete these before any final version of the paper.

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1 Introduction

The best approximation problem, BAP, arises in many areas of optimization and approximation theory. In particular, we study finding the best approximation x^* to a given point v from a polyhedral set, $P \subset \mathbb{R}^n$, in the n-dimensional Euclidean space; namely, find $x^*(v) \in \mathbb{R}^n$ such that

$$x^{*}(v) = \underset{x \in P}{\operatorname{argmin}} \|x - v\|.$$
(1.1)

There is an abundance of theory, algorithms, and applications for this problem, see e.g., [4, 13, 22], [6, Chap. 6], and the references therein. The optimum point $x^*(v)$ is the projection of v onto the polyhedral set P and is known to be unique. In this work we follow a Newton type approach of an *elegant* compact optimality condition, even though the corresponding Jacobian resulting from the optimality conditions is possibly a generalized Jacobian and/or singular. We include a regularization, as well as an inexact approach for large-scale problems. Empirical evidence illustrates the surprising success of this approach.

We include several applications. In particular, we solve large-scale linear programming, (LP), problems using a parametrized best approximation problem. This introduces an efficient finitely converging, stepping stone external path following algorithm. In addition, we consider large-scale systems of triangle inequalities. In our applications we do not assume differentiability of our optimality conditions and/or nonsingularity of the generalized Jacobian. We introduce a Newton type

approach for our applications that overcomes the nonsmooth difficulties by applying regularization and scaling. We then provide extensive testing and comparisons to illustrate the surprisingly high efficiency, accuracy, and speed of our proposed method.

1.1 Main Contributions

- (i) First, we present the basics for the best approximation problem, see Theorem 2.1 below. This includes an application of the Moreau decomposition that yields a single elegant equation that captures all three KKT optimality conditions: primal and dual feasibility and complementary slackness. This emphasizes the equivalence of this single equation (2.4) in the small dimensional dual variable y to solving the entire KKT optimality conditions. We include a comparison with interior point methods in Remark 2.2.
- (ii) Second, we present the nonsmooth, regularized Newton method. No line search is used. (See Section 2.1.1 below.)
- (iii) We show that the regularization from a modified, simplified, Levenberg-Marquardt, LM, method yields a descent direction. (See Lemma 2.5 below.)
- (iv) We present our empirical test results that include an external path following approach to solving large-scale linear programs that fully exploits sparsity. This is based on efficiently solving the BAP subproblems accurately and applying sensitivity analysis. We compare our results with several codes in the literature. The details are in Section 5 below.
- (v) We compare computationally our algorithm with the Halpern-Lions-Wittmann-Bauschke, (HLWB), algorithm that belongs to a class of projection methods usually developed and investigated in the field of fixed point theory.

1.2 Related Work

Our approach uses a special decomposition from the optimality conditions that allows for a Newton method with a cone projection applied to a system whose size is of the order of the number of linear equality constraints forming the polyhedron P. This approach first appeared in infinite dimensional Hilbert space applications, e.g., [11,17,18,44], where the projection mapping is differentiable, and typically P is the intersection of a cone and a linear manifold. The approach was applied to a parametrized quadratic problem to solve finite-dimensional linear programs in [53]. (See our application Section 4.1, below. In this finite-dimensional case differentiability was lost.) The approach in infinite-dimensional Hilbert spaces was followed up and extended in the theory of partially finite programs in [9, 10] and the many references therein. Further references are given in [3,37,52].

As mentioned above, differentiability is lost in the finite-dimensional cases, see e.g., in [53]. This led to the introduction of semismoothness [45]. In particular, semismoothness for a nondifferentiable Newton type method is introduced and applied in [47, 48]. Further applications for nearest doubly stochastic and nearest Euclidean distance matrices are presented in [2, 33]. A regularized semismooth approach for general composite convex programs is given in [54].

Differentiability properties are nontrivial as discussed in, e.g., [32]. A characterization of differentiability in terms of normal cones is given in [24]. Further results and connections to semismoothness are in, e.g., [28, 32]. A survey presentation on differentiability properties can be found at the link [50].

2 Projection onto a Polyhedral Set

We begin with the projection onto the polyhedral set given in standard form, since every polyhedron can be transformed into this form. Suppose we are given $v \in \mathbb{R}^n, b \in \mathbb{R}^m, A \in \mathbb{R}^{m \times n}$, rank A = mand no columns of A are 0. We define the following projection onto a polyhedral set, i.e., the best approximation problem, BAP to the generalized simplex,

(P)

$$\begin{aligned}
x^*(v) &:= \operatorname{argmin}_x \quad \frac{1}{2} \|x - v\|^2 \\
& \text{s.t.} \quad Ax = b \\
x \in \mathbb{R}^n_+, \quad (2.1)
\end{aligned}$$

optimal value: $p^*(v) = \frac{1}{2} ||x^*(v) - v||^2$,

i.e., the optimum and optimal value are, respectively, $x^*(v), p^*(v)$; and \mathbb{R}^n_+ is the nonnegative orthant. We now proceed to derive the regularized nonsmooth Newton method, (RNNM) to solve (2.1).

2.1 Basic Theory and Algorithm

In this section we briefly describe the properties of problem (2.1) as well as some background and motivation behind using a generalized Newton method. We assume that

$$P := \{ x \in \mathbb{R}^n_+ : Ax = b \} \neq \emptyset.$$

$$(2.2)$$

Problem (2.1) has a strongly convex smooth objective function and nonempty closed convex constraint set. Therefore, the optimal value is finite, uniquely attained, and strong duality holds. In the following, we precisely formulate this conclusion.

Throughout the rest of the paper we set¹

$$F(y) := A(v + A^T y)_+ - b, \quad f(y) := \frac{1}{2} \|F(y)\|^2.$$
(2.3)

Theorem 2.1. Consider the generalized simplex best approximation problem (2.1) with primal optimal value and optimum $p^*(v)$ and $x^*(v)$, respectively. Then the following hold:

(i) The optimum $x^*(v)$ exists and is unique. Moreover, strong duality holds and the dual problem of (2.1) is the maximization of the dual functional, $\phi(y, z)$:

$$p^{*}(v) = d^{*}(v) := \max_{\substack{z \in \mathbb{R}^{n}_{+} \\ y \in \mathbb{R}^{m}}} \phi(y, z) := -\frac{1}{2} \left\| z + A^{T} y \right\|^{2} + y^{T} (Av - b) - z^{T} v.$$

¹Let $x \in \mathbb{R}^n$. Here and elsewhere we use x_+ (respectively x_-) to denote the projection of the vector x onto the nonnnegative orthant defined as $x_+ = (\max\{0, x_i\})_{i=1}^n$ (respectively onto the nonpositive orthant defined by $x_- = (\min\{0, x_i\})_{i=1}^n$).

(ii) Let $y \in \mathbb{R}^m$. Then

$$F(y) = 0 \iff y \in \operatorname*{argmin}_{u} f(u) \text{ and } x^*(v) = (v + A^T y)_+.$$
(2.4)

Proof. Recall that the Lagrangian L(x, y, z) for (2.1), and its gradient, are respectively

$$L(x, y, z) = \frac{1}{2} \|x - v\|^2 + y^T (b - Ax) - z^T x, \quad \nabla_x L(x, y, z) = x - v - A^T y - z.$$
(2.5)

(i): The solution of the problem (2.1) is a projection onto a nonempty polyhedral set, which is a closed and convex set, see (2.2). Therefore, the optimum exists and is unique and strong duality holds, i.e., there is a zero duality gap and the dual is attained.

Let x be a stationary point of the Lagrangian i.e., $\nabla_x L(x, y, z) = 0$. Then by (2.5) we have the following equivalent representation

$$x = v + A^T y + z$$

It then follows that at a stationary point x we have

$$\begin{split} L(x,y,z) &= \frac{1}{2} \left\| v + A^T y + z - v \right\|^2 + y^T (b - A(v + A^T y + z)) - z^T (v + A^T y + z) \\ &= \frac{1}{2} \left\| A^T y + z \right\|^2 + y^T b - y^T A v - (A^T y)^T (A^T y + z) - z^T v - z^T (A^T y + z) \\ &= \frac{1}{2} \left\| A^T y + z \right\|^2 + y^T b - y^T A v - (A^T y + z)^T (A^T y + z) - z^T v \\ &= -\frac{1}{2} \left\| z + A^T y \right\|^2 + y^T (b - A v) - z^T v. \end{split}$$

The Lagrangian dual is

$$d^{*} = \max_{y \in \mathbb{R}^{n}, z \in \mathbb{R}^{n}_{+}} \min_{x \in \mathbb{R}^{n}_{+}} L(x, y, z) \quad (= \frac{1}{2} ||x - v||^{2} + y^{T}(b - Ax) - z^{T}x)$$

$$= \max_{x \in \mathbb{R}^{n}_{+}, y \in \mathbb{R}^{m}, z \in \mathbb{R}^{n}_{+}} \{L(x, y, z) : \nabla_{x}L(x, y, z) = 0\}$$

$$= \max_{x \in \mathbb{R}^{n}_{+}, y \in \mathbb{R}^{m}, z \in \mathbb{R}^{n}_{+}} \{L(x, y, z) : x = v + A^{T}y + z\}$$

$$= \max_{y \in \mathbb{R}^{m}, z \in \mathbb{R}^{n}_{+}} -\frac{1}{2} ||z + A^{T}y||^{2} + y^{T}(b - Av) - z^{T}v.$$

Moreover, $p^* := p^*(v) = d^* := d^*(v)$, and the dual value is attained.

(ii): Now the KKT optimality conditions for the primal-dual variables (x, y, z) are²:

$$\begin{aligned} \nabla_x L(x, y, z) &= x - v - A^T y - z = 0, \ z \in \mathbb{R}^n_+, & \text{(dual feasibility)} \\ \nabla_y L(x, y, z) &= A x - b = 0, \ x \in \mathbb{R}^n_+, & \text{(primal feasibility)} \\ \nabla_z L(x, y, z) &\cong x \in (\mathbb{R}^n_+ - z)^+. & \text{(complementary slackness } z^T x = 0) \end{aligned}$$

The above KKT conditions can be rewritten as :

$$\begin{pmatrix} x - v - A^T y - z \\ Ax - b \\ z^T x \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \quad x, z \in \mathbb{R}^n_+, y \in \mathbb{R}^m.$$
(2.6)

It follows from the dual feasibility that $v + A^T y = x - z = x + (-z)$. Together with the complementary slackness we have

²Let $S \subset \mathbb{R}^n$. We use $S^+ = \{\phi : \langle \phi, s \rangle \ge 0, \forall s \in S\}$ to denote the (nonnegative) polar cone of the set S.

$$x^T z = 0, x, z \in \mathbb{R}^n_+, -z \in \mathbb{R}^n_- = (\mathbb{R}^n_+)^+,$$

and we learn that x - z is the Moreau decomposition of $v + A^T y$. That is

$$x = (v + A^T y)_+$$
 and $-z = (v + A^T y)_-$; equivalently, $z = -(v + A^T y)_-$. (2.7)

Substituting for $x = (v + A^T y)_+$ we obtain a simplification of the optimality conditions in (2.6) as follows

$$A(v + A^T y)_+ = b, \ x = (v + A^T y)_+ \implies z = -(v + A^T y)_-, \ z^T x = 0, \ x, z \in \mathbb{R}^n_+, \ x - v - A^T y - z = 0,$$

equivalently; F(y) = 0, for some $y \in \mathbb{R}^m$.

For the converse, let $y \in \mathbb{R}^m$ be given and suppose that F(y) = 0. Let $\bar{x} = (v + A^T y)_+$. Therefore, \bar{x} is primal feasible. Let $\bar{z} = -(v + A^T y)_-$. We get nonnegative feasibility and complementary slackness: $\bar{z} \ge 0$, $\bar{z}^T \bar{x} = 0$. And,

$$(v + A^T y) = \bar{x} - \bar{z} \implies \bar{x} - v - A^T y - z = 0,$$

i.e., dual feasibility holds. The KKT conditions now imply that $\bar{x}(v)$ is optimal. Moreover, F(y) = 0 implies that $y \in \operatorname{argmin}_{u} f(u)$, i.e., y solves the nonlinear least squares problem.

Remark 2.2. Interior point methods use perturbed KKT conditions with $z^T x = 0$ in (2.6) replaced by $z_j x_j = \mu, x_j > 0, z_j > 0, \forall j$, where $\mu > 0$ is the log-barrier parameter. A Newton step is taken with backtracking to stay strictly feasible. Therefore, our method is equivalent to fixing $\mu = 0$ throughout the iterations and not staying strictly feasible for x, z. This is comparable to the predictor step in predictor-corrector methods, or to affine scaling method.

2.1.1 Nonlinear Least Squares; Jacobians

The BAP as described in (2.1) is equivalent to the minimization of f(y) in (2.3), i.e., to a nonlinear least squares problem where the nonlinearity arises from the projection.

This system can be recharacterized by introducing the (possibly nonsmooth) projection of a vector p onto the nonnegative, respectively nonpositive, orthant denoted $p_+ = \operatorname{argmin}_x\{||x - p|| : x \ge 0\}$, respectively $p_- = \operatorname{argmin}_x\{||x - p|| : x \le 0\}$. In general, we can define the *Moreau* decomposition of p with respect to \mathbb{R}^n_+ as $p = p_+ + p_-$, $p_+^T p_- = 0$.

Note that in the differentiable case the gradient of the squared residual f(y) in (2.3) is

$$\nabla f(y) = (F'(y))^* F(y),$$

where $(\cdot)^*$ denotes the adjoint (here adjoint is transpose) and F' denotes the Jacobian matrix. We note that we have differentiability of the function $h(w) := w_+$ if, and only if, $\{i : w_i = 0\} = \emptyset$ if, and only if, $w - w_+$ is in the relative interior of the normal cone of \mathbb{R}^n_+ at w_+ (negative of the polar cone at w_+), see [50, Page 7], [24].

We now discuss the framework of nonsmooth terminology needed for generalized gradients of a general function $H : \mathbb{R}^n \to \mathbb{R}^n$.

Definition 2.3 ((local) Lipschitz continuity). Let $\Omega \subseteq \mathbb{R}^n$. A function $H : \Omega \to \mathbb{R}^n$ is Lipschitz continuous on Ω if there exists K > 0 such that

$$||H(y) - H(z)|| \le K ||y - z||, \, \forall y, z \in \Omega.$$

H is locally Lipschitz continuous on Ω if for each $x \in \Omega$ there exists a neighbourhood *U* of *x* such that *H* is Lipschitz continuous on *U*.

Let $\Omega \subseteq \mathbb{R}^n$. It follows from Rademacher's Theorem [25, 49] that if $H : \Omega \to \mathbb{R}^n$ is locally Lipschitz on Ω then H is Frechét differentiable almost everywhere on Ω . Following Clarke [19, Def. 2.6.1], we recall the following definition of the generalized Jacobian³.

Definition 2.4 (generalized Jacobian). Suppose that $H : \mathbb{R}^m \to \mathbb{R}^m$ is locally Lipschitz.

Let D_H be the set of points where H is differentiable. Let H'(y) be the usual Jacobian matrix at $y \in D_H$. The generalized Jacobian of H at y, $\partial H(y)$, is the convex hull⁴ of the set of all matrices obtained as limits of usual Jacobians, defined as follows

$$\partial H(y) := \operatorname{conv} \left\{ \lim_{\substack{y_i \to y \\ y_i \in D_H}} H'(y_i) \right\}.$$

In addition, $\partial H(y)$ is called nonsingular if every $V \in \partial H(y)$ is nonsingular.

We now return to the nonlinear least squares problem (2.3) with functions f and F. In the differentiable case, the Gauss-Newton direction is the solution of the (consistent) Gauss-Newton equation⁵

$$F'(y))^*(F'(y))\Delta y = -(F'(y))^*F(y).$$
(equivalently invertible case, $F'(y)\Delta y = -F(y)).$ (2.8)

In the sequel A^{\dagger} denotes the generalized (Moore-Penrose) inverse of a matrix A. Solving for the best least squares solution Δy in (2.8) yields

$$\Delta y = -F'(y)^{\dagger} F(y). \tag{2.9}$$

Therefore, the directional derivative of f in the direction Δy satisfies

$$\begin{aligned} \Delta y^T \nabla f(y) &= (F'(y))^{\dagger} F(y))^T (-(F'(y))^* F(y)) \\ &= -\|\operatorname{Proj}_{\operatorname{range}((F'(y))^*)} F(y))\|^2 \\ &< 0, \quad \text{if } F(y) \notin \operatorname{null}((F'(y))^*), \end{aligned}$$
(2.10)

where $\operatorname{Proj}_{\Omega}(u)$ denotes the orthogonal projection of the point u onto the set Ω . We conclude in the differentiable case that: the Gauss-Newton direction Δy is a descent direction when $F(y) \neq 0$.

The Levenberg-Marquardt, LM, method is a popular method for handling singularity in F'(y)by using the substitution/regularization $(F'(y))^*F'(y) \leftarrow ((F'(y))^*F'(y)) + \lambda I, \lambda > 0$. We now see

³For our application we restrict ourselves to square Jacobians.

⁴Let $S \subset \mathbb{R}^n$. The convex hull of S, denoted $\operatorname{conv}(S)$ is the smallest convex set containing S.

⁵The Gauss-Newton direction is the minimum of the quadratic model $f(y + \Delta y) \approx f(y) + \nabla f(y)^T \Delta y + \frac{1}{2} \Delta y^T ((F'(y))^* F'(y)) \Delta y$, i.e., the higher order quadratic terms are ignored, e.g., [27]. This is particularly suitable here as the higher order terms involve the F(y) that is converging to zero.

that we maintain a descent direction with a similar simplified approach if the basic assumption in (2.11) holds. This simplified approach avoids the product $(F'(y))^*F'(y)$ and thus avoids increased ill-conditioning and loss of sparsity.

Lemma 2.5. Consider the nonlinear least squares problem in (2.3). Let $y \in \mathbb{R}^m$, with F differentiable at y. Let $\lambda > 0$ and let Δy be the (unique) solution of

$$(F'(y) + \lambda I)\Delta y = -F(y).$$

Then F'(y) is positive semidefinite, $F'(y) \succeq 0$, and moreover, Δy is the simplified LM direction and is a descent direction if, and only if,

$$F(y) \neq 0. \tag{2.11}$$

Proof. For simplicity, set J = J(y) = F'(y). By the feasibility assumption for (1.1), we conclude that $0 = \min_{y} f(y)$ and that the basic assumption satisfies

$$F(y) \neq 0 \iff JF(y) \neq 0.$$
 (2.12)

We observe that J is symmetric positive semidefinite follows from the definitions; see (2.16) below. Let $J = UDU^T$ denote the orthogonal spectral decomposition. The simplified regularization of LM type uses $(J + \lambda I)\Delta y = -F$. Therefore,

$$\Delta y = -(J + \lambda I)^{-1} F = -U (D + \lambda I)^{-1} U^T F.$$

Therefore, the directional derivative of f at y in the direction of Δy is

$$\begin{aligned} \Delta y^T \nabla f(y) &= -\left(U \, (D + \lambda I)^{-1} \, U^T F \right)^T \, (U D U^T F) \\ &= -(U^T F)^T \, (D + \lambda I)^{-1} \, D(U^T F) \\ &= -(U^T F)^T D^{1/2} \, (D + \lambda I)^{-1} \, D^{1/2} (U^T F) \\ &< 0 \quad \Longleftrightarrow \quad (D^{1/2} U^T) F \neq 0. \end{aligned}$$

By (2.12), the latter is not zero if, and only if, (2.11) holds. This completes the proof.

2.1.2 Well Conditioned Generalized Jacobian

Recall the optimality conditions derived following (2.6). If we denote the orthogonal projection operator onto the nonnegative orthant by $\mathcal{P}_+ w = w_+$, then

$$Aw_{+} = A(\mathcal{P}_{+}w) = (A\mathcal{P}_{+})w_{+} = (A\mathcal{P}_{+})(\mathcal{P}_{+}w) = \sum_{w_{i}>0} w_{i}A_{i}.$$

Here A_i is the *i*-th column of A. Thus, we see that at points where the projection is differentiable, the columns of A that are chosen correspond to the positive variables of w. We note that

$$v + A^T y > 0 \implies F'(\Delta y) = AIA^T \Delta y = AA^T \Delta y.$$

Define the three index sets, \mathcal{I}_+ , \mathcal{I}_0 , \mathcal{I}_- , respectively, by

$$\mathcal{I}_{+,0,-} := \mathcal{I}_{+,0,-}(y) = \{i : (v + A^T y)_i > 0, = 0, < 0\}.$$

Then, for sufficiently small Δy we can ignore \mathcal{I}_{-} to get

$$\begin{aligned} F(y + \Delta y) - F(y) &= A(v + A^T(y + \Delta y))_+ - A(v + A^Ty)_+ \\ &= \sum_{i \in \mathcal{I}_+(y + \Delta y)} (v + A^T(y + \Delta y))_i A_i - \sum_{i \in \mathcal{I}_+(y)} (v + A^Ty)_i A_i \\ &= \sum_{i \in \mathcal{I}_+(y)} (A^T \Delta y)_i A_i + \sum_{i \in \mathcal{I}_+(y + \Delta y) \cap \mathcal{I}_0(y)} (v + A^T(y + \Delta y))_i A_i \\ &= \sum_{i \in \mathcal{I}_+(y)} A_i A_i^T \Delta y + \sum_{i \in \mathcal{I}_+(y + \Delta y) \cap \mathcal{I}_0(y)} (v + A^T(y + \Delta y))_i A_i \\ &= \sum_{i \in \mathcal{I}_+(y)} A_i A_i^T \Delta y + \sum_{i \in \mathcal{I}_+(y + \Delta y) \cap \mathcal{I}_0(y)} (A^T \Delta y)_i A_i \\ &= \sum_{i \in \mathcal{I}_+(y)} A_i A_i^T \Delta y + \sum_{i \in \mathcal{I}_+(y + \Delta y) \cap \mathcal{I}_0(y)} A_i A_i^T \Delta y. \end{aligned}$$

We note that the first summation is over the fixed index set $\mathcal{I}_+(y)$, while the second is dependent on $(A^T \Delta y)_i > 0$. Suppose that $A_{\mathcal{I}_0}^T \Delta y = e_i$ is consistent for each $i \in \mathcal{I}_0$. Then we can add or not add the corresponding column to the generalized Jacobian. This means we only need a maximum linearly independent subset of the columns $A_{\mathcal{I}_0}$. Let $\overline{\mathcal{I}}_0 \subseteq \mathcal{I}_0$ be a maximum linearly independent subset⁶.

Following [33] with the change using *licols* and $\overline{\mathcal{I}}_0$, we define the following set

$$\mathcal{U}(y) := \left\{ u \in \mathbb{R}^n : u_i \in \left\{ \begin{array}{ll} \{1\}, & \text{if } i \in \mathcal{I}_+ \\ [0,1], & \text{if } i \in \bar{\mathcal{I}}_0 \\ \{0\}, & \text{if } i \in \mathcal{I}_- \cup (\mathcal{I}_0 \setminus \bar{\mathcal{I}}_0) \end{array} \right\}.$$
(2.13)

Then the generalized Jacobian of the nonlinear system at $y \in \mathbb{R}^m$ is given by the set

$$\partial F(y) = \{ A \operatorname{Diag}(u) A^T : u \in \mathcal{U}(y) \}.$$
(2.14)

Let $y_0 \in \mathbb{R}^m$. Here Diag is the diagonal matrix formed from u. The nonsmooth Newton method for solving F(y) = 0 consists of the following iterative process.

$$y^{k+1} = y^k - V_k^{-1} F(y^k), \, V_k \in \partial F(y^k).$$
(2.15)

Here V_k is a generalized Jacobian (matrix) taken from the generalized Jacobian $\partial F(y^k)$.

We note that, defining M = Diag(u) with $u \in \mathcal{U}(y)$, we have

$$AMA^{T} = \sum_{i \in \mathcal{I}_{+} \cup \bar{\mathcal{I}}_{0}} u_{i}A_{i}A_{i}^{T}, \quad u_{i} = 1, i \in \mathcal{I}_{+}, \, u_{i} \in [0, 1], i \in \bar{\mathcal{I}}_{0}.^{7}$$
(2.16)

Note that for an index set \mathcal{T} , $A_{\mathcal{T}}$ denotes the submatrix of A formed using the columns indexed by \mathcal{T} .

Remark 2.6. Since we have freedom in choosing the values $u_i \in [0, 1], i \in \overline{I}_0$, we follow the optimal diagonal scaling in [21, Prop. 2.1(v)], [34, Thm. 5.2] to minimize a condition number, and choose the generalized Jacobian by setting

$$u_i = \min\{1, 1/||A_i||^2\}, \, \forall i \in \bar{\mathcal{I}}_0.$$

 $^{^{6}}$ We use the variant of the QR decomposition *licols* to extract a *nice* subset of linearly independent columns.

⁷Note that for positive diagonal M, and rectangular B, the ranks of $B, BM, (BM)(BM)^T$ are all the same.

This means that the generalized Jacobian matrix we choose is nonsingular if, and only if, $A_{\mathcal{I}_+\cup\mathcal{I}_0}$ is full rank m. Moreover, for large problems we expect $||A_i|| > 1$ and therefore $u_i < 1$. This goes against the intuitive choice of making u_i as large as possible, i.e., = 1. Note that all elements of $\partial F(y)$ are invertible if, and only if, $A_{\mathcal{I}_+}$ is invertible; while there exists an invertible element if, and only if, $A_{\mathcal{I}_+\cup\mathcal{I}_0}$ is full rank m.

2.1.3 Vertices and Polar Cones

In our numerical tests we can decide on the characteristics of the optimal solution using the properties of (degenerate) vertices.

Lemma 2.7 (vertex and polar cone). Suppose that $x(y) = (v + A^T y)_+ \in P$, where $y \in \mathbb{R}^m$. Then the following are equivalent:

- (i) x(y) is a vertex of P;
- (ii) $A_{\mathcal{I}_+(y)}$ is full column rank;
- (iii) $\begin{bmatrix} A_{\mathcal{I}_{+}} & A_{\mathcal{I}_{0}\cup\mathcal{I}_{-}} \\ 0 & I_{\mathcal{I}_{0}\cup\mathcal{I}_{-}} \end{bmatrix}$ is full column rank n.

Moreover:

- (a) the corresponding generalized Jacobian in (2.16), Remark 2.6, is nonsingular if x(y) is a nondegenerate vertex;
- (b) the (nonnegative) polar cone of the feasible set P at x = x(y) is

$$(P-x)^{+} = \{ w : w = A^{T}u + z, \, u \in \mathbb{R}^{m}, \, z \in \mathbb{R}^{n}_{+}, \, x^{T}z = 0 \}.$$

$$(2.17)$$

Proof. Without loss of generality we can permute the columns of A and corresponding components of x and have $A = \begin{bmatrix} A_{\mathcal{I}_+} & A_{\mathcal{I}_0} & A_{\mathcal{I}_-} \end{bmatrix}$. We know that x(y) is a vertex (equivalently an extreme point, a basic feasible solution) if, and only if $A_{\mathcal{I}_+}$ can be completed to a basis matrix if, and only if, the active set is full rank n. The active set of constraints is

$$\begin{bmatrix} A_{\mathcal{I}_{+}} & A_{\mathcal{I}_{0}\cup\mathcal{I}_{-}} \\ 0 & I_{\mathcal{I}_{0}\cup\mathcal{I}_{-}} \end{bmatrix} x = \begin{pmatrix} b \\ 0 \end{pmatrix}.$$
(2.18)

This has the unique solution x(y) if, and only if, $A_{\mathcal{I}_+}$ is full column rank. This shows the three equivalences items (i) to (iii), as well as the nonsingularity of the generalized Jacobian that we choose as claimed in item (a).

From the optimality conditions we have that the gradient of the objective satisfies

$$x - v = A^T y + \sum_{j \in \mathcal{I}_0 \cup \mathcal{I}_-} z_j e_j,$$

where e_j is the *j*-th unit vector. And we know that x - v is in the polar cone at x if, and only if, x is optimal. Therefore, this yields the description of the polar cone at x as claimed in item (b).

Remark 2.8 (degeneracy of optimal solutions). Let x be a boundary point of P. Then the polar cone of P at x is given in (2.17). Moreover, x is the optimal solution of (2.1) if, and only if, $x - v \in (P - x)^+$, i.e., we can choose v with

$$v = x - A^T u - z, \ z \ge 0, \ z^T x = 0.$$

In fact, we can choose z so that x + z > 0 and have no degeneracy or choose z = 0 and have high degeneracy. For these choices we still get x optimal. As mentioned above, it is shown in [24] that

 $x^*(v)$ is differentiable at $\bar{v} \iff (x^*(\bar{v}) - \bar{v}) \in \operatorname{relint}(P - x^*(\bar{v}))^+$,

where relint refers to the relative interior. This justifies our use of the Levenberg-Marquardt regularization.

The pseudocodes for solving (2.1) using the exact and inexact nonsmooth Newton methods are presented below in Appendix A in Algorithms A.1 and A.2, respectively.

3 Cyclic HLWB Projection for Best Approximation

A notable aspect of this work is the computational comparison of our semismooth algorithm with the method of Halpern-Lions-Wittmann-Bauschke, (HLWB). The convergence analysis of the method has its roots in the field of fixed point theory. For the readers' convenience we provide a brief description and some relevant references.

Problem 3.1 (The best approximation problem for linear inequalities). Given an $m \times n$ matrix A and a vector $b \in \mathbb{R}^m$ such that

$$Q := \{ x \in \mathbb{R}^n : Ax \le b \} \ne \emptyset, \tag{3.1}$$

and a point $v \in \mathbb{R}^n$, $v \notin Q$, called the anchor point, find the orthogonal projection of v onto Q, denoted by $P_Q(v)$.

The set Q is the intersection of m half-spaces. Denote the *i*-th half-space of (3.1) by

$$H_i := \{ x \in R^n : x^T a^i \le b_i \}, \tag{3.2}$$

where a^i is the *i*-th row of A and b_i is the *i*-th component of b. The orthogonal projection of a point $v \in \mathbb{R}^n$ onto H_i , denoted by $P_i(v)$, is

$$P_i(v) = v + \min\left\{0, \frac{b_i - x^T a^i}{\|a^i\|^2}\right\} a^i.$$
(3.3)

The HLWB algorithm for this problem is a *projection method* that employs projections onto the individual half-spaces of (3.2) and makes use of a sequence of, so called, steering parameters.

Definition 3.2 (steering sequence). A real sequence $(\sigma_k)_{k=0}^{\infty}$ is called a steering sequence if it has the following properties:

$$\sigma_{k} \in [0,1] \text{ for all } k \ge 0, \text{ and } \lim_{k \to \infty} \sigma_{k} = 0,$$

$$\sum_{k=0}^{\infty} \sigma_{k} = \infty, \qquad (or \ equivalently, \ \prod_{k=0}^{\infty} (1 - \sigma_{k}) = 0), \qquad (3.4)$$

$$\sum_{k=0}^{\infty} |\sigma_{k+1} - \sigma_{k}| < \infty.$$

Observe that although $\sigma_k \in [0, 1]$, the definition rules out the option of choosing all σ_k equal to zero or all equal to one because of contradictions with the other properties. The third property in (3.4) was introduced by Wittmann, see, e.g., the review paper of López, Martin-Márquez and Xu [40].

Algorithm 3.1 cyclic HLWB algorithm for linear inequalities Initialization: Choose an arbitrary initialization point $x_0 \in \mathbb{R}^n$ Iterative Step: Given the current iterate x_k , calculate the next iterate x_{k+1} by

$$x_{k+1} = \sigma_k v + (1 - \sigma_k) P_{i_k}(x_k), \tag{3.5}$$

where v is the given anchor point, $i_k = k \mod m+1$ and $(\sigma_k)_{k=0}^{\infty}$ is a steering sequence.

The HLWB algorithm has a much broader formulation that applies to the BAP with respect to the common fixed points set of a family of firmly nonexpansive (FNE) operators presented in Bauschke [4]; see also Bauschke and Combettes [6, Chap. 30]. For more on the BAP, see, e.g., Deutsch's book [22]. The family of iterative projection methods for the BAP includes, in addition to the HLWB method, also Dykstra's algorithm [12], [6, Theorem 30.7], Haugazeau's algorithm [29], [6, Corollary 30.15], and Hildreth's algorithm [31,36]. There are also simultaneous versions of some of these algorithms available, see, e.g., [13]. A string-averaging HLWB algorithm, which encompasses the sequential, the simultaneous and other variants of the HLWB algorithm, recently appeared in [14].

More on applications of BAP and the HLWB algorithm are given in Appendix C.

4 Applications

We consider several applications of the best approximation problem, (2.1). Of special interest is the following approach to solving a linear program, (LP).

4.1 Solving Linear Programs

We consider a maximization primal LP in standard equality form

(PLP)
$$p_{LP}^* := \max_{s.t.} c^T x$$
$$x \in \mathbb{R}^m_+.$$
(4.1)

The dual LP is

(DLP)
$$d_{LP}^* := \min_{s.t.} b^T y$$
$$s.t. \quad A^T y - z = c \in \mathbb{R}^n$$
$$z \in \mathbb{R}^n_+.$$
(4.2)

We assume that A is full row rank and that the optimal value is finite. Note that the fundamental theorem of linear programming now guarantees that strong duality holds for both the primal and dual problems, i.e., equality $p_{LP}^* = d_{LP}^*$ holds and both optimal values are *attained*.

We now see in Lemma 4.1 that the solution to (PLP) is the limit of the sequence of projections of the vectors $v_R = Rc \in \mathbb{R}^n$ onto the feasible set as⁸ $R \uparrow \infty$.

Lemma 4.1 ([41–43,53]). Let the given LP data be A, b, c with finite optimal value p_{LP}^* . For each R > 0 define

$$\begin{aligned}
x^*(R) &:= \operatorname{argmin}_x \quad \frac{1}{2} \|x - Rc\|^2 \\
s.t. \quad Ax &= b \in \mathbb{R}^m \\
x \in \mathbb{R}^n_+.
\end{aligned} \tag{4.3}$$

Then x^* is the minimum norm solution of (PLP) if, and only if, there exists $\overline{R} > 0$ such that

$$R \ge \bar{R} \implies x^* = x^*(R) = \operatorname{argmin}\left\{\frac{1}{2} \|x - Rc\|^2 : Ax = b, x \in \mathbb{R}^n_+\right\}.$$
(4.4)

Remark 4.2. Note that the objective function in (4.3) when expanded is equivalent to $R(-c^T x + \frac{1}{2R} ||x||^2) + (\frac{1}{2} ||Rc||^2)$, i.e., this is equivalent to minimizing $-c^T x + \frac{1}{2R} ||x||^2$, an exact regularization of the original LP (4.1), e.g., [26, 51]. In fact, using a Lagrange multiplier argument, we observe that this is equivalent to adding a trust region constraint $||x||^2 \leq \delta$ to the LP. The trust region radius δ is inversely proportional to the regularization parameter $\frac{1}{2R}$ and so directly proportional to R, for $R \leq \overline{R}$, where \overline{R} is given in Lemma 4.1. We note that if δ is too small, we would have an infeasible problem. Equivalently, if R is too small, then the BAP solution $x^*(R)$ is not near the optimal solution x^* of the LP.

In our application, we ignore the regularization property but exploit the fact that we can solve the BAP efficiently for each R.

We would like an R that is not too large but large enough so that $Rc > ||x^*||$. We use the following estimate to start our algorithm:

$$R = \min\left\{50, \frac{\sqrt{mn} \|b\|}{1 + \|c\|}\right\}.$$
(4.5)

To avoid numerical complications from large numbers, we consider the following equivalent problem that uses the scaling $\frac{1}{B}b$ rather than Rc.

Corollary 4.3. Let $A, b, c, R, x^*(R)$ be defined as in Lemma 4.1. Then

$$\frac{1}{R}x^*(R) = w^*(R) := \operatorname{argmin}_w \quad \frac{1}{2} \|w - c\|^2 \\
s.t. \quad Aw = \frac{1}{R}b \in \mathbb{R}^m \\
w \in \mathbb{R}^n_+.$$
(4.6)

Proof. From

$$||x - Rc||^{2} = R^{2} \left\| \frac{1}{R}x - c \right\|^{2} = R^{2} ||w - c||^{2}, x = Rw$$

⁸Note that our algorithm identifies infeasibility, but we do not consider that aspect in this paper.

we substitute for x in (4.3) and obtain: $A(Rw) = b \iff Aw = \frac{1}{R}b$. The result follows from the observation that argmin does not change after discarding the constant R^2 .

4.1.1 Warm Start; Stepping Stone External Path Following

We consider the scaling in Corollary 4.3 and recall the relation between the scaling for c with variable x:

$$x(R) = Rw(R).$$

(To simplify notation, we ignore the optimality symbol $(\cdot)^*$.) The optimality conditions from Theorem 4.6 for w = w(R) in Corollary 4.3 are:

$$\begin{pmatrix} w - c - A^T y - z \\ A w - \frac{1}{R} b \\ z^T w \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \quad w, z \in \mathbb{R}^n_+, y \in \mathbb{R}^m.$$
(4.7)

We conclude that

 $\lim_{R \to \infty} \operatorname{Proj}_{\operatorname{range}(A^T)} w(R) = 0, \lim_{R \to \infty} Rw(R) = x^*, \text{ the optimum of the LP.}$

The optimality conditions are now

$$w = c + A^T y + z, \ b = ARw = AR(c + A^T y)_+, \quad w^T z = 0, \ w, z \ge 0.$$
 (4.8)

This means that ||w|| is an estimate for the error in dual feasibility, i.e., an estimate for the accuracy of Rw as the optimum of the original LP.

Given the current R and the approximate optimal triplet (w(R), y(R), z(R)), we would like to find a good new $R_n \ge R$ and a corresponding y_n to send to the projection algorithm for a warm start process. We use sensitivity analysis for the best approximation problem.

Theorem 4.4. Suppose R > 0 is given and the triplet (w, y, z) = (w(R), y(R), z(R)) is primal-dual optimal for (4.6); i.e., satisfies (4.7). Let

$$\mathcal{N} = \mathcal{N}(z) = \{i : z_i > 0\}, \ \mathcal{B} = \mathcal{B}(w) = \{i : w_i > 0\}, \ \mathcal{Z} = \mathcal{Z}(w, z) = \{i : w_i = z_i = 0\}; \\ e = \begin{pmatrix} b_{\mathcal{B}} - Rw_{\mathcal{B}} \\ -(b_{\mathcal{N}} + Rz_{\mathcal{N}}) \end{pmatrix}, \quad f = \begin{pmatrix} Rb_{\mathcal{B}} \\ -Rb_{\mathcal{N}} \end{pmatrix},$$
(4.9)

where $b_{\mathcal{B}}, b_{\mathcal{N}}$ are defined in (4.13) and (4.16), respectively. Then the maximum value for increasing R and maintaining both optimality and the indices in the bases sets $\mathcal{B}, \mathcal{N}, \mathcal{Z}$ is

$$R_n = \min\{f_i/e_i : e_i > 0, f_i > 0, \forall i\}.$$
(4.10)

The corresponding changes $\Delta w, \Delta y, \Delta z$ that result in $w + \Delta w, y + \Delta y, z + \Delta z$ still optimal for R_n are given in the proof in (4.13), (4.12), (4.16), respectively.

Moreover, if $R_n = \infty$, then the optimal solution of the **LP** has been found.

Proof. We first want to find the maximum increase in R that keeps the current basis \mathcal{B} optimal for (4.6), i.e., we maintain

$$z_i \ge 0, \forall i \in \mathcal{N}, w_i \ge 0, \forall i \in \mathcal{B}, w_i = z_i = 0, \forall i \in \mathcal{Z}.$$

To maintain the feasibility from the three basis sets in (4.9), we have

$$A_{\mathcal{B}}(w_{\mathcal{B}} + \Delta w_{\mathcal{B}}) = \frac{1}{R_n}b \implies A_{\mathcal{B}}\Delta w_{\mathcal{B}} = \left(\frac{1}{R_n} - \frac{1}{R}\right)b$$

$$w_{\mathcal{B}} + \Delta w_{\mathcal{B}} - c_{\mathcal{B}} - A_{\mathcal{B}}^T(y + \Delta y) = 0 \implies \Delta w_{\mathcal{B}} = A_{\mathcal{B}}^T(\Delta y) \implies A_{\mathcal{B}}\Delta w_{\mathcal{B}} = A_{\mathcal{B}}A_{\mathcal{B}}^T(\Delta y) = \left(\frac{R-R_n}{RR_n}\right)b$$

$$-c_{\mathcal{Z}} - A_{\mathcal{Z}}^T(y + \Delta y) = 0 \implies A_{\mathcal{Z}}^T(\Delta y) = 0$$

$$-c_{\mathcal{N}} - A_{\mathcal{N}}^T(y + \Delta y) - (z_{\mathcal{N}} + \Delta z_{\mathcal{N}}) = 0 \implies \Delta z_{\mathcal{N}} = -A_{\mathcal{N}}^T(\Delta y).$$

$$(4.11)$$

We have two equations to solve for Δy . When strict complementarity fails, we choose a full column rank matrix $V_{\mathcal{Z}}$ that satisfies range $(V_{\mathcal{Z}}) = \operatorname{null}(A_{\mathcal{Z}}^T)$; otherwise $V_{\mathcal{Z}} = I$. Then we solve to get

$$\Delta y_p := V_{\mathcal{Z}} \left(A_{\mathcal{B}} A_{\mathcal{B}}^T V_{\mathcal{Z}} \right)^{\dagger} b, \ \Delta y := \left(\frac{R - R_n}{RR_n} \right) \Delta y_p.^9 \tag{4.12}$$

Note that a solution exists since $b \in \operatorname{range}(A_{\mathcal{B}})^{10}$ We now have

$$-w_{\mathcal{B}} \leq \Delta w_{\mathcal{B}} = A_{\mathcal{B}}^{T} \left(\frac{R - R_{n}}{RR_{n}}\right) \Delta y_{p} = -\left(\frac{R_{n} - R}{RR_{n}}\right) A_{\mathcal{B}}^{T} \Delta y_{p} = :-\left(\frac{R_{n} - R}{RR_{n}}\right) b_{\mathcal{B}}.$$
 (4.13)

We get that

$$(R_n - R)b_{\mathcal{B}} \le (RR_n)w_{\mathcal{B}} \iff R_n(b_{\mathcal{B}} - Rw_{\mathcal{B}}) \le Rb_{\mathcal{B}}.$$
(4.14)

To find the maximum R_n and check that it is not $R_n = \infty$, we use an **LP** type ratio test. We set the two vectors to be

$$e_{\mathcal{B}} = (b_{\mathcal{B}} - Rw_{\mathcal{B}}), f_{\mathcal{B}} = Rb_{\mathcal{B}}.$$

Note that the inequalities in (4.14) hold trivially for $R_n = R$. For simplicity of notation, we ignore the subscript \mathcal{B} and use e, f. Therefore, we cannot have both $e_i > 0, f_i \leq 0$. We choose R_n to be the maximum that satisfies the ratio test, i.e., we get:

$$R_n = \min_{i} \{ f_i / e_i : f_i > 0, e_i > 0, i \in \mathcal{B} \},$$
(4.15)

where the minimum over the empty set is by definition $+\infty$. Note that $\max_i \{f_i/e_i : f_i < 0, e_i < 0, i \in \mathcal{B}\} \leq R_n$ always holds since $R_n = R > 0$ satisfies the inequality. Moreover, the result simplifies in the nondegenerate case as we have

$$A_{\mathcal{B}}^{T}\left(\frac{R-R_{n}}{RR_{n}}\right)\Delta y_{p} = -\left(\frac{R_{n}-R}{RR_{n}}\right)A_{\mathcal{B}}^{\dagger}b = -\left(\frac{R_{n}-R}{RR_{n}}\right)b_{\mathcal{B}}, \quad b_{\mathcal{B}} = A_{\mathcal{B}}^{\dagger}b.$$

⁹Note that in applications we can include indices from \mathcal{Z} in \mathcal{B} . This allows for a greater choice for $\Delta y, \Delta w_B$.

¹⁰In the nondegenerate case we get a simplification since $A_{\mathcal{B}}^T \left(A_{\mathcal{B}} A_{\mathcal{B}}^T \right)^{\dagger} = A_{\mathcal{B}}^{\dagger}$.

We can then set $R_n = \infty$ if $A_{\mathcal{B}}$ is full column rank or $b_{\mathcal{B}} = w_{\mathcal{B}}$, i.e., we have the (best) least squares solution.

Similarly we now need a ratio test for z_N to maintain dual feasibility and nonnegativity. Note that we set $\Delta z_i = \Delta w_i = 0, \forall i \in \mathbb{Z}$. We have

$$-z_{\mathcal{N}} \leq \Delta z_{\mathcal{N}} = -A_{\mathcal{N}}^{T} \left(\frac{R-R_{n}}{RR_{n}}\right) \Delta y_{p} = \left(\frac{R_{n}-R}{RR_{n}}\right) A_{\mathcal{N}}^{T} \Delta y_{p} =: \left(\frac{R_{n}-R}{RR_{n}}\right) b_{\mathcal{N}}.$$
 (4.16)

We get that

$$(R_n - R)b_{\mathcal{N}} \ge -(RR_n)z_{\mathcal{N}} \iff R_n(-b_{\mathcal{N}} - Rz_{\mathcal{N}}) \le -Rb_{\mathcal{N}}$$

We again find the maximum R_n and check that we do not have $R_n = \infty$ using an LP type ratio test. We set the two vectors to be $e_{\mathcal{N}} = -(b_{\mathcal{N}} + Rz_{\mathcal{N}})$, $f_{\mathcal{N}} = -Rb_{\mathcal{N}}$. Recall that the inequality holds trivially for $R_n = R$. Again, for simplicity of notation, we ignore the subscript \mathcal{N} and use e, f. Therefore, we cannot have $e_i > 0, f_i \leq 0$. We choose R_n to be the maximum that satisfies:

$$\max\{f_i/e_i, \text{ if } f_i < 0, e_i < 0, i \in \mathcal{N}\} \le R_n = \min\{f_i/e_i, \text{ if } f_i > 0, e_i > 0, i \in \mathcal{N}\}.$$

We choose R_n as the minimum of the above two values found.

Finally, if $R_n = \infty$, then the bases do not change as R increases to infinity, i.e., the optimal bases have been found.

The above Theorem 4.4 illustrates the external path following algorithm that we are using. The theorem finds specific values of R, stepping stones on the path, where the current choice of columns of A changes. Once we find that the next stepping stone is at infinity, we know that we have found the optimal choice of columns of A. Thus, we have an external path following algorithm with parameter R but we only choose specific points on this path to step on. The algorithm is particularly efficient for nondegenerate problems, $\mathcal{Z} = \emptyset$, where the sensitivity analysis is accurate. For highly degenerate problems, restricting $\Delta w_i = \Delta z_i = 0, \forall i \in \mathcal{Z}$, can severely restrict increasing R, see Section 5.3 below.

4.1.2 Upper and Lower Bounds for the LP Problem

The optimal solution from the projection problems (4.3) and (4.6) provides a feasible x, and we get the corresponding LP lower bound $c^T x^*(R)$. The upper bound is not as easy and more important in stopping the algorithm.

Note that in Section 4.1.1 primal feasibility and complementary slackness hold for x(R) = Rwand z, and this is identical for the LP problem. Therefore, we need to find y_{LP} to satisfy the LP dual feasibility

$$z_{\mathsf{LP}} = A^T y_{\mathsf{LP}} - c \ge 0.$$

But, from the projection problem optimality conditions we have

$$A^{T}(-y) = z + c - w, \ 0 \le z = A^{T}(-y) - c + w, \ w \ge 0.$$

As seen above, this means that in the limit, w is small and we do get dual feasibility $y(R) \to y_{LP}$. But at each iteration we actually have

$$z - w = A^T(-y) - c, \ z, w \ge 0, z^T w = 0, \quad y \cong y_R.$$
 (4.17)

We can write the required dual feasibility equations using the indices for $w_i > 0$.

$$A_i^T y - c_i \in \begin{cases} \{0\}, & \text{if } w_i > 0, \\ \mathbb{R}_+, & \text{if } w_i = 0. \end{cases}$$

Recall the definitions of \mathcal{N}, \mathcal{B} in (4.9). Then for a given y_R from the optimality conditions from the projection problem (4.17), we consider the nearest dual LP feasible system with unknowns $z \geq 0, y_{LP}$. Note that we are using the projection with free variables, Section 4.2.

Lemma 4.5. Let w, y, z be approximate optimal solutions from (4.8) and \mathcal{B} the support defined in (4.9). Consider the following BAP for the given dual variables.

$$\begin{pmatrix} y_{\mathsf{LP}}^{*} \\ z_{\mathsf{LP}}^{*} \end{pmatrix} \in \operatorname{argmin} \quad \frac{1}{2} \| (-y) - y_{\mathsf{LP}} \|^{2} + \frac{1}{2} \| 0 - (z_{\mathsf{LP}})_{\mathcal{B}} \|^{2} + \frac{1}{2} \| z_{\mathcal{N}} - (z_{\mathsf{LP}})_{\mathcal{N}} \|^{2}$$

$$s.t. \quad \begin{bmatrix} A_{\mathcal{B}}^{T} & -I & 0 \\ A_{\mathcal{N}}^{T} & 0 & -I \end{bmatrix} \begin{pmatrix} y_{\mathsf{LP}} \\ (z_{\mathsf{LP}})_{\mathcal{B}} \\ (z_{\mathsf{LP}})_{\mathcal{N}} \end{pmatrix} = \begin{pmatrix} c_{\mathcal{B}} \\ c_{\mathcal{N}} \end{pmatrix}$$

$$y_{\mathsf{LP}} \ free, \ z_{\mathsf{LP}} = \begin{pmatrix} (z_{\mathsf{LP}})_{\mathcal{B}} \\ (z_{\mathsf{LP}})_{\mathcal{N}} \end{pmatrix} \ge 0.$$

$$(4.18)$$

Then the optimal value of the LP (4.1) satisfies the upper bound

$$p_{\mathsf{LP}}^* \leq b^T y_{\mathsf{LP}}^*.$$

Moreover, suppose that $z_{\mathcal{B}} = 0$. Then equality holds and the **LP** is solved with primal-dual optimum pair (w, y_{LP}) .

Proof. Recall that the optimal value p_{LP}^* is finite. The proof of the bound follows from weak duality in linear programming. Equality follows from the optimality conditions since primal feasibility and complementary slackness hold with w.

4.2 **Projection and Free Variables**

For many applications, some of the variables are free and not all the variables are in the objective function. We consider these two cases. Note this can arise when the objective is a general least squares problem, e.g., $\min ||Bx - c||^2$ and we add the constraint Bx - w = 0 and substitute the free variable w into the objective function.

4.2.1 Projection with Free Variables

We first consider the problem with some of the variables free:

(P)

$$\begin{aligned}
x(v) &:= \operatorname{argmin}_{x_1, x_2} \quad \frac{1}{2} \|x - v\|^2, \quad x = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}, \, v = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}, \\
s.t. \quad Ax = b \in \mathbb{R}^m \\
x_1 \in \mathbb{R}^{n_1}_+, \, x_2 \in \mathbb{R}^{n_2},
\end{aligned}$$
(4.19)

optimal value: $p_f^*(v) = \frac{1}{2} \|x(v) - v\|^2$,

Theorem 4.6. Consider the generalized simplex best approximation problem with free variables (4.19). Assume that the feasible set is nonempty. Then the optimum x(v) exists and is unique. Moreover, let

$$F_f(y) := A \left(\frac{\left((v + A^T y)_1 \right)_+}{(v + A^T y)_2} \right) - b, \quad f_f(y) = \frac{1}{2} \|F_f(y)\|^2.$$
(4.20)

Then $F_f(y) = 0 \iff y \in \operatorname{argmin} f_f(y)$, and

$$x(v) = \begin{pmatrix} ((v + A^T y)_1)_+ \\ (v + A^T y)_2 \end{pmatrix}, \text{ for any root } F_f(y) = 0.$$
(4.21)

Let $p_f^*(v) = \frac{1}{2} ||x(v) - v||^2$ denote the primal optimal value. Then strong duality holds and the dual problem of (4.19) is the maximization of the dual functional, $\phi_f(y, z_1)$:

Proof. We modify the proof of Theorem 2.1. The Lagrangian, $L_f(x, y, z)$ for (4.19) is

$$L_f(x, y, z) = \frac{1}{2} \|x - v\|^2 + y^T (b - Ax) - z_1^T x_1, \quad \nabla_x L_f(x, y, z) = x - v - A^T y - \begin{pmatrix} z_1 \\ 0 \end{pmatrix}.$$
(4.22)

Solving for a stationary point means

$$0 = \nabla_x L_f(x, y, z) \implies x = v + A^T y + z, \quad z = \begin{pmatrix} z_1 \\ 0 \end{pmatrix}.$$

Therefore, with this definition of z, we still have at a stationary point that

$$\begin{split} L_f(x,y,z) &= \frac{1}{2} \left\| v + A^T y + z - v \right\|^2 + y^T (b - A(v + A^T y + z)) - z^T (v + A^T y + z) \\ &= \frac{1}{2} \left\| A^T y + z \right\|^2 + y^T b - y^T A v - (A^T y)^T (A^T y + z) - z^T v - z^T (A^T y + z) \right\| \\ &= \frac{1}{2} \left\| A^T y + z \right\|^2 + y^T b - y^T A v - (A^T y + z)^T (A^T y + z) - z^T v \\ &= -\frac{1}{2} \left\| z + A^T y \right\|^2 + y^T (b - A v) - z^T v. \end{split}$$

As in Theorem 2.1, the problem (4.19) is a projection onto a nonempty polyhedral set, a closed and convex set. The optimum exists and is unique and strong duality holds, i.e., there is a zero duality gap $p_f^* = d_f^*$, and the dual value is attained. The Lagrangian dual is

$$d^* = \max_{z_1 \in \mathbb{R}^{n_1}_+, y} \min_x \quad L_f(x, y, z) = \frac{1}{2} \|x - v\|^2 + y^T (b - Ax) - z_1^T x_1$$

$$= \max_{z_1 \in \mathbb{R}^{n_1}_+, y, x} \quad \{L_f(x, y, z_1) : \nabla_x L_f(x, y, z_1) = 0\}$$

$$= \max_{z_1 \in \mathbb{R}^{n_1}_+, y, x} \quad \{L_f(x, y, z) : x = v + A^T y + z\}$$

$$= \max_{z_1 \in \mathbb{R}^{n_1}_+, y} \quad -\frac{1}{2} \|z + A^T y\|^2 + y^T (b - Av) - z^T v.$$

Therefore, we derive the *KKT optimality conditions* for the primal dual variables (x, y, z) with $z = \begin{pmatrix} z_1 \\ 0 \end{pmatrix}, x_1 \ge 0, z_1 \ge 0$, as follows $\nabla_x L_f(x, y, z) = x - v - A^T y - z = 0$, (dual feasibility) $\nabla_y L_f(x, y, z) = Ax - b = 0$, (primal feasibility) $\nabla_z L_f(x, y, z) \cong x \in (\mathbb{R}^n_+ - z)^+$. (complementary slackness $z_1^T x_1 = 0$)

The standard KKT optimality conditions for primal-dual variables (x, y, z) can be rewritten as:

$$\begin{pmatrix} x - v - A^T y - z \\ Ax - b \\ z^T x \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \quad x_1, z_1 \in \mathbb{R}^{n_1}_+, y \in \mathbb{R}^m, z = \begin{pmatrix} z_1 \\ 0 \end{pmatrix}.$$

Note $v + A^T y = x - z = x + (-z)$. Therefore this is a Moreau decomposition of $v + A^T y$, with $x^T z = 0, x, z \in \mathbb{R}^n_+, x = (v + A^T y)_+$. Therefore, we get $A(v + A^T y)_+ = b$, where we modify the definition of + so that we project only the first part corresponding to x_1 onto the nonnegative orthant $\mathbb{R}^{n_1}_+$ and then this means $z_1 = -((v + A^T y)_1)_-$.

We see that the optimality conditions

$$A\begin{pmatrix} ((v+A^Ty)_1)_+\\ (v+A^Ty)_2 \end{pmatrix} = b, \ x_1 = ((v+A^Ty)_1)_+, \ x_2 = (v+A^Ty)_2$$

imply that

$$z = -(v + A^T y)_{-}, \ z^T x = 0, x, \ z \in \mathbb{R}^n_+, x - v - A^T y - z = 0,$$

i.e., $F_f(y) = 0$, for some $y \in \mathbb{R}^m$.

For a vertex, a basic feasible solution, we need n active constraints. The equality constraints Ax = b account for m, leaving n - m to choose among $1, 2, \ldots, n_1$, the constrained variables in x_1 . This leaves

 $m_1 = n_1 - (n - m) = m - (n - n_1) = m - n_2 \implies m_1 = m - n_2$, basic variables.

4.3 Triangle Inequalities

We can obtain an efficient projection onto a large set of triangle inequalities that arise as cuts in graph problems, e.g., [46]. We let G = (V, E) denote a graph with vertex set V and edge set E, and define the sets:

$$\mathcal{T} := \{ (u, v, w) : u < v < w \in V \},\$$

and the corresponding *triangle inequalities*, where the weight vector $x = (x_{uv})_{uv \in E}$ here has two indices for the edge uv connecting vertices u, v,

$$(I) \left\{ \begin{array}{l} x_{vw} - x_{uv} - x_{uw} \leq 0 \\ x_{uw} - x_{uv} - x_{vw} \leq 0 \\ x_{uv} - x_{vw} - x_{uw} \leq 0 \\ \forall (u, v, w) \in \mathcal{T} \\ 0 \leq x_{uv} \leq 1, \, \forall (u, v) \in E \end{array} \right\}.$$
(4.23)

We could rewrite this as a standard feasibility-seeking problem or as a best approximation problem, i.e., given an \bar{x} we want to find the nearest point to \bar{x} that is in a subset of triangle inequalities defined by the matrix T, namely with slacks s, t and e the vector of ones,

$$\min \frac{1}{2} \|x - \bar{x}\|^2 \text{ s.t. } Tx + s = 0, x + t = e, \ x, t \ge 0, \ s \ge 0.$$

We generated and solved random problems. The algorithm was very efficient though we do not report the details here.

5 Numerics

In this section we compare the Regularized Nonsmooth Newton Method, (RNNM), (exact and inexact) with the HLWB method [4] described in Section 3, MATLAB's *lsqlin* interior point solver, and the *quadratic programming proximal augmented Lagrangian method*, (QPPAL) [39]. Recall our BAP, (2.1), and the pseudocode for HLWB in Algorithm A.3 in Appendix A. We show in our experiments that RNNM (exact) significantly outperforms the other methods. These experiments are performed with an i7-4930k @ 3.2GHz, 16 GBs of RAM, and MATLAB 2022b software.

Before comparing the differences in performance of the algorithms we are experimenting with, we elaborate on our implementation of the HLWB method, see also Section 3. HLWB projects onto individual convex sets and computes the next iterate, x^{k+1} , by taking a specific convex combination. This combination is determined by a sequence of steering parameters, as defined in Definition 3.2, and the initial point v, commonly referred to as the anchor point in Problem 3.1. Traditionally, each projection is called an *iteration*, and the collection of these iterations is defined as a *sweep* [6]. In the context of problem (2.1), HLWB is iterating onto one of the hyperplanes (sets) defined by the rows of A, denoted a^{i_k} , as well as the nonnegative orthant. We complete a sweep once we project onto all the hyperplanes and onto the nonnegative orthant. (See steps 13-15 of Algorithm A.3.) Thus, we relate one sweep of HLWB with one iteration of RNNM.

5.1 Time Complexity

Since RNNM is a second-order method and HLWB is a first-order method, we now discuss theoretical time complexity differences. From the RNNM algorithm, Algorithm A.1, we can see that worst-case time complexity is $O(m^3 + m^2 n)^{11}$ flops, of which every step but solving the linear system is

¹¹See Algorithm A.1 lines 4-12, the total time complexity respectively is: $m^2n + m^2 + m^3 + n + 2n + mn + 2n + mn + n + m + 1 = m^2n + m^3 + m^2 + 2mn + 5n + m + 1 = O(m^3 + m^2n)$.

efficiently parallelizable. It is worth mentioning that in line 7 of Algorithm A.1, the linear system we are solving is positive definite and sparse. Therefore, it can be solved efficiently using the Cholesky decomposition. From the HLWB algorithm, Algorithm A.3, we can see that worst-case time complexity per iteration is O(mn) and per sweep is $O(m^2n)$, of which every step is efficiently parallelizable.¹²

From the perspective of theoretical time complexity it would be easy to assume that HLWB is the preferable algorithm as each of it's iterations are composed of operations that are completely parallelizable and each first-order sweep has an overall lower time-complexity. However, without performing numerical tests with varying parameters m and n, we cannot yet conclude how a firstorder method compares to a second-order method in terms of desired performance, especially as mand n get extremely large as observed in practice.

5.2 Comparison of Algorithms

When performing our numerical experiments, we refer to the discussion on techniques for comparisons of algorithms given in [8]. In particular, we include performance profiles [23], and tables of the performances for RNNM (exact and inexact), HLWB, *lsqlin*, and for QPPAL.

We compare the HLWB algorithm to RNNM by generating a test problem with the form specified in (2.1). In this test problem, the anchor v lies in the relative interior of the normal cone (negative of the polar cone) of a vertex of the feasible polyhedron. Therefore, the vertex is the closest point to v. Additionally, to ensure meaningful comparisons, we set ||A|| = 1 and ||v|| = 1 as no convergence results for RNNM solving (2.1) have been proven, as far as we know.

The RNNM algorithm starts with initializing $x_0 \leftarrow (v + A^T y_0)_+$, where either $y_0 = 0_m$ or we are given a y_0 for a warm start (as discussed in our LP application). Then, $x_0 \leftarrow (v + A^T y_0)_+$ reduces to $x_0 \leftarrow \max(v, 0)$ in the initialization stage of RNNM. Therefore, to ensure all algorithms start at the same point, we initialize $x_0 \leftarrow \max(v, 0)$ for HLWB, and provide $x_0 \leftarrow \max(v, 0)$ as a warm start for MATLAB's *lsqlin* solver. Since QPPAL performs an ADMM warm-start, there is no way to provide a warm start point for it.

Since RNNM solves a reduced KKT condition for a convex problem, the term $\frac{||F(y_k)||}{1+||b||}$ is a sufficient relative residual to serve as a stopping condition for RNNM. Since HLWB is a first order method, its stopping criterion is measured at the end of a sweep, rather than at the end of an iteration. Furthermore, HLWB does not have any proper stopping criterion, but converges in the limit. Therefore, we use the relative primal feasibility residual, i.e., $\frac{||A\hat{x}_k - b||}{1+||b||}$, as the stopping criterion. Note that we use y_k instead of x_k in the stopping criterion as \hat{x}_k is nonnegative at the end of every sweep. The *lsqlin* solver uses first-order optimality conditions. As in *lsqlin*, QPPAL uses first-order optimality conditions, and we report the relative optimality gap, $|p^* - d^*|/(1 + (|p^*| + |d^*|)/2)$ for the relative residual of QPPAL. Before discussing the generation of the problems, it is worth noting that we are choosing to use QPPAL's Cholesky decomposition direct solver instead of its inexact solver. In addition, we increase the maximum number of iterations for the two phases of QPPAL to match the maximum number of sweeps the other methods utilize. Furthermore, we inform QPPAL that the quadratic has Q = I, the identity.

¹²See Algorithm A.3 lines 5-12; the total time complexity respectively per iteration that projects onto a half space is (2n+2)+1+(n+2)+(mn+m+1) = mn+3n+m+6 = O(mn) flops. Similarly, the total time complexity respectively per iteration that projects onto the nonnegative orthant is: n+1+(n+2)+(mn+m+1) = mn+2n+m+4 = O(mn) flops of which all flops are efficiently parallelizable. Therefore, in terms of sweeps the HLWB method computes $m(mn+3n+m+6) + mn+2n+m+4 = m^2n+4mn+m^2+2n+7m+4 = O(m^2n)$ flops.

In Section 5.2.1, we generate problems such that v lies in the relative interior of the normal cone of a nondegenerate vertex. We also experiment with degenerate vertices, but observe very similar results. These tests, and the performance of the RNNM algorithm help to motivate the theory and potential practice of using RNNM for LP applications, as seen in Section 5.3.

For the performance profiles in Section 5.2.1, we use the following notation from [8]. Let P denote our set of problems with varying m, n, and density. Similarly, let S represent our set of solvers, RNNM (exact and inexact), HLWB, *lsqlin*, and QPPAL. We define the performance measure $t_{p,s} > 0$ for each pair $(p, s) \in P \times S$ as the computational time of solver s to solve problem p. For each problem $p \in P$ and solver $s \in S$, we define the performance ratio as

$$r_{p,s} = \begin{cases} \frac{t_{p,s}}{\min\{t_{p,s} : s \in S\}}, & \text{if convergence test passed,} \\ \infty, & \text{if convergence test failed.} \end{cases}$$

The solver s that performs the best on problem p will have a performance ratio of 1. Solvers that perform worse than s on problem p will satisfy $t_{p,s} > 1$. In other words, the larger the performance ratio, the worse the solver performed on problem p.

The performance profile of a solver s is defined as

$$\rho_s(\tau) = \frac{1}{|P|} \operatorname{size} \{ p \in P : r_{p,s} \le \tau \}$$

Therefore, $\rho_s(\tau)$ represents the relative portion of time in which the performance ratio $r_{p,s}$ for solver s is within a factor $\tau \in \mathbb{R}$ of the best possible performance ratio.

5.2.1 Numerical Comparisons

We tested the algorithms with optimal solutions at: nondegenerate vertices, degenerate vertices and non-vertices. They all exhibited similar results. Therefore, we present results restricted to nondegenerate vertices. We begin with choosing v for (2.1) such that the optimum is uniquely a nondegenerate vertex of P. In the tables below we vary m, n, and the problem density to illustrate the changes in each solver's performance. A data point in each table is the arithmetic mean of 5 randomly generated problems of the specified parameters that also satisfy ||A|| = 1, ||v|| = 0.1. For example, the first row of Table 5.1 represents a problem with parameters m = 500, n = 3000, and a density of 0.0081, and each solver will solve 5 randomly generated problems of the form discussed in (2.1), and the average time and relative residual from solving all 5 problems is displayed in the table. The desired stopping tolerance for the tables and performance profiles is $\varepsilon = 10^{-14}$ and maximum iterations (sweeps) is 2000 for all solvers. Lastly, it should be noted that the regularization parameter of RNNM for these experiments is chosen in an adaptive way. It takes into account the relative residual as defined in line 13 of Algorithm A.1, the norm of the Newton direction, and the norm of v. The purpose of this is to decrease the amount of regularization as we approach the optimal solution while accounting for the norms of the Newton direction and v. This regularization parameter is explicitly defined as

$$\lambda_{k+1} = \operatorname{mean}\left(\left(10^{-2}F_k\right)\max(1, \log_{10}(\|d_k\|)), \left(10^{-3}F_k\right)\max(1, \log_{10}(\|v\|)), 10^{-3}F_k\right),$$
(5.1)

where F_k is the relative residual at iteration k, and d_k is the Newton direction.

From Tables 5.1 to 5.3, the empirical evidence demonstrates the superiority of the RNNM (exact) approach over the other solvers. Since the RNNM's reduced KKT system is $m \times m$ and solved using the Cholesky Decomposition, it's performance should be affected most noticeabley as m varies or density increases. This theoretical observation can be seen in Tables 5.1 to 5.3, as the RNNM (exact and inexact) algorithm is slower to converge for increasing m and density,

but is not affected by an increase in n.

From Figure 5.1 the empirical evidence shows similar results to the tables, but better demonstrates the differences in performance between RNNM (exact) and the other solvers. The problems in Figure 5.1a are similar to those of Table 5.1 except *m* varies by 100 from 100 to 2000. Similarly, the problems in Figure 5.1b have *n* varying by 100 from 3000 to 5000, and Figure 5.1c has density varying by 1% from 1% to 100%. In every performance profile, the RNNM (exact) algorithm clearly outperforms the other solvers in our experiments, with RNNM (inexact) performing well for an inexact method on mid-sized problems. Conversely, HLWB is relatively slow on these problems. This can be attributed to its linear convergence rate. Due to it's linear convergence, it will perform a large number of sweeps, which can amount to millions of iterations on certain problems with large *m*. Performance profiles can be found in Appendix B.1 with the stopping tolerances $\varepsilon = 10^{-2}$, 10^{-4} , to illustrate that RNNM (exact) outperforms HLWB and *lsqlin* at different tolerances, but QPPAL remains competitive.

Table 5.1: Varying problem sizes m; comparing computation time and relative residuals.

1	Specific	ations			Time (s)		Rel. Resids.					
m	n	% density	Exact	Inexact	HLWB	lsqlin	QPPAL	Exact	Inexact	HLWB	lsqlin	QPPAL
500	3000	8.1e-01	4.23e-02	1.51e-01	1.54e + 02	3.77e + 00	1.14e + 00	1.96e-16	8.26e-16	2.25e-04	7.26e-17	1.72e-17
1000	3000	8.1e-01	4.40e-01	9.97e-01	3.71e+02	5.37e + 00	2.15e+00	2.70e-16	1.95e-15	2.14e-04	3.87e-17	2.70e-17
1500	3000	8.1e-01	1.17e+00	3.23e+00	6.09e + 02	7.02e+00	4.69e + 00	3.41e-17	6.73e-16	2.27e-04	3.95e-17	1.16e-17
2000	3000	8.1e-01	2.49e+00	7.51e+00	8.67e + 02	1.02e+01	7.81e+00	6.11e-17	3.11e-17	2.24e-04	3.14e-17	-2.74e-17

Table 5.2: Varying problem sizes n; comparing computation time and relative residuals.

	Specific	cations			Time (s)		Rel. Resids.					
m	n	% density	Exact	Inexact	HLWB	lsqlin	QPPAL	Exact	Inexact	HLWB	lsqlin	QPPAL
200	3000	8.1e-01	3.12e-03	3.69e-02	4.45e + 01	3.50e + 00	8.66e-01	8.64e-18	7.39e-17	2.56e-04	6.52e-16	5.89e-17
200	3500	8.1e-01	3.08e-03	4.05e-02	5.17e + 01	4.93e + 00	1.00e+00	9.07e-18	1.26e-17	2.78e-04	1.23e-15	2.15e-17
200	4000	8.1e-01	3.24e-03	3.70e-02	5.82e + 01	7.31e+00	1.09e+00	1.46e-16	8.91e-16	2.80e-04	3.21e-16	-9.18e-18
200	4500	8.1e-01	3.99e-03	4.17e-02	6.58e + 01	1.01e+01	1.18e+00	1.80e-15	2.05e-16	3.13e-04	4.61e-17	1.71e-16

Table 5.3: Varying problem density; comparing computation time and relative residuals.

	Specific	cations			Time (s)		Rel. Resids.					
m	n	% density	Exact	Inexact	HLWB	lsqlin	QPPAL	Exact	Inexact	HLWB	lsqlin	QPPAL
300	1000	25	5.69e-02	2.66e-01	4.55e + 01	3.30e-01	1.20e + 00	2.83e-17	1.14e-17	1.50e-04	8.61e-17	5.99e-17
300	1000	50	5.43e-02	2.28e-01	5.39e + 01	3.08e-01	1.82e + 00	1.23e-16	1.97e-17	1.44e-04	8.08e-16	1.42e-17
300	1000	75	7.75e-02	2.86e-01	5.36e + 01	3.16e-01	1.49e + 01	4.83e-16	1.72e-17	1.62e-04	3.49e-16	-3.43e-16
300	1000	100	7.27e-02	2.47e-01	4.65e + 01	3.00e-01	2.54e + 02	5.66e-16	2.15e-17	1.63e-04	1.91e-15	1.04e-14



Figure 5.1: Performance profiles for problems with varying m, n, and densities for nondegenerate vertex solutions.

5.3 Solving Large Sparse Linear Programs

We now apply (4.3) and Theorem 4.4 to solve large-scale randomly generated LPs, and problems from the NETLIB dataset. We call this method the *stepping stones external path following algorithm*, (SSEPF), and note that we use the estimate for a starting R given in (4.5). The stepping stones are found using R_n in (4.10). We add a small decreasing scalar to R_n to ensure that we change the basis of A at each iteration. For simplicity, we restrict ourselves to nondegenerate LPs for the randomly generated problems.

We compare SSEPF with the MATLAB *linprog* code, using both the dual simplex and the interior-point algorithms. We also compare with Mosek's dual simplex and interior point method, and with the semismooth Newton inexact proximal augmented Lagrangian method, (SNIPAL) [38]. We use randomly generated problems scaled so that ||A|| = 1, and the optimal solution x^* satisfies $||x^*|| = 1$. A data point in Table 5.4 is the arithmetic mean of 5 randomly generated problems of the specified parameters. We exclude instances where a method fails to provide a solution from Table 5.4 for clarity, but these instances are plotted in Figure 5.2 as a failure to converge. Since the smallest stopping tolerance allowed by *linprog* is $\varepsilon = 10^{-10}$, a linear program is considered successfully solved in the performance profile of Figure 5.2 if the optimality gap is less than or equal

to $\varepsilon = 10^{-8}$. The maximum number of iterations for *linprog* and Mosek is the default number, and for SNIPAL it is 2000. The relative residual shown in Table 5.4 is the sum of the relative primal feasibility, dual feasibility, and complementary slackness. In other words, let (x^*, y^*, z^*) be the optimal solution an algorithm returns, then the relative residual as shown in the table is

$$\frac{\|Ax^* - b\|}{1 + \|b\|} + \frac{\|z^* - A^Ty^* + c\|}{1 + \|c\|} + \frac{(x^*)^Tz^*}{1 + \max(\|x^*\|, \|z^*\|)}$$

When discussing the performance of SSEPF, it should be noted that we are using the exact RNNM direction to solve the BAP subproblem, and using (5.1) to compute the regularization parameter. We denote this in Table 5.4 and Figure 5.2 as SSEPF-RNNM. Furthermore, we use the abbreviations Linprog DS and Linprog IPM to refer to *linprog's* dual simplex and interior point method, respectively. Likewise, we use similar abbreviations for Mosek.

From Table 5.4, the empirical evidence demonstrates that the stepping stone approach performs better than MATLAB's dual simplex and interior point method on most problems, and has proven to be quite competitive with Mosek's dual simplex and interior point method. This becomes more evident as

the sizes of the problems grow and the problems become sparser. In other words, we see that our code fully exploits sparsity in LP. This can be seen when observing the performance of SSEPF-RNNM with respect to time on the rows of Table 5.4 where the problem density decreases. Despite the increase in problem dimension, the decrease in density leads to an increase in performance in comparison to the previous row. Another thing to notice is that in rows 5-9 of Table 5.4, *linprog's* interior point method and Mosek's dual simplex method failed to converge to a solution after having reached the default maximum number of iterations.

In Section 5.2.1, the performance profiles were constructed by looking at smaller intervals of varying m, n and density. For example Table 5.1 shows results where m varies by increments of 500, but in Figure 5.1a m varies by increments of 100. Since *linprog*'s interior point method and Mosek's dual simplex method struggled with obtaining the desired primal feasibility, as seen in Table 5.4, Figure 5.2 shows the performance of each solver with respect to all 50 problems instead of examining the average performance.

It is important to note that the performance profile exhibits more failed solutions from the dual simplex and interior point methods of MATLAB. We have tried taking the maximum of the primal feasibility, dual feasibility, and complementary slackness returned by MATLAB's *linprog* function instead of the sum, and both revealed equivalent results. In other words, we are not sure why there are more problems failing at this tolerance than reported by MATLAB, but it further distinguishes our stepping stone approach from MATLAB's *linprog* algorithms. Mosek, and more specifically Mosek's interior point method is very competitive, as Figure 5.2 shows. Unfortunately, SNIPAL failed to converge on every problem in this dataset. We have seen it converge successfully on some random linear programming problems, but none of the ones that we generated in our Numerical Experiments section. It is not noting that the table which shows the average performance of 5 randomly generated problems with respect to a set of parameters indicates that SSEPF-RNNM performs better than Mosek's interior point method in 7 out of 10 rows in the table.

_															
Г	5	Specificat	tions			Time	(s)		Rel. Resids.						
Г	m	n	% density	SSEPF-RNNM	Linprog DS	Linprog IPM	MOSEK DS	MOSEK IPM	SNIPAL	SSEPF-RNNM	Linprog DS	Linprog IPM	MOSEK DS	MOSEK IPM	SNIPAL
Γ	2e + 03	5e+03	1.0e-01	8.94e-02	3.09e-02	4.50e-02	1.46e-01	1.64e-01	6.90e+00	3.38e-17	2.63e-16	4.88e-09	1.31e-16	1.53e-16	2.14e-04
Γ	2e + 03	1e+04	1.0e-01	9.64e-02	4.84e-02	7.53e-02	1.49e-01	1.93e-01	8.31e+00	2.82e-17	6.00e-16	1.60e-04	1.31e-16	2.89e-16	1.72e-04
Γ	2e + 03	1e+05	1.0e-01	1.68e-01	3.91e-01	7.45e-01	5.41e-01	6.56e-01	1.94e+01	1.48e-17	7.45e-17	1.72e-05	8.84e-17	8.57e-17	1.55e-04
Г	5e + 03	1e+04	1.0e-01	9.97e+01	2.08e-01	1.39e+01	4.26e-01	2.65e+00	5.54e + 01	5.55e-17	4.16e-16	5.02e-07	1.67e-14	3.20e-16	2.29e-04
Γ	5e + 03	1e+05	1.0e-01	7.64e+01	7.24e-01	1.42e+02	1.12e+00	8.51e+00	7.85e+01	2.36e-17	9.31e-11	6.38e-05	3.13e-16	1.79e-16	1.58e-04
Γ	5e+03	5e+05	1.0e-01	2.30e+02	6.97e + 00	6.54e + 02	7.02e+00	1.52e+01	1.70e+02	1.52e-17	1.87e-10	3.73e-05	3.92e-16	1.68e-16	1.48e-04
Γ	2e + 04	1e+05	1.0e-02	6.32e-01	9.46e-01	5.68e + 00	1.05e+00	2.49e+00	4.28e + 01	1.36e-17	3.55e-06	4.33e-07	1.99e-06	1.28e-16	1.42e-04
Γ	2e + 04	5e+05	1.0e-02	6.66e-01	4.46e + 00	3.78e + 01	5.63e + 00	9.28e + 00	1.23e+02	8.48e-18	3.37e-06	8.83e-07	1.36e-06	2.89e-16	1.10e-04
Γ	2e + 04	1e+06	1.0e-02	1.85e+00	9.30e+00	6.50e + 01	1.17e+01	1.59e+01	2.06e+02	7.08e-18	4.34e-06	6.27e-06	1.76e-06	9.65e-17	1.12e-04
Γ	1e + 05	1e + 07	1.0e-03	7.38e+00	1.06e + 01	6.14e + 00	9.35e + 01	9.60e + 01	1.56e + 03	1.39e-18	1.39e-18	1.39e-18	1.76e-17	1.76e-17	5.90e-05

Table 5.4: LP application results averaged on 5 randomly generated problems per row.



Figure 5.2: Performance Profiles for LP application with respect to all problems.

We also consider the first five problems in alphabetical order from the subset of the NETLIB dataset where primal strict feasibility (PSF) holds [35, Sect. 4.2.2]. We then check dual strict feasibility (DSF) and include the value of the constant we obtain from solving the theorem of the alternative, i.e., a large, respectively small, constant indicates an algebraically *fat*, respectively *thin*, feasible set. Failure, or near failure, of strict feasibility correlates with the difficulty of the numerics. We successfully solve two of the five problems. We think that the difficulties from the NETLIB dataset is due to the dual feasible set being very thin for some problems. For example, in Table 5.5, the problems 25fv47 and lotfi have a very thin feasible set in the dual problem.

It is important to note that the performance of SSEPF-RNNM on the blend problem is signifcantly worse than the other solvers. A common issue with SSEPF-RNNM when solving the blend problem as well as rows 4-6 of Table 5.4 is that at certain tolerances, RNNM uses the maximum number of iterations (2000) to solve the BAP subproblem. In other words, even though we are performing a warm-start with the solution from the previous BAP subproblem, RNNM can fail to converge to the desired relative tolerance. However, even though RNNM failed to converge, it still provides a solution that is very close to the optimal solution, i.e., instead of solving the BAP subproblem to within a relative tolerance of 10^{-14} , it returns a solution that is within a relative tolerance of 10^{-12} or 10^{-13} . There are at least two solutions to this issue. First, we can decrease the length of the Newton step when the iteration count is large. Using this heuristic shows significant improvement in performance when solving the blend problem. Secondly, if RNNM fails to converge to within the specified relative tolerance of 10^{-14} , we can try a larger relative tolerance, such as 10^{-13} . This strategy has shown to be crucial when trying to solve problems like 25fv47, where we are not able to solve the BAP subproblem with high accuracy due to it's thin dual feasible

Problem:	Primal Strict Feas.	Dual Strict Feas.
25fv47	2.00e-01	2.01e-17
afiro	9.00e+00	1.19e-01
blend	7.30e-02	3.49e-03
israel	3.71e+00	1.38e-03
lotfi	1.00e+00	1.89e-10

Table 5.5: Primal and Dual strict feasibility of NETLIB problems.

			Time	(s)			Rel. Resids.						
Problem:	SSEPF-RNNM	Linprog DS	Linprog IPM	MOSEK DS	MOSEK IPM	SNIPAL	SSEPF-RNNM	Linprog DS	Linprog IPM	MOSEK DS	MOSEK IPM	SNIPAL	
25fv47	Inf	2.01e-01	1.01e-01	3.76e-01	1.54e-01	1.20e+01	Inf	2.30e-15	2.25e-15	5.51e-16	1.09e-14	7.36e-05	
afiro	2.62e-02	7.71e-03	2.91e-03	9.16e-02	9.01e-02	9.81e-02	1.97e-16	3.67e-16	8.62e-14	7.49e-17	1.43e-13	9.39e-11	
blend	1.42e+02	8.48e-03	3.81e-03	9.12e-02	9.03e-02	1.58e+00	5.37e-15	4.78e-14	1.31e-13	1.33e-15	1.63e-15	1.30e-03	
israel	Inf	1.07e-02	2.79e-02	9.33e-02	9.82e-02	3.27e + 00	Inf	7.15e-16	8.44e-14	6.57e-16	8.93e-12	5.21e-05	
lotfi	Inf	9.63e-03	7.86e-03	9.41e-02	9.43e-02	2.00e+00	Inf	4.61e-14	3.38e-14	1.17e-16	9.05e-13	4.35e-05	

Table 5.6: LP application results on the NETLIB problems.



Figure 5.3: Performance Profiles for LP application with respect to the Netlib problems.

Our algorithm has difficulties with highly degenerate problems where the optimal solution is not unique. Moreover, the optimal solution of minimum norm that our algorithm finds can fail strict complementarity with many $x_i + z_i = 0$. The loss of strict complementarity results in a generalized Jacobian with low rank as few columns of A are chosen in (2.16). Additionally, the sensitivity analysis of Theorem 4.4 has difficulty increasing R. Finally, the failure of strict complementarity indicates that the gradient at optimality is not in the relative interior of the normal cone, Lemma 2.7, Item (b), indicating failure of differentiability of the projection.

6 Conclusion

In this paper we considered the theory and applications of the "best approximation problem" of finding the projection of a point onto a polyhedral set. We studied an elegant optimality condition, derived using the Moreau decomposition, that allowed for a, possibly both nonsmooth and singular, Newton type method. However, this needed a perturbation of a max-rank choice of a generalized Jacobian, i.e., application of nonsmooth analysis and regularization. The regularization guaranteed a descent direction but the method was not necessarily monotonically decreasing. We presented extensive comparisons with the HLWB algorithm approach, e.g., [4], and found that, in our experiments, our method outperformed HLWB in both speed and accuracy.

We discussed several applications including solving large, sparse, linear programs. The preliminary tests we performed were very efficient and outperformed the other codes we used for comparison both in speed and accuracy. Our algorithmic approach can be considered as a *stepping stone external path following* method since we follow an external path with parameter R in the objective function; but we only consider a discrete number of points on the path found using sensitivity analysis. We discovered that very few stepping stones are needed, often just one suffices.

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A Pseudocodes for Generalized Simplex

The pseudocodes described in Algorithms A.1 to A.3 solve (2.1) using the exact and inexact nonsmooth Newton methods RNNM, respectively.

Algorithm A.1 BAP of v for constraints $Ax = b, x \ge 0$; exact Newton direction

Require: $v \in \mathbb{R}^n, y_0 \in \mathbb{R}^m, (A \in \mathbb{R}^{m \times n}, \operatorname{rank}(A) = m), b \in \mathbb{R}^m, \varepsilon > 0, \text{ maxiter} \in \mathbb{N}.$ 1: **Output.** Primal-dual opt.: $x_{k+1}, (y_{k+1}, z_{k+1})$ 2: Initialization. $k \leftarrow 0, x_0 \leftarrow (v + A^T y_0)_+, z_0 \leftarrow (x_0 - (v + A^T y_0))_+,$ $F_0 = Ax_0 - b$, stopcrit $\leftarrow ||F_0|| / (1 + ||b||)$ 3: while $((\text{stopcrit} > \varepsilon) \& (k \le \text{maxiter}))$ do $V_{k} = \sum_{i \in \mathcal{I}_{+}} A_{i} A_{i}^{T} + \sum_{i \in \bar{\mathcal{I}}_{0}} \frac{1}{\|A_{i}\|^{2}} A_{i} A_{i}^{T}$ 4: $\lambda = \min(1e^{-3}, \text{ stopcrit})$ 5: $\bar{V} = (V_k + \lambda I_m)$ 6: solve pos. def. system $\overline{V}d = -F_k$ for Newton direction d 7: 8: updates $y_{k+1} \leftarrow y_k + d$ 9: $x_{k+1} \leftarrow (v + A^T y_{k+1})_+$ 10: $z_{k+1} \leftarrow (x_{k+1} - (v + A^T y_k))_+$ 11: $F_{k+1} \leftarrow Ax_{k+1} - b$ (residual) 12:stopcrit $\leftarrow \|F_{k+1}\|/(1+\|b\|)$ 13: $k \leftarrow k + 1$ 14:15: end while

Algorithm A.2 BAP of v for constraints $Ax = b, x \ge 0$, inexact Newton direction

Require: $v \in \mathbb{R}^n, y_0 \in \mathbb{R}^m, (A \in \mathbb{R}^{m \times n}, \operatorname{rank}(A) = m), b \in \mathbb{R}^m, \varepsilon > 0, \text{ maxiter} \in \mathbb{N}.$ 1: Output. Primal-dual: $x_{k+1}, (y_{k+1}, z_{k+1})$ 2: Initialization. $k \leftarrow 0, x_0 \leftarrow (v + A^T y_0)_+, z_0 \leftarrow (x_0 - (v + A^T y_0))_+,$ $\delta \in (0,1], \nu \in [1+\frac{\delta}{2},2]$, and a sequence θ such that $\theta_k \ge 0$ and $\sup_{k\in\mathbb{N}} \theta_k < 1$ $F_0 = Ax_0 - b$, stopcrit $\leftarrow ||F_0|| / (1 + ||b||)$ 3: while $((\text{stopcrit} > \varepsilon) \& (k \le \text{maxiter}))$ do $V_k = \sum_{i \in \mathcal{I}_+} A_i A_i^T + \sum_{i \in \bar{\mathcal{I}}_0} \frac{1}{\|A_i\|^2} A_i A_i^T$ 4: $\lambda = (\text{stopcrit})^{\delta}$ 5: $\bar{V} = (V_k + \lambda I_m)$ 6: solve $\bar{V}d = -F_k$ for Newton direction d such that residual $||r_k|| \le \theta_k ||F_k||^{\nu}$ 7: 8: updates $y_{k+1} \leftarrow y_k + d$ 9: $x_{k+1} \leftarrow (v + A^T y_{k+1})_+$ 10: $z_{k+1} \leftarrow (x_{k+1} - (v + A^T y_k))_+$ 11: $F_{k+1} \leftarrow Ax_{k+1} - b$ (residual) 12:13:stopcrit $\leftarrow \|F_{k+1}\|/(1+\|b\|)$ $k \leftarrow k+1$ 14:15: end while

Algorithm A.3 Extended HLWB algorithm

Require: $v \in \mathbb{R}^n$, $(A \in \mathbb{R}^{m \times n}, \operatorname{rank}(A) = m)$, $b \in \mathbb{R}^m$, $\varepsilon > 0$, maxiter $\in \mathbb{N}$. 1: Output. x_{k+1} 2: Initialization. $k \leftarrow 0$, $msweeps \leftarrow 0$ $x_0 \leftarrow max(v, 0)$, $\hat{x}_0 \leftarrow x_0$, $i_0 = 1$ stopcrit $\leftarrow ||A\hat{x}_0 - b|| / (1 + ||b||) (= ||F_0|| / (1 + ||b||))$ 3: while ((stopcrit > ε) & ($k \le$ maxiter)) do if $1 \leq i_k \leq m$ then 4: $\hat{x}_{k} = x_{k} + \frac{b_{i_{k}} - a_{i_{k}}^{T} x_{k}}{\|a_{i_{k}}\|^{2}} a_{i_{k}}$ 5:6: else 7: $\hat{x}_k = \max(0, x_k)$ end if 8: updates 9: $\sigma_k = \frac{1}{k+1}$ 10: $x_{k+1} \leftarrow \sigma_k v + (1 - \sigma_k) \hat{x}_k$ 11: stopcrit $\leftarrow ||A\hat{x}_k - b|| / (1 + ||b||)$ 12:if $k \pmod{m+1} = 0$ then 13:msweeps = msweeps + 114:end if 15: $i_k = k \pmod{m} + 1$ 16:17: end while

B Additional Performance Profiles

B.1 Nondegenerate



Figure B.1: Performance Profiles for varying m for nondegenerate vertex solutions.



Figure B.2: Performance Profiles for varying n for nondegenerate vertex solutions.



Figure B.3: Performance Profiles for varying density for nondegenerate vertex solutions.

B.2 Degenerate

Table B.1: Varying problem sizes m and comparing computation time with relative residual for degenerate vertex solutions.

Specifications				Rel. Resids.								
m	n	% density	Exact	Inexact	HLWB	lsqlin	QPPAL	Exact	Inexact	HLWB	lsqlin	QPPAL
500	3000	8.1e-01	4.23e-02	1.51e-01	1.54e + 02	3.77e + 00	1.14e + 00	1.96e-16	8.26e-16	2.25e-04	7.26e-17	1.72e-17
1000	3000	8.1e-01	4.40e-01	9.97e-01	3.71e+02	5.37e + 00	2.15e+00	2.70e-16	1.95e-15	2.14e-04	3.87e-17	2.70e-17
1500	3000	8.1e-01	1.17e+00	3.23e + 00	6.09e + 02	7.02e + 00	4.69e + 00	3.41e-17	6.73e-16	2.27e-04	3.95e-17	1.16e-17
2000	3000	8.1e-01	2.49e+00	7.51e+00	8.67e + 02	1.02e+01	7.81e+00	6.11e-17	3.11e-17	2.24e-04	3.14e-17	-2.74e-17

Table B.2: Varying problem sizes n and comparing computation time with relative residual for degenerate vertex solutions.

Specifications			Time (s)					Rel. Resids.				
m	n	% density	Exact	Inexact	HLWB	lsqlin	QPPAL	Exact	Inexact	HLWB	lsqlin	QPPAL
200	3000	8.1e-01	3.12e-03	3.69e-02	4.45e + 01	3.50e + 00	8.66e-01	8.64e-18	7.39e-17	2.56e-04	6.52e-16	5.89e-17
200	3500	8.1e-01	3.08e-03	4.05e-02	5.17e + 01	4.93e+00	1.00e+00	9.07e-18	1.26e-17	2.78e-04	1.23e-15	2.15e-17
200	4000	8.1e-01	3.24e-03	3.70e-02	5.82e + 01	7.31e+00	1.09e+00	1.46e-16	8.91e-16	2.80e-04	3.21e-16	-9.18e-18
200	4500	8.1e-01	3.99e-03	4.17e-02	6.58e + 01	1.01e+01	1.18e+00	1.80e-15	2.05e-16	3.13e-04	4.61e-17	1.71e-16

Table B.3: Varying problem density and comparing computation time with relative residual for degenerate vertex solutions.

Specifications			Time (s)					Rel. Resids.				
m	n	% density	Exact	Inexact	HLWB	lsqlin	QPPAL	Exact	Inexact	HLWB	lsqlin	QPPAL
300	1000	25	5.69e-02	2.66e-01	4.55e+01	3.30e-01	1.20e + 00	2.83e-17	1.14e-17	1.50e-04	8.61e-17	5.99e-17
300	1000	50	5.43e-02	2.28e-01	5.39e + 01	3.08e-01	1.82e + 00	1.23e-16	1.97e-17	1.44e-04	8.08e-16	1.42e-17
300	1000	75	7.75e-02	2.86e-01	5.36e + 01	3.16e-01	1.49e + 01	4.83e-16	1.72e-17	1.62e-04	3.49e-16	-3.43e-16
300	1000	100	7.27e-02	2.47e-01	4.65e + 01	3.00e-01	2.54e + 02	5.66e-16	2.15e-17	1.63e-04	1.91e-15	1.04e-14



Figure B.4: Performance Profiles for varying m for degenerate vertex solutions.



Figure B.5: Performance Profiles for varying n for degenerate vertex solutions.



Figure B.6: Performance Profiles for varying density for degenerate vertex solutions.

\mathbf{C} Applications of the BAP and the HLWB algorithm

The BAP and the HLWB algorithm play important roles in mathematical and technological problems. We give two examples.

- 1. Finding best approximation pairs for two intersections of closed convex sets
 - The problem of finding a best approximation pair of two sets, which in turn generalizes the well-known convex feasibility problem [5], has a long history that dates back to work by Cheney and Goldstein in 1959 [16]. This problem was recently revisited in [1] where an alternating HLWB (A-HLWB) algorithm was proposed and studied that can be used when the two sets are finite intersections of half-spaces. Motivated by that [7] presented alternative algorithms that utilize projection and proximity operators. Their modeling framework is able to accommodate even convex sets and their numerical experiments indicate that these methods are competitive and in some cases superior to the A-HLWB algorithm. The practical importance of the problem of finding a best approximation pair of two sets stems from its relevance to real-world situations wherein the feasibility-seeking modeling is used and there are two disjoint constraints sets. One set represents "hard" constraints, i.e., constraints the must be met, while the other set represents "soft" constraints which should be observed as much as possible, see, e.g., [20]. Under such circumstances, the desire to find a point in the hard constraints set that will be closest to the set of soft constraints leads to the problem of finding a best approximation pair of the two sets.
- 2. Least intensity modulated treatment plan in radiotherapy In the fully-discretized modelling of the intensity-modulated radiation therapy (IMRT) treatment planning problem the irradiated body is discretized into voxels and the external radiation field is discretized into beamlets. This is represented by a system of linear inequalities as in (3.2) with nonnegativity constraints. The unknown vector x represents radiation intensities and if it is a solution of the linear feasibility problem then it fulfills all the planning prescriptions dictated by the oncologist. In such a feasibility-seeking approach several solutions are acceptable but a solution that is closest to the origin will use the least possible intensities that still fulfill the constraints. Delivering an acceptable treatment plan with less radiation intensities is preferable and so one replaces the feasibility-seeking problem by a BAP of approximating the origin by a point from the feasible sets, i.e., by seeking the projection of the origin onto the feasible set. Such an approach was used, e.g., in [55] where a simultaneous version of Hildreth's sequential algorithm for norm minimization over linear inequalities, [31, 36], [15, Algorithm 6.5.2] was combined with a norm-minimizing image reconstruction algorithm of Herman and Lent [30], called ART4 (Algebraic Reconstruction Technique 4), which handles in a special effective manner interval inequalities.

Data Availability and Conflict of Interest Statement

The codes for generating both the data and the output is available at the paper link at URL www.math.uwaterloo.ca/~hwolkowi/henry/reports/ABSTRACTS.html or by request from one of the authors.

The authors declare no competing interests.

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