Proximal Distance Algorithms: Theory and Examples

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Abstract

Proximal distance algorithms combine the classical penalty method of constrained minimization with distance majorization. If \( f(x) \) is the loss function, and \( C \) is the constraint set in a constrained minimization problem, then the proximal distance principle mandates minimizing the penalized loss \( f(x) + \frac{\rho}{2} \text{dist}(x, C)^2 \) and following the solution \( x_\rho \) to its limit as \( \rho \) tends to \( \infty \). At each iteration the squared Euclidean distance \( \text{dist}(x, C)^2 \) is majorized by the spherical quadratic \( \|x - P_C(x_k)\|^2 \), where \( P_C(x_k) \) denotes the projection of the current iterate \( x_k \) onto \( C \). The minimum of the surrogate function \( f(x) + \frac{\rho}{2} \|x - P_C(x_k)\|^2 \) is given by the proximal map \( \text{prox}_{\frac{1}{\rho} f}(P_C(x_k)) \). The next iterate \( x_{k+1} \) automatically decreases the original penalized loss for fixed \( \rho \). Since many explicit projections and proximal maps are known, it is straightforward to derive and implement novel optimization algorithms in this setting. These algorithms can take hundreds if not thousands of iterations to converge, but the stereotyped nature of each iteration makes proximal distance algorithms competitive with traditional algorithms. For convex problems, we prove global convergence. Our numerical examples include a) linear programming, b) nonnegative quadratic programming, c) projection to the closest kinship matrix, d) projection onto a second-order cone constraint, e) calculation of Horn’s copositive matrix index, f) linear complementarity programming, and g) sparse principal components analysis. The proximal distance algorithm in each case is competitive or superior in speed to traditional methods.

Key words and phrases: constrained optimization, EM algorithm, majorization, projection, proximal map

Math Subject Classifications: 90C59, 90C26, 65K05

1 Introduction

The solution of constrained optimization problems is part science and part art. As mathematical scientists explore the largely uncharted territory of high-dimensional nonconvex problems, it is imperative to consider new methods. The current paper studies a class of optimization algorithms that combine the classical penalty method of optimization [5,17] with the notion of a proximal operator [3,43,48]. The formula

\[
\text{prox}_f(y) = \arg\min_x \left[ f(x) + \frac{1}{2} \|x - y\|^2 \right]
\]  

(1)
defines the proximal map of a function \( f(x) \). Here \( \| \cdot \| \) is the standard Euclidean norm, and \( f(x) \) is typically assumed to be closed and convex. Projection onto a closed convex set \( C \) is realized by choosing \( f(x) \) to be the \( 0/\infty \) indicator \( \delta_C(x) \) of \( C \). It is possible to drop the convexity assumption if \( f(x) \) is nonnegative or coercive. In so doing, \( \text{prox}_f(y) \) may become multi-valued. For example, the minimum distance from a non-convex set to an exterior point can be attained at multiple boundary points. The point \( x \) in the definition (1) can be restricted to a subset \( S \) of Euclidean space by replacing \( f(x) \) by \( f(x) + \delta_S(x) \), where \( \delta_S(x) \) is the indicator of \( S \). One of the virtues of exploiting proximal operators is that they have been thoroughly investigated. For a large number of functions \( f(x) \), the map \( \text{prox}_{cf}(y) \) is either given by an exact formula or calculable by an efficient algorithm for all \( c > 0 \). The known formulas tend to be highly accurate. This is a plus because the classical penalty method suffers from roundoff error for large values of the penalty constant. Although the penalty method seldom delivers exquisitely accurate solutions, moderate accuracy suffices for many problems.

The derivation of our proximal distance algorithms hinges on the majorization-minimization (MM) principle [28, 36]. In minimizing a function \( f(x) \), the MM principle exploits a surrogate function \( g(x \mid x_k) \) that majorizes \( f(x) \) around the current iterate \( x_k \). Majorization mandates both domination \( g(x \mid x_k) \geq f(x) \) for all feasible \( x \) and tangency \( g(x_k \mid x_k) = f(x_k) \) at the anchor \( x_k \). If \( x_{k+1} \) minimizes \( g(x \mid x_k) \), then the descent property \( f(x_{k+1}) \leq f(x_k) \) follows from the string of inequalities and equalities

\[
f(x_{k+1}) \leq g(x_{k+1} \mid x_k) \leq g(x_k \mid x_k) = f(x_k).
\]

Clever selection of the surrogate \( g(x \mid x_{k+1}) \) can lead to a simple algorithm with an explicit update that requires little computation per iterate. The number of iterations until convergence of an MM algorithm depends on how tightly \( g(x \mid x_k) \) hugs \( f(x) \). Constraint satisfaction is built into any MM algorithm. If maximization of \( f(x) \) is desired, then the objective \( f(x) \) should dominate the surrogate \( g(x \mid x_k) \) subject to the tangency condition. The next iterate \( x_{k+1} \) is then chosen to maximize \( g(x \mid x_k) \). The minorization-maximization version of the MM principle guarantees the ascent property.

There are ample precedents in the optimization literature for the proximal distance principle. Proximal gradient algorithms have been employed for many years in many contexts, including projected Landweber, alternating projection onto the intersection of two or more closed convex sets, the alternating-direction method of multipliers (ADMM), and fast iterative shrinkage thresholding algorithms (FISTA) [4, 16, 35]. Applications of distance majorization are more recent [15]. Our recent presentation [38] to the 2014 International Congress of Mathematicians introduced the proximal distance algorithm. The current paper expands on that preliminary treatment and fills in many gaps of theory and practice. It has been a learning experience melding the classical penalty method with distance majorization. Details of implementation such as Nesterov acceleration matter in performance. We have found that squared distance penalties tend to work better than our original exact penalties. In the presence of convexity, it is now clear that every proximal distance algorithm reduces to a proximal gradient algorithm. Hence, convergence analysis can appeal to a venerable body of convex theory. This does not to imply that the proximal distance algorithm is limited to convex problems. In fact, its most important applications may well be to nonconvex problems. The focus of this paper is on practical exploration of the proximal distance algorithm. We do not attempt to extend classical convergence arguments to nonconvex problems. This challenge is an active area of research for many highly talented mathematicians.
2 Derivation

The generic problem of minimizing a function $f(x)$ over a closed set $C$ can be attacked by distance majorization. The penalty method seeks the minimum point of a penalized version $f(x) + \rho q(x)$ of $f(x)$ and then follows the solution vector $x_\rho$ as $\rho$ tends to $\infty$. In the limit one recovers the constrained solution. If the constraint set $C$ equals an intersection $\bigcap_{i=1}^m C_i$ of closed sets, then it is natural to define the penalty $q(x) = \frac{1}{2m} \sum_{i=1}^m \text{dist}(x, C_i)^2$. Distance majorization gives the surrogate function

$$g_\rho(x | x_k) = f(x) + \frac{\rho}{2m} \sum_{i=1}^m \|x - P_{C_i}(x_k)\|^2$$

for an irrelevant constant $c_k$. If we put $y_k = \frac{1}{m} \sum_{i=1}^m P_{C_i}(x_k)$, then by definition the minimum of the surrogate $g_\rho(x | x_k)$ occurs at the proximal point

$$x_{k+1} = \text{prox}_{\rho^{-1} f}(y_k).$$

We call this MM algorithm the proximal distance algorithm. The penalty $q(x)$ is generally smooth because

$$\nabla \frac{1}{2} \text{dist}(x, C)^2 = x - P_C(x)$$

at any point $x$ where the projection $P_C(x)$ is single valued [9,37].

For the special case of projection of an external point $z$ onto the intersection $C$ of the closed sets $C_i$, one should take $f(x) = \frac{1}{2} \|z - x\|^2$. The proximal distance iterates then obey the explicit formula

$$x_{k+1} = \frac{1}{1 + \rho}(z + \rho y_k).$$

Linear programming with arbitrary convex constraints is another simple case. Here $f(x) = v^t x$, and the update reduces to

$$x_{k+1} = y_k - \frac{1}{\rho} v.$$

If the proximal map is impossible to calculate, but $\nabla f(x)$ is known to be Lipschitz with constant $L$, then one can substitute the standard majorization

$$f(x) \leq f(x_k) + df(x_k)(x - x_k) + \frac{L}{2} \|x - x_k\|^2$$

for $f(x)$. Minimizing the sum of the loss majorization plus the penalty majorization leads to the MM update

$$x_{k+1} = \frac{1}{L + \rho} [-\nabla f(x_k) + L x_k + \rho y_k]$$

for $f(x)$. This is a gradient descent algorithm without an intervening proximal map.
The proximal distance algorithm can also be applied to unconstrained problems. For example, consider the problem of minimizing a penalized loss $\ell(x) + p(Ax)$. The presence of the linear transformation $Ax$ in the penalty complicates optimization. The strategy of parameter splitting introduces a new variable $y$ and minimizes $\ell(x) + p(y)$ subject to the constraint $y = Ax$. If $P_M(z)$ denotes projection onto the manifold $M = \{z = (x, y) : Ax = y\}$, then the constrained problem can be solved approximately by minimizing the function

$$\ell(x) + p(y) + \frac{\rho}{2} \text{dist}(z, M)^2$$

for large $\rho$. If $P_M(z_k)$ consists of two subvectors $u_k$ and $v_k$ corresponding to $x_k$ and $y_k$, then the proximal distance updates are

$$x_{k+1} = \text{prox}_{\rho^{-1}\ell}(u_k) \quad \text{and} \quad y_{k+1} = \text{prox}_{\rho^{-1}p}(v_k).$$

When the matrix $A$ has dimensions $r \times s$, one can attack the projection problem by differentiating the Lagrangian

$$\mathcal{L}(x, y, \lambda) = \frac{1}{2} \|x - u\|^2 + \frac{1}{2} \|y - v\|^2 + \lambda^t (Ax - y).$$

To solve the stationarity equations

$$0 = x - u + A^t \lambda \quad \text{and} \quad 0 = y - v - \lambda,$$

we multiply the first by $A$, subtract it from the second, and substitute $Ax = y$. This generates the identity

$$0 = Au - v - (AA^t + I_r) \lambda$$

with solution

$$\lambda = (AA^t + I_r)^{-1}(Au - v).$$

The values $x = u - A^t \lambda$ and $y = v + \lambda$ are then immediately available. This approach is preferred when $r < s$. In the opposite case $r > s$, it makes more sense to directly minimize the function

$$f(x) = \frac{1}{2} \|x - u\|^2 + \frac{1}{2} \|Ax - v\|^2.$$ 

This leads to the solution

$$x = (A^t A + I_s)^{-1}(A^t v + u).$$

The advantage here is that the matrix $A^t A + I_s$ is now $s \times s$ rather than $r \times r$. \hfill \Box

3 Convergence and Acceleration

In the presence of convexity, the proximal distance algorithm reduces to a proximal gradient algorithm. This follows from the representation

$$y = \frac{1}{m} \sum_{i=1}^m P_{C_i}(x) = x - \frac{1}{m} \sum_{i=1}^m \left[ x - P_{C_i}(x) \right] = x - \nabla q(x)$$
involving the penalty \( q(x) \). Thus, the proximal distance algorithm can be expressed as

\[
x_{k+1} = \text{prox}_{\rho^{-1}f}[x_k - \nabla q(x_k)].
\]

In this regard, there is the implicit assumption that \( \nabla q(x) \) is Lipschitz with constant 1. This is indeed the case. According to the Moreau decomposition \([3]\), for a single closed convex set \( C \)

\[
\nabla q(x) = x - P_C(x) = \text{prox}_{\delta_C^*}(x),
\]

where \( \delta_C^*(x) \) is the Fenchel conjugate of the indicator function

\[
\delta_C(x) = \begin{cases} 
0 & x \in C \\
\infty & x \notin C.
\end{cases}
\]

Because proximal operators of closed convex functions are nonexpansive \([3]\), the result follows for a single set. For the general penalty \( q(x) \) with \( m \) sets, the Lipschitz constants are scaled by \( m^{-1} \) and added to produce an overall Lipschitz constant of 1.

Proximal gradient algorithms can be painfully slow to converge. This fact suggests that one should slowly send \( \rho \) to \( \infty \) and refuse to wait until convergence occurs for any given \( \rho \). It also suggests that Nesterov acceleration may vastly improve the chances for convergence. Nesterov acceleration for the general proximal gradient algorithm with loss \( f(x) \) and penalty \( p(x) \) takes the form

\[
z_k = x_k + \frac{k - 1}{k + d - 1}(x_k - x_{k-1})
\]

\[
x_{k+1} = \text{prox}_{L^{-1}f}[z_k - L^{-1}\nabla p(z_k)],
\]

(3)

where \( L \) is the Lipschitz constant for \( \nabla p(x) \) and \( d \) is typically chosen to be 3. Nesterov acceleration achieves an \( O(n^{-2}) \) convergence rate \([51]\), which is vastly superior to the \( O(n^{-1}) \) rate achieved by ordinary gradient descent. The Nesterov update possesses the desirable property of preserving affine constraints. In other words, if \( Ax_{k-1} = b \) and \( Ax_k = b \), then \( Az_k = b \) as well. In cases not covered by current convex theory, we will accelerate our proximal distance algorithms by applying the algorithm map \( M(x) \) to the shifted point \( z_k \), yielding the accelerated update \( x_{k+1} = M(z_k) \). The recent paper of Ghadimi and Lan \([22]\) extends Nesterov acceleration to this more general setting.

Newton’s method offers another possibility for acceleration. This depends on the differentiability of the gradient

\[
\nabla f(x) + \frac{\rho}{m} \sum_{i=1}^{m} [x - P_{C_i}(x)].
\]

Unfortunately, the second differential

\[
d^2 f(x) + \frac{\rho}{m} \sum_{i=1}^{m} [I - dP_{C_i}(x)]
\]

may not exist globally. For some sets \( C \), the differential \( dP_C(x) \) is trivial to calculate. For instance, when \( P_C(x) = Mx + b \) is affine, the identity \( dP_C(x) = M \) holds. In the case of projection onto the set \( \{x : Ax = b\} \), the matrix \( M \) takes the form \( M = I - A'(AA')^{-1}A \). If \( C \) is a sparsity set, and \( P_C(x) \) reduces to a single point, then \( dP_C(x) \) is a diagonal matrix whose \( i \)th diagonal entry is 1 when \( |x_i| \) is
sufficiently large and 0 otherwise. When $C$ is a nonnegativity set, and no entry of $x$ is 0, $dP_C(x)$ is diagonal with $i$th diagonal entry 1 for $x_i$ positive and 0 for $x_i$ negative. To its detriment, Newton’s method requires a great deal of linear algebra per iteration in high-dimensional problems. There is also no guarantee that the second differential is positive definite, even for convex problems.

Finally, it is worth proving that the proximal distance algorithm converges in the presence of convexity. Our convergence analysis relies on well-known operator results [3]. Proximal operators in general and projection operators in particular are nonexpansive and averaged. By definition an averaged operator $M(x) = \alpha x + (1 - \alpha)N(x)$ is a convex combination of a nonexpansive operator $N(x)$ and the identity operator $I$. The averaged operators on $\mathbb{R}^m$ with $\alpha \in (0, 1)$ form a convex set closed under functional composition. Furthermore, $M(x)$ and the base operator $N(x)$ share their fixed points. The celebrated theorem of Krasnosel’skii [34] and Mann [41] says that if an averaged operator $M(x) = \alpha x + (1 - \alpha)N(x)$ possesses one or more fixed points, then the iteration scheme $x_{k+1} = M(x_k)$ converges to a fixed point.

Consider minimization of the penalized loss

$$f(x) + \frac{\rho}{2m} \sum_{i=1}^{m} \text{dist}(x, C_i)^2.$$ 

By definition the proximal distance iterate is given by

$$x_{k+1} = \text{prox}_{\frac{1}{\rho} f}(y_k),$$

where $y_k = \frac{1}{m} \sum_{i=1}^{m} P_{C_i}(x_k)$. The algorithm map is an averaged operator, being the composition of two averaged operators. Hence, the Krasnosel’skii-Mann theorem guarantees convergence to a fixed point if one or more exist. Now $y$ is a fixed point if and only if

$$f(y) + \frac{\rho}{2m} \sum_{i=1}^{m} \|y - P_S(y)\|^2 \leq f(x) + \frac{\rho}{2m} \sum_{i=1}^{m} \|x - P_S(y)\|^2$$

for all $x$. In the presence of convexity, this is equivalent to the directional derivative inequality

$$0 \leq d_v f(y) + \frac{\rho}{m} \sum_{i=1}^{m} [y - P_{C_i}(y)]^t v = d_v \left[f(y) + \frac{\rho}{2m} \sum_{i=1}^{m} \text{dist}(y, C_i)^2\right]$$

for all $v$, which is in turn equivalent to $y$ minimizing the convex penalized loss. Minimum points, and therefore, fixed points exist.

Convergence of the overall proximal distance algorithm is tied to the convergence of the classical penalty method [5]. In this context the loss is $f(x)$, and the penalty is $q(x) = \frac{1}{2m} \sum_{i=1}^{m} \text{dist}(x, C_i)^2$. Assuming the objective $f(x) + \rho q(x)$ is coercive, the theory mandates that the solution path $x_\rho$ is bounded and any cluster point of the path attains the minimum value of $f(x)$ subject to the constraints. Furthermore, if $f(x)$ is coercive and possesses a unique minimum point in the constraint set $C$, then the path $x_\rho$ converges to that point.
4 Examples

The following examples highlight the versatility of proximal distance algorithms in a variety of convex and non-convex settings. Programming details matter in solving these problems. Individual programs are not necessarily long, but care must be exercised in projecting onto constraints, choosing tuning schedules, folding constraints into the domain of the loss, implementing acceleration, and declaring convergence. All of our examples are coded in the Julia programming language. Whenever possible, competing software was run in the Julia environment via the Julia module MathProgBase [19, 40]. The sparse PCA problem relies on the software of Witten et al. [54], which is coded in R. Convergence is tested at iteration \( k \) by the two criteria

\[
|f(x_k) - f(x_{k-1})| \leq \epsilon_1[|f(x_{k-1})| + 1] \quad \text{and} \quad \text{dist}(x_k, C) \leq \epsilon_2,
\]

where \( \epsilon_1 = 10^{-6} \) and \( \epsilon_2 = 10^{-4} \) are typical values. The number of iterations until convergence is about 1000 in most examples. This handicap is offset by the simplicity of each stereotyped update. Our code is available as supplementary material to this paper. Readers are encouraged to try the code and adapt it to their own examples.

4.1 Linear Programming

This interesting special case is harder to get right than one might first suspect. The best tactic seems to be to roll the standard affine constraints \( Ax = b \) into the domain of the loss function \( v^t x \). The standard nonnegativity requirement \( x \geq 0 \) is achieved by penalization. Let \( x_k \) be the current iterate and \( y_k = (x_k)_+ \) be its projection onto \( \mathbb{R}^n_+ \). Derivation of the proximal distance algorithm relies on the Lagrangian

\[
v^t x + \frac{\rho}{2} \|x - y_k\|^2 + \lambda^t (Ax - b).
\]

One can multiply the stationarity equation

\[
0 = v + \rho(x - y_k) + A^t \lambda
\]

by \( A \) and solve for the Lagrange multiplier \( \lambda \) in the form

\[
\lambda = (AA^t)^{-1}(\rho Ay_k - \rho b - Av).
\]

Inserting this value into the stationarity equation gives the MM update

\[
x_{k+1} = y_k - \frac{1}{\rho} v - A^t (AA^t)^{-1} \left( Ay_k - b - \frac{1}{\rho} Av \right).
\]

Table 1 compares the accelerated proximal distance algorithm to the open-source Splitting Cone Solver (SCS) [45] and the interior point method implemented in the commercial Gurobi solver. The first seven rows of the table summarize linear programs with dense data \( A, b, \) and \( v \). The bottom six rows rely on random sparse matrices \( A \) with sparsity level 0.01. For dense problems, the proximal distance algorithm starts the penalty constant \( \rho \) at 1 and doubles it every 100 iterations. Because we precompute and cache the pseudoinverse \( A^t (AA^t)^{-1} \) of \( A \), the update (6) reduces to vector additions and matrix-vector multiplications.

For sparse problems the proximal distance algorithm updates \( \rho \) by a factor of 1.5 every 50 iterations. To avoid computing large pseudoinverses, we appeal to the LSQR variant of the conjugate gradient method.
Table 1: CPU times and optima for linear programming. Here $m$ is the number of constraints, $n$ is the number of variables, PD is the accelerated proximal distance algorithm, SCS is the Splitting Cone Solver, and Gurobi is the Gurobi solver. After $m = 512$ the constraint matrix $A$ is initialized to be sparse with sparsity level 0.01.

| Dimensions | Optima | CPU Seconds |
|------------|--------|-------------|
| $m$ | $n$ | PD | SCS | Gurobi | PD | SCS | Gurobi |
| 2 | 4 | 0.2629 | 0.2629 | 0.2629 | 0.0018 | 0.0004 | 0.0012 |
| 4 | 8 | 1.0455 | 1.0456 | 1.0455 | 0.0022 | 0.0012 | 0.0011 |
| 8 | 16 | 2.4513 | 2.4514 | 2.4513 | 0.0167 | 0.0024 | 0.0013 |
| 16 | 32 | 3.4226 | 3.4225 | 3.4223 | 0.0472 | 0.0121 | 0.0014 |
| 32 | 64 | 6.2398 | 6.2397 | 6.2398 | 0.0916 | 0.0165 | 0.0028 |
| 64 | 128 | 14.671 | 14.671 | 14.671 | 0.1554 | 0.0643 | 0.0079 |
| 128 | 256 | 27.116 | 27.116 | 27.116 | 0.3247 | 0.8689 | 0.0406 |
| 256 | 512 | 58.501 | 58.494 | 58.494 | 0.6064 | 2.9001 | 0.2773 |
| 512 | 1024 | 135.35 | 135.34 | 135.34 | 1.4651 | 5.0410 | 1.9607 |
| 1024 | 2048 | 254.50 | 254.47 | 254.47 | 4.7953 | 4.7158 | 0.9544 |
| 2048 | 4096 | 533.27 | 533.23 | 533.23 | 12.482 | 23.495 | 10.121 |
| 4096 | 8192 | 991.74 | 991.67 | 991.67 | 52.300 | 84.860 | 93.687 |
| 8192 | 16384 | 2058.7 | 2058.5 | 2058.5 | 456.50 | 430.86 | 945.75 |

[46, 47] to solve the linear system (5). The optima of all three methods agree to 4 digits of accuracy. It is hard to declare an absolute winner in these comparisons. Gurobi clearly performs best on low-dimensional problems, but it may not scale quite as well as SCS and the proximal distance algorithm. In large sparse regimes the proximal distance algorithm and SCS perform equally well. If high accuracy is not a concern, then the proximal distance algorithm is easily accelerated with a more aggressive update schedule for $\rho$.

### 4.2 Nonnegative Quadratic Programming

In nonnegative quadratic programming (NQP) one minimizes the objective function $f(x) = \frac{1}{2}x^TAx + b^Tx$ subject to $x \geq 0$ for a positive definite matrix $A$. As in Example 4.1, projection onto the nonnegative cone is accomplished by the max operator $(x)_+$. For a given value of the penalty constant $\rho$, the proximal distance update is

$$x_{k+1} = (\rho I + A)^{-1} [\rho(x_k)_+ - b].$$

Naïvely solving the linear system at every iteration leads to suboptimal performance. Two alternatives exist, depending on whether $A$ is dense or sparse. If $A$ is dense, then one should compute the spectral decomposition $A = VDV^T$ once and cache it. The update (7) becomes

$$x_{k+1} = V (\rho I + D)^{-1} V^T [\rho(x_k)_+ - b].$$

The diagonal matrix $\rho I + D$ is trivial to invert. The remaining operations reduce to matrix-vector multiplications, which are substantially cheaper than repeated matrix inversions. Extraction of the spectral decomposition of $A$ becomes prohibitive as the dimension of $A$ increases. To compute the update (7) efficiently for large sparse matrices, we consequently apply LSQR.
Table 2: CPU times and optima for nonnegative quadratic programming. Here \( n \) is the number of variables, PD is the accelerated proximal distance algorithm, IPOPT is the Ipopt solver, and Gurobi is the Gurobi solver. After \( n = 512 \), the constraint matrix \( A \) is sparse.

| Dimensions | Optima | CPU Seconds |
|------------|--------|-------------|
|            | PD     | IPOPT       | Gurobi | PD     | IPOPT | Gurobi |
| 2          | -0.0015 | -0.0014     | -0.0014 | 0.0042 | 0.0025 | 0.0031 |
| 4          | -0.6070 | -0.6070     | -0.6070 | 0.0002 | 0.0028 | 0.0017 |
| 8          | -0.6840 | -0.6834     | -0.6834 | 0.0064 | 0.0036 | 0.0024 |
| 16         | -0.6235 | -0.6234     | -0.6235 | 0.0872 | 0.0037 | 0.0022 |
| 32         | -0.1936 | -0.1934     | -0.1936 | 0.0864 | 0.0041 | 0.0030 |
| 64         | -0.3368 | -0.3364     | -0.3368 | 0.1121 | 0.0054 | 0.0059 |
| 128        | -0.5344 | -0.5337     | -0.5344 | 0.1698 | 0.0124 | 0.0326 |
| 256        | -0.4969 | -0.4956     | -0.4969 | 0.3001 | 0.0512 | 0.0760 |
| 512        | -0.4716 | -0.4689     | -0.4716 | 0.8104 | 0.2617 | 0.3720 |
| 1024       | -26271  | -26277      | -26277  | 12.7841 | 0.2575 | 0.3685 |
| 2048       | -26000  | -26024      | -26024  | 29.6108 | 2.2635 | 2.2506 |
| 4096       | -56138  | -56272      | -56272  | 57.9576 | 23.850  | 17.452 |
| 8192       | -52960  | -53025      | -53025  | 126.145  | 242.90  | 164.90 |
| 16384      | -108677 | -108837     | -108837 | 425.017 | 2596.3  | 1500.4 |

Table 2 compares the performance of the proximal distance algorithm for NQP to the open source nonlinear interior point solver Ipopt \([52, 53]\) and the interior point method of Gurobi. Test problems were generated by filling an \( n \times n \) matrix \( M \) and an \( n \)-vector \( b \) with standard normal deviates. We then set \( A = M^T M + 0.001 I \). For sparse problems we set the sparsity level of \( M \) to be \( \log_{10}(n)/n \). Our setup ensures that \( A \) has full rank and that the quadratic program has a solution. For dense matrices, we start \( \rho \) at 1 and multiply it by 1.5 every 200 iterations. For sparse problems, we start \( \rho \) at \( 10^{-4} \) and multiply it by 1.5 every 100 iterations. Table 2 suggests that the proximal distance algorithm and the interior point solvers perform equally well on small dense problems. However, in high-dimensional and low-accuracy environments, the proximal distance algorithm provides better performance.

4.3 Closest Kinship Matrix

In genetics studies, kinship is measured by the fraction of genes two individuals share identical by descent. For a given pedigree, the kinship coefficients for all pairs of individuals appear as entries in a symmetric kinship matrix \( Y \). This matrix possesses three crucial properties: a) it is positive semidefinite, b) its entries are nonnegative, and c) its diagonal entries are \( \frac{1}{2} \) unless some pedigree members are inbred. Inbreeding is the exception rather than the rule. Kinship matrices can be estimated empirically from SNP (single nucleotide polymorphisms) data, but there is no guarantee that the three highlighted properties are satisfied. Hence, it helpful to project \( Y \) to the nearest qualifying matrix.

This projection problem is best solved by folding the positive semidefinite constraint into the domain of the Frobenius loss function \( \frac{1}{2}\|X - Y\|_F^2 \). As we shall see, the alternative of imposing two penalties rather than one is slower and less accurate. Projection onto the constraints implied by conditions b) and c) is trivial. All diagonal entries \( x_{ii} \) of \( X \) are reset to \( \frac{1}{2} \), and all off-diagonal entries \( x_{ij} \) are reset to \( \max\{x_{ij}, 0\} \).
Table 3: CPU times and optima for the closest kinship matrix problem. Here the kinship matrix is \( n \times n \), PD1 is the proximal distance algorithm, PD2 is the accelerated proximal distance, PD3 is the accelerated proximal distance algorithm with the positive semidefinite constraints folded into the domain of the loss, and Dykstra is Dykstra’s adaptation of alternating projections. All times are in seconds.

| Size | PD1 Loss | PD1 Time | PD2 Loss | PD2 Time | PD3 Loss | PD3 Time | Dykstra Loss | Dykstra Time |
|------|---------|---------|---------|---------|---------|---------|-------------|--------------|
| 2    | 1.64    | 0.36    | 1.64    | 0.01    | 1.64    | 0.01    | 1.64        | 0.00         |
| 4    | 2.86    | 0.10    | 2.86    | 0.01    | 2.86    | 0.01    | 2.86        | 0.00         |
| 8    | 18.77   | 0.21    | 18.78   | 0.03    | 18.78   | 0.03    | 18.78       | 0.00         |
| 16   | 45.10   | 0.84    | 45.12   | 0.18    | 45.12   | 0.12    | 45.12       | 0.02         |
| 32   | 169.58  | 4.36    | 169.70  | 0.61    | 169.70  | 0.52    | 169.70      | 0.37         |
| 64   | 837.85  | 16.77   | 838.44  | 2.90    | 838.43  | 2.63    | 838.42      | 4.32         |
| 128  | 3276.41 | 91.94   | 3279.44 | 18.00   | 3279.25 | 14.83   | 3279.23     | 19.73        |
| 256  | 14029.07| 403.59  | 14045.30| 89.58   | 14043.59| 64.89   | 14043.46    | 72.79        |

If \( P(X_k) \) denotes the current projection, then the proximal distance algorithm minimizes the surrogate

\[
g(X | X_k) = \frac{1}{2} \| X - Y \|_F^2 + \frac{\rho}{2} \| X - P(X_k) \|_F^2
\]

\[
= \frac{1 + \rho}{2} \left\| X - \frac{1}{1 + \rho} Y - \frac{\rho}{1 + \rho} P(X_k) \right\|_F^2 + c_k,
\]

where \( c_k \) is an irrelevant constant. The minimum is found by extracting the spectral decomposition \( U D U^t \) of \( \frac{1}{1 + \rho} Y + \frac{\rho}{1 + \rho} P(X_k) \) and truncating the negative eigenvalues. This gives the update \( X_{k+1} = UD + U^t \) in obvious notation. This proximal distance algorithm and its Nesterov acceleration are simple to implement in a numerically oriented language such as Julia. The most onerous part of the calculation is clearly the repeated eigen-decompositions.

Table 3 compares three versions of the proximal distance algorithm to Dykstra’s algorithm [11]. Higham proposed Dykstra’s algorithm for the related problem of finding the closest correlation matrix [25]. In Table 3 algorithm PD1 is the unadorned proximal distance algorithm, PD2 is the accelerated proximal distance, and PD3 is the accelerated proximal distance algorithm with the positive semidefinite constraints folded into the domain of the loss. On this demanding problem, these algorithms are comparable to Dykstra’s algorithm in speed but slightly less accurate. Acceleration of the proximal distance algorithm is effective in reducing both execution time and error. Folding the positive semidefinite constraint into the domain of the loss function leads to further improvements. The data matrices \( M \) in these trials were populated by standard normal deviates and then symmetrized by averaging opposing off-diagonal entries. In algorithm PD1 we set \( \rho_k = \max\{1.2^k, 2^{22}\} \). In the accelerated versions PD2 and PD3 we started \( \rho \) at 1 and multiplied it by 5 every 100 iterations. At the expense of longer compute times, better accuracy can be achieved by all three proximal distance algorithms with a less aggressive update schedule.

### 4.4 Projection onto a Second-Order Cone Constraint

Second-order cone programming is one of the unifying themes of convex analysis [2, 39]. It revolves around conic constraints of the form \( \{ u : \| Au + b \| \leq c^t u + d \} \). Projection of a vector \( x \) onto such a constraint
is facilitated by parameter splitting. In this setting parameter splitting introduces a vector \( w \), a scalar \( r \), and the two affine constraints \( w = Au + b \) and \( r = c^T u + d \). The conic constraint then reduces to the Lorentz cone constraint \( ||w|| \leq r \), for which projection is straightforward [10]. If we concatenate the parameters into the single vector

\[
y = \begin{pmatrix} u \\ w \\ r \end{pmatrix}
\]

and define \( L = \{ y : ||w|| \leq r \} \) and \( M = \{ y : w = Au + b \text{ and } r = c^T u + d \} \), then we can rephrase the problem as minimizing \( \frac{1}{2} ||x - u||^2 \) subject to \( y \in L \cap M \). This is a fairly typical set projection problem except that the \( w \) and \( r \) components of \( y \) are missing in the loss function.

Taking a cue from Example 4.1, we incorporate the affine constraints in the domain of the objective function. If we represent projection onto \( L \) by \( P \left( \begin{pmatrix} w_k \\ r_k \end{pmatrix} \right) = \begin{pmatrix} \tilde{w}_k \\ \tilde{r}_k \end{pmatrix} \), then the Lagrangian generated by the proximal distance algorithm amounts to

\[
\mathcal{L} = \frac{1}{2} ||x - u||^2 + \frac{\rho}{2} \left( \begin{pmatrix} w - \tilde{w}_k \\ r - \tilde{r}_k \end{pmatrix} \right)^2 + \lambda^T (Au + b - w) + \theta (c^T u + d - r).
\]

This gives rise to a system of three stationarity equations

\[
\begin{align*}
0 &= u - x + A^T \lambda + \theta c \\
0 &= \rho (w - \tilde{w}_k) - \lambda \\
0 &= \rho (r - \tilde{r}_k) - \theta.
\end{align*}
\]

Solving for the multipliers \( \lambda \) and \( \theta \) in equations (9) and (10) and substituting their values in equation (8) yield

\[
\begin{align*}
0 &= u - x + \rho A^T (w - \tilde{w}_k) + \rho (r - \tilde{r}_k)c \\
&= u - x + \rho A^T (Au + b - \tilde{w}_k) + \rho (c^T u + d - \tilde{r}_k)c.
\end{align*}
\]

This leads to the MM update

\[
\begin{align*}
u_{k+1} &= (\rho^{-1} I + A^T A + cc^T)^{-1} [\rho^{-1} x + A^T (\tilde{w}_k - b) + (\tilde{r}_k - d)c].
\end{align*}
\]

The updates \( w_{k+1} = Au_{k+1} + b \) and \( r_{k+1} = c^T u_{k+1} + d \) follow from the constraints.

Table 4 compares the proximal distance algorithm to SCS and Gurobi. Echoing previous examples, we tailor the update schedule for \( \rho \) differently for dense and sparse problems. Dense problems converge quickly and accurately when we set \( \rho_0 = 1 \) and double \( \rho \) every 100 iterations. Sparse problems require a greater range and faster updates of \( \rho \), so we set \( \rho_0 = 0.01 \) and then multiply \( \rho \) by 2.5 every 10 iterations. For dense problems, it is clearly advantageous to cache the spectral decomposition of \( A^T A + cc^T \) as suggested in Example 4.2. In this regime, the proximal distance algorithm is as accurate as Gurobi and nearly as fast. SCS is comparable to Gurobi in speed but notably less accurate.
Table 4: CPU times and optima for the second-order cone projection. Here \( m \) is the number of constraints, \( n \) is the number of variables, PD is the accelerated proximal distance algorithm, SCS is the Splitting Cone Solver, and Gurobi is the Gurobi solver. After \( m = 512 \) the constraint matrix \( A \) is initialized with sparsity level 0.01.

| Dimensions | Optima | CPU Seconds |
|------------|--------|-------------|
|            | PD     | SCS         | Gurobi     | PD     | SCS         | Gurobi     |
| 2          | 4      | 0.10598     | 0.10607    | 0.10598 | 0.0043     | 0.0103     | 0.0026     |
| 4          | 8      | 0.00000     | 0.00000    | 0.00000 | 0.0003     | 0.0009     | 0.0022     |
| 8          | 16     | 0.88988     | 0.88991    | 0.88988 | 0.0557     | 0.0011     | 0.0027     |
| 16         | 32     | 2.16514     | 2.16520    | 2.16514 | 0.0725     | 0.0012     | 0.0040     |
| 32         | 64     | 3.03855     | 3.03864    | 3.03853 | 0.0952     | 0.0019     | 0.0094     |
| 64         | 128    | 4.86894     | 4.86962    | 4.86895 | 0.1225     | 0.0065     | 0.0403     |
| 128        | 256    | 10.5863     | 10.5843    | 10.5863 | 0.1975     | 0.0810     | 0.0868     |
| 256        | 512    | 31.1039     | 31.0965    | 31.1039 | 0.5463     | 0.3995     | 0.3405     |
| 512        | 1024   | 27.0483     | 27.0475    | 27.0483 | 3.7667     | 1.6692     | 2.0189     |
| 1024       | 2048   | 1.45578     | 1.45569    | 1.45569 | 0.5352     | 0.3691     | 1.5489     |
| 2048       | 4096   | 2.22936     | 2.22930    | 2.22921 | 1.0845     | 2.4531     | 5.5521     |
| 4096       | 8192   | 1.72306     | 1.72202    | 1.72209 | 3.1404     | 17.272     | 15.204     |
| 8192       | 16384  | 5.36191     | 5.36116    | 5.36144 | 13.979     | 133.25     | 88.024     |

With a large sparse constraint matrix \( A \), extraction of its spectral decomposition becomes prohibitive. If we let \( E = (\rho^{-1/2} I - A^t c) \), then we must solve a linear system of equations defined by the Gramian matrix \( G = EE^t \). There are three reasonable options for solving this system. The first relies on computing and caching a sparse Cholesky decomposition of \( G \). The second computes the QR decomposition of the sparse matrix \( E \). The R part of the QR decomposition coincides with the Cholesky factor. Unfortunately, every time \( \rho \) changes, the Cholesky or QR decomposition must be redone. The third option is the conjugate gradient algorithm. In our experience the QR decomposition offers superior stability and accuracy. When \( E \) is very sparse, the QR decomposition is often much faster than the Cholesky decomposition because it avoids forming the dense matrix \( A^t A \). Even when only 5% of the entries of \( A \) are nonzero, 90% of the entries of \( A^t A \) can be nonzero. If exquisite accuracy is not a concern, then the conjugate gradient method provides the fastest update. Table 4 reflects this choice.

4.5 Copositive Matrices

A symmetric matrix \( M \) is copositive if its associated quadratic form \( x^t M x \) is nonnegative for all \( x \geq 0 \). Copositive matrices find applications in numerous branches of the mathematical sciences [6]. All positive semidefinite matrices and all matrices with nonnegative entries are copositive. The variational index

\[
\mu(M) = \min_{\|x\|=1, \ x \geq 0} x^t M x
\]

is one key to understanding copositive matrices [26]. The constraint set \( S \) is the intersection of the unit sphere and the nonnegative cone \( \mathbb{R}_+^n \). Projection of an external point \( y \) onto \( S \) splits into three cases. When all components of \( y \) are negative, then \( P_S(y) = e_i \), where \( y_i \) is the least negative component of \( y \), and \( e_i \) is
the standard unit vector along coordinate direction \( i \). The origin \( 0 \) is equidistant from all points of \( S \). If any component of \( y \) is positive, then the projection is constructed by setting the negative components of \( y \) equal to 0, and standardizing the truncated version of \( y \) to have Euclidean norm 1.

As a test case for the proximal distance algorithm, consider the Horn matrix [24]

\[
M = \begin{bmatrix}
1 & -1 & 1 & 1 & -1 \\
-1 & 1 & -1 & 1 & 1 \\
1 & -1 & 1 & -1 & 1 \\
1 & 1 & -1 & 1 & -1 \\
-1 & 1 & 1 & -1 & 1
\end{bmatrix}.
\]

The value \( \mu(M) = 0 \) is attained for the vectors \( \frac{1}{\sqrt{2}}(1, 1, 0, 0, 0)^t \), \( \frac{1}{\sqrt{6}}(1, 2, 1, 0, 0)^t \), and equivalent vectors with their entries permuted. Matrices in higher dimensions with the same Horn pattern of 1’s and -1’s are copositive as well [29]. A Horn matrix of odd dimension cannot be written as a positive semidefinite matrix, a nonnegative matrix, or a sum of two such matrices.

The proximal distance algorithm minimizes the criterion

\[
g(x | x_k) = \frac{1}{2} x^t M x + \frac{\rho}{2} \| x - P_S(x_k) \|^2
\]

and generates the updates

\[
x_{k+1} = (M + \rho I)^{-1} \rho P_S(x_k).
\]

It takes a gentle tuning schedule to get decent results. The choice \( \rho_k = 1.2^k \) converges in 600 to 700 iterations from random starting points and reliably yields objective values below \( 10^{-5} \) for Horn matrices. The computational burden per iteration is significantly eased by exploiting the cached spectral decomposition of \( M \). Table 5 compares the performance of the proximal distance algorithm to the Mosek solver on a range of Horn matrices. Mosek uses semidefinite programming to decide whether \( M \) can be decomposed into a sum of a positive semidefinite matrix and a nonnegative matrix. If not, Mosek declares the problem infeasible. Nesterov acceleration improves the final loss for the proximal distance algorithm, but it does not decrease overall computing time.

Testing for copositivity is challenging because neither the loss function nor the constraint set is convex. The proximal distance algorithm offers a fast screening device for checking whether a matrix is copositive. On random 1000 \( \times \) 1000 symmetric matrices \( M \), the method invariably returns a negative index in less than two seconds of computing time. Because the vast majority of symmetric matrices are not copositive, accurate estimation of the minimum is not required. Table 6 summarizes a few random trials with lower-dimensional symmetric matrices. In higher dimensions, Mosek becomes non-competitive, and Nesterov acceleration is of dubious value.

### 4.6 Linear Complementarity Problem

The linear complementarity problem [44] consists of finding vectors \( x \) and \( y \) with nonnegative components such that \( x^t y = 0 \) and \( y = Ax + b \) for a given square matrix \( A \) and vector \( b \). The natural loss function is \( \frac{1}{2} \| y - Ax - b \|^2 \). To project a vector pair \((u, v)\) onto the nonconvex constraint set, one considers each component pair \((u_i, v_i)\) in turn. If \( u_i \geq \max\{v_i, 0\} \), then the nearest pair \((x, y)\) has components
Table 5: CPU times (seconds) and optima for approximating the Horn variational index of a Horn matrix. Here \( n \) is the size of Horn matrix, PD is the proximal distance algorithm, aPD is the accelerated proximal distance algorithm, and Mosek is the Mosek solver.

| Dimension | Optima       | CPU Seconds |
|-----------|--------------|-------------|
| \( n \)  | PD           | aPD         | Mosek       |
| 4         | 0.000000     | 0.000000    | feasible    | 0.5555 | 0.0124 | 2.7744 |
| 5         | 0.000000     | 0.000000    | infeasible  | 0.0039 | 0.0086 | 0.0276 |
| 8         | 0.000021     | 0.000000    | feasible    | 0.0059 | 0.0083 | 0.0050 |
| 9         | 0.000045     | 0.000000    | infeasible  | 0.0055 | 0.0072 | 0.0082 |
| 16        | 0.000377     | 0.000001    | feasible    | 0.0204 | 0.0237 | 0.0185 |
| 17        | 0.000441     | 0.000001    | infeasible  | 0.0204 | 0.0378 | 0.0175 |
| 32        | 0.001610     | 0.000007    | feasible    | 0.0288 | 0.0288 | 0.1211 |
| 33        | 0.002357     | 0.000009    | infeasible  | 0.0242 | 0.0346 | 0.1294 |
| 64        | 0.054195     | 0.000026    | feasible    | 0.0415 | 0.0494 | 3.6284 |
| 65        | 0.006985     | 0.000026    | infeasible  | 0.0431 | 0.0551 | 2.7862 |

Table 6: CPU times and optima for testing the copositivity of random symmetric matrices. Here \( n \) is the size of matrix, PD is the proximal distance algorithm, aPD is the accelerated proximal distance algorithm, and Mosek is the Mosek solver.

| Dimension | Optima       | CPU Seconds |
|-----------|--------------|-------------|
| \( n \)  | PD           | aPD         | Mosek       |
| 4         | -0.391552    | -0.391561   | infeasible  | 0.0029 | 0.0031 | 0.0024 |
| 8         | -0.911140    | -2.050316   | infeasible  | 0.0037 | 0.0044 | 0.0045 |
| 16        | -1.680697    | -1.680930   | infeasible  | 0.0199 | 0.0272 | 0.0062 |
| 32        | -2.334520    | -2.510781   | infeasible  | 0.0261 | 0.0242 | 0.0441 |
| 64        | -3.821927    | -3.628060   | infeasible  | 0.0393 | 0.0437 | 0.6559 |
| 128       | -5.473609    | -5.475879   | infeasible  | 0.0792 | 0.0798 | 38.3919 |
| 256       | -7.956365    | -7.551814   | infeasible  | 0.1632 | 0.1797 | 456.1500 |
Table 7: CPU times (seconds) and optima for the linear complementarity problem with randomly generated data. Here $n$ is the size of matrix, PD is the accelerated proximal distance algorithm, and Gurobi is the Gurobi solver.

| Dimension | Optima |
|-----------|--------|
|           | CPU Seconds |
|           | PD | Mosek | PD | Mosek |
| 4         | 0.000000 | 0.000000 | 0.0230 | 0.0266 |
| 8         | 0.000000 | 0.000000 | 0.0062 | 0.0079 |
| 16        | 0.000000 | 0.000000 | 0.0269 | 0.0052 |
| 32        | 0.000000 | 0.000000 | 0.0996 | 0.4303 |
| 64        | 0.000074 | 0.000000 | 2.6846 | 360.5183 |

If $v_i \geq \max\{u_i, 0\}$, then the nearest pair has components $(x_i, y_i) = (0, v_i)$. Otherwise, $(x_i, y_i) = (0, 0)$. At each iteration the proximal distance algorithm minimizes the criterion

$$\frac{1}{2}\|y - Ax - b\|^2 + \frac{\rho}{2}\|x - \bar{x}_k\|^2 + \frac{\rho}{2}\|y - \bar{y}_k\|^2,$$

where $(\bar{x}_k, \bar{y}_k)$ is the projection of $(x_k, y_k)$ onto the constraint set. The stationarity equations become

$$0 = -A^t(y - Ax - b) + \rho(x - \bar{x}_k)$$
$$0 = y - Ax - b + \rho(y - \bar{y}_k).$$

Substituting the value of $y$ from the second equation into the first equation leads to the updates

$$x_{k+1} = [(1 + \rho)I + A^tA]^{-1}[A^t(\bar{y}_k - b) + (1 + \rho)\bar{x}_k]$$
$$y_{k+1} = \frac{1}{1 + \rho}(Ax_{k+1} + b) + \frac{\rho}{1 + \rho}\bar{y}_k.$$

The linear system (12) can be solved in low to moderate dimensions by computing and caching the spectral decomposition of $A^tA$ and in high dimensions by the conjugate gradient method. Table 7 compares the performance of the proximal gradient algorithm to the Gurobi solver on some randomly generated problems.

### 4.7 Sparse Principal Components Analysis

Let $X$ be an $n \times p$ data matrix gathered on $n$ cases and $p$ predictors. Assume the columns of $X$ are centered to have mean 0. Principal component analysis (PCA) [27, 49] operates on the sample covariance matrix $S = \frac{1}{n}X^tX$. Here we formulate a proximal distance algorithm for sparse PCA (SPCA), which has attracted substantial interest in the machine learning community [8, 7, 18, 30, 31, 54, 55]. According to a result of Ky Fan [20], the first $q$ principal components (PCs) $u_1, \ldots, u_q$ can be extracted by maximizing the function $\text{tr}(U^tSU)$ subject to the matrix constraint $U^tU = I_q$, where $u_i$ is the $i$th column of the $p \times q$ matrix $U$. This constraint set is called a Stiefel manifold. One can impose sparsity by insisting that any given column $u_i$ have at most $r$ nonzero entries. Alternatively, one can require the entire matrix $U$ to have at most $r$ nonzero entries. The latter choice permits sparsity to be distributed non-uniformly across columns.
Extraction of sparse PCs is difficult for three reasons. First, the Stiefel manifold $M_q$ and both sparsity sets are nonconvex. Second, the objective function is concave rather than convex. Third, there is no simple formula or algorithm for projecting onto the intersection of the two constraint sets. Fortunately, it is straightforward to project onto each separately. Let $P_{M_q}(U)$ denote the projection of $U$ onto the Stiefel manifold. It is well known that $P_{M_q}(U)$ can be calculated by extracting a partial singular value decomposition $U = V \Sigma W^t$ of $U$ and setting $P_{M_q}(U) = V W^t$ \[23\]. Here $V$ and $W$ are orthogonal matrices of dimension $p \times q$ and $q \times q$, respectively, and $\Sigma$ is a diagonal matrix of dimension $q \times q$. Let $P_{S_r}(U)$ denote the projection of $U$ onto the sparsity set $S_r = \{ V : v_{ij} \neq 0 \text{ for at most } r \text{ entries of each column } v_i \}$.

Because $P_{S_r}(U)$ operates column by column, it suffices to project each column vector $u_i$ to sparsity. This entails nothing more than sorting the entries of $u_i$ by magnitude, saving the $r$ largest, and sending the remaining $p-r$ entries to 0. If the entire matrix $U$ must have at most $r$ nonzero entries, then $U$ can be treated as a concatenated vector during projection.

The key to a good algorithm is to incorporate the Stiefel constraints into the domain of the objective function \[32, 33\] and the sparsity constraints into the distance penalty. Thus, we propose decreasing the criterion

$$f(U) = -\frac{1}{2} \tr(U^t SU) + \frac{\rho}{2} \dist(U, S_r)^2.$$  

at each iteration subject to the Stiefel constraints. The loss can be majorized via

$$-\frac{1}{2} \tr(U^t SU) = -\frac{1}{2} \tr[(U - U_k)^t S(U - U_k)] - \tr(U^t SU_k) + \frac{1}{2} \tr(U_k^t SU_k)\leq -\tr(U^t SU_k) + \frac{1}{2} \tr(U_k^t SU_k)$$  

because $S$ is positive semidefinite. The penalty is majorized by

$$\frac{\rho}{2} \dist(U, S_r)^2 \leq -\rho \tr[U^t P_{S_r}(U_k)] + c_k$$  

up to an irrelevant constant $c_k$ since the squared Frobenius norm satisfies the relation $\|U^t U\|_F^2 = q$ on the Stiefel manifold. It now follows that $f(U)$ is majorized by

$$\frac{1}{2} \|U - SU_k - \rho P_{S_r}(U_k)\|_F^2$$  

up to an irrelevant constant. Accordingly, the Stiefel projection

$$U_{k+1} = P_{M_q}[SU_k + \rho P_{S_r}(U_k)]$$  

provides the next MM iterate.

Figures 1 and 2 compare the proximal distance algorithm to the SPC function from the R package PMA \[54\]. The breast cancer data from PMA provide the data matrix $X$. The data consist of $p = 19, 672$ RNA measurements on $n = 89$ patients. The two figures show computation times and the proportion of variance explained (PVE) by the $p \times q$ loading matrix $U$. For sparse PCA, PVE is defined as $\tr(X_q^t X_q) / \tr(X^t X)$, where $X_q = XU(U^t U)^{-1}U^t$ \[50]. When the loading vectors of $U$ are orthogonal, this criterion reduces
Figure 1: Proportion of variance explained by $q$ PCs for each algorithm. Here PD1 is the accelerated proximal distance algorithm enforcing matrix sparsity, PD2 is the accelerated proximal distance algorithm enforcing column-wise sparsity, and SPC is the orthogonal sparse PCA method from PMA.
Figure 2: Computation times for $q$ PCs for each algorithm. Here PD1 is the accelerated proximal distance algorithm enforcing matrix sparsity, PD2 is the accelerated proximal distance algorithm enforcing column-wise sparsity, and SPC is the orthogonal sparse PCA method from PMA.
to the familiar definition $\text{tr}(U^t X^t X U) / \text{tr}(X^t X)$ of PVE for ordinary PCA. The proximal distance algorithm enforces either matrix-wise or column-wise sparsity. In contrast, SPC enforces only column-wise sparsity via the constraint $\|u_i\|_1 \leq c$ for each column $u_i$ of $U$. We take $c = 8$. The number of nonzeroes per loading vector output by SPC dictates the sparsity level for the column-wise version of the proximal distance algorithm. Summing these counts across all columns dictates the sparsity level for the matrix version of the proximal distance algorithm.

Figures 1 and 2 demonstrate the superior PVE and computational speed of both proximal distance algorithms versus SPC. The type of projection does not appear to affect the computational performance of the proximal distance algorithm, as both versions scale equally well with $q$. However, the matrix projection, which permits the algorithm to more freely assign nonzeroes to the loadings, attains better PVE than the more restrictive column-wise projection. For both variants of the proximal distance algorithm, Nesterov acceleration improves both fitting accuracy and computational speed, especially as the number of PCs $q$ increases.

5 Discussion

The proximal distance algorithm applies to a host of problems. In addition to the linear and quadratic programming examples considered here, our previous paper [38] derives and tests algorithms for binary piecewise-linear programming, $\ell_0$ regression, matrix completion [12, 13, 14, 42], and sparse precision matrix estimation [21]. Other potential applications immediately come to mind. An integer linear program in standard form can be expressed as minimizing $c^t x$ subject to $Ax + s = b$, $s \geq 0$, and $x \in \mathbb{Z}^p$. The latter two constraints can be combined in a single constraint for which projection is trivial. The affine constraints should be folded into the domain of the objective. Integer programming is NP hard, so that the proximal distance algorithm just sketched is merely heuristic. Integer linear programming includes traditional NP hard problems such as the traveling salesman problem, the vertex cover problem, set packing, and Boolean satisfiability. It will be interesting to see if the proximal distance principle is competitive in meeting these challenges. Our experience with the closest lattice point problem [11] and the eight queens problem suggests that the proximal distance algorithm can be too greedy for hard combinatorial problems. The nonconvex problems solved in this paper are in some vague sense easy combinatorial problems.

The behavior of a proximal distance algorithm depends critically on a sensible tuning schedule for increasing $\rho$. Starting $\rho$ too high puts too much stress on satisfying the constraints. Incrementing $\rho$ too quickly causes the algorithm to veer off the solution path guaranteed by the penalty method. Given the chance of roundoff error even with double precision arithmetic, it is unwise to take $\rho$ all the way to $\infty$. Trial and error can help in deciding whether a given class of problems will benefit from an aggressive update schedule and strict or loose convergence criteria. In problems with little curvature such as linear programming, more conservative updates are probably prudent. Both the closest kinship matrix problem and the SPCA problem document the value of folding constraints into the domain of the loss. In the same spirit it is wise to minimize the number of constraints. A single penalty for projecting onto the intersection of two constraint sets is almost always preferable to two penalties for their separate projections. Exceptions to this rule occur when projection onto the intersection is hard. The integer linear programming problem mentioned previously illustrates these ideas.

Our earlier proximal distance algorithms ignored acceleration. In many cases the solutions produced had very low accuracy. The realization that convex proximal distance algorithms can be phrased as proximal gradient algorithms convinced us to try Nesterov acceleration. We now do this routinely on the subproblems with $\rho$ fixed. This typically forces tighter path following and a reduction in overall computing times. Our
examples generally bear out the contention that Nesterov acceleration is useful in nonconvex problems. However, the value of acceleration often lies in improving the quality of a solution as much as it does in increasing the rate of convergence. Of course, acceleration cannot prevent convergence to an inferior local minimum.

We hope readers will sense the potential of the proximal distance principle. This simple idea offers insight into many existing algorithms and a straightforward path in devising new ones. Effective proximal and projection operators usually spell the difference between success and failure. The number and variety of such operators is expanding quickly as the field of optimization relinquishes its fixation on convexity. The current paper research leaves many open questions about tuning schedules, rates of convergence, and acceleration in the face of nonconvexity. We welcome the contributions of other mathematical scientists in unraveling these mysteries and in inventing new proximal distance algorithms.

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