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The indefinite proximal gradient method

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Abstract: We introduce a variant of the proximal gradient method in which the quadratic term is diagonal but may be indefinite, and is safeguarded by a trust region. Our method is a special case of the proximal quasi-Newton trust-region method of Aravkin et al. [3]. We provide closed-form solution of the step computation in certain cases where the nonsmooth term is separable and the trust region is defined in the infinity norm, so that no iterative subproblem solver is required. Our analysis expands upon that of [3] by generalizing the trust-region approach to problems with bound constraints. We provide an efficient open-source implementation of our method, named TRDH, in the Julia language in which Hessians approximations are given by diagonal quasi-Newton updates. TRDH evaluates one standard proximal operator and one indefinite proximal operator per iteration. We also analyze and implement a variant named iTRDH that performs a single indefinite proximal operator evaluation per iteration. We establish that iTRDH enjoys the same asymptotic worst-case iteration complexity as TRDH. We report numerical experience on unconstrained and bound-constrained problems, where TRDH and iTRDH are used both as standalone and subproblem solvers. Our results illustrate that, as standalone solvers, TRDH and iTRDH improve upon the quadratic regularization method R2 of [3] but also sometimes upon their quasi-Newton trust-region method, referred to here as TR-R2, in terms of smooth objective value and gradient evaluations. On challenging nonnegative matrix factorization, binary classification and data fitting problems, TRDH and iTRDH used as subproblem solvers inside TR improve upon TR-R2 for at least one choice of diagonal approximation.

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Dedicatory: In honor and memory of our colleague and friend Daniela di Serafino.

1 Introduction

We consider the nonsmooth regularized problem

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} \ f(x) + h(x) \quad \text{subject to } \ell \leqslant x \leqslant \mathfrak{u}, \tag{1}$$

where $\ell \in (\mathbb{R} \cup \{-\infty\})^n$, $\mathfrak{u} \in (\mathbb{R} \cup \{+\infty\})^n$ with $\ell \leqslant \mathfrak{u}$ componentwise, $f: \mathbb{R}^n \to \mathbb{R}$ is continuously differentiable on an open set containing $[\ell,\mathfrak{u}]$, and $\mathfrak{h}: \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ is proper and lower semicontinuous (lsc). A component $\ell_\mathfrak{t} = -\infty$ or $\mathfrak{u}_\mathfrak{t} = +\infty$ indicates that $\mathfrak{x}_\mathfrak{t}$ is unbounded below or above, respectively. Both f and h may be nonconvex. Typically, h is nonsmooth and serves to identify a local minimizer of f with desirable features, such as sparsity.

Numerical methods for (1) are typically based on the proximal-gradient method [21]. Aravkin et al. [3] provide an overview of recent works focusing on (1) where both f and h may be nonconvex, to which we refer the reader. In addition, they propose two methods: an adaptive quadratic regularization approach named R2, which may be viewed as a proximal-gradient method with adaptive step size, and a quasi-Newton trust-region method named TR in which the subproblem consist in minimizing a quadratic approximation of f about the current iterate regularized by a model of h inside a trust region. Typically, an explicit solution to the subproblem is not known, and an iterative procedure must be used—the authors use R2. Aravkin et al. [2] develop a similar approach designed for applications where f is a least-squares residual. They propose a trust-region and a regularization approach. Again, they use R2 as subproblem solver.

In both R2 and the traditional proximal-gradient method, a uniformly positively scaled ∇f is used to compute a step, and that computation relies on the proximal operator—see Section 2 for precise definitions. Some authors consider positive-definite diagonal gradient scaling—see below. In the present research, we contend that generalizing the definition of the proximal operator by allowing a diagonal scaling of ∇f , and even permitting negative scaling factors, continues to allow us to derive analytical solutions for several nonsmooth terms of interest in applications. Moreover, such potentially indefinite scaling might allow the model to better capture inherent nonconvexity in f about the current iterate. We devise a trust-region method based on those ideas and name it TRDH, which stands for *trust-region method with diagonal Hessian approximations*. At every iteration, our method performs the evaluation of both a classical proximal operator and a generalized proximal operator with indefinite diagonal scaling. However, it is possible to modify TRDH slightly to devise a variant that requires a single generalized proximal operator evaluation per iteration while preserving the asymptotic worst-case evaluation complexity bound. We name the variant iTRDH, which stands for *indefinite trust-region method with diagonal Hessian*.

Diagonal gradient scaling could be referred to as diagonal quasi-Newton, and though the literature appears to be thin on that subject, there exist a few references. Diagonal Hessian approximations range from a multiple of the identity, as in the traditional proximal-gradient or the spectral gradient method, to approximations computed based on a relaxed secant equation. We go into more details in Section 4.

Because we use the ℓ_{∞} -norm to define the trust region, we are able to treat bound constraints naturally, by taking the intersection of $[\ell, u]$ with the trust region. Our generalized *indefinite* proximal operators must take the indicator of the resulting box into account together with h, or a model thereof.

A by-product of the present research is an efficient software implementation of TRDH and iTRDH, both as standalone solvers, and as subproblem solvers for use inside TR. TRDH and iTRDH can use several diagonal Hessian approximations: the multiple of the identity given by the spectral gradient approximation, and two diagonal quasi-Newton approximations based on the weak secant equation. Our open-source implementations in Julia are available from https://github.com/JuliaSmoothOptimizers/RegularizedOptimization.jl.

We report numerical experience conducted with TRDH, iTRDH, TR-TRDH and TR-iTRDH on a range of unconstrained and bound-constrained problems, where TR-TRDH and TR-iTRDH refer to TRDH and iTRDH used as subsolvers in TR. Our general conclusion is that for at least one choice of a diagonal Hessian approximation, TRDH and iTRDH outperform R2 in terms of evaluations of f and ∇f . In addition, for at least one choice of a diagonal Hessian approximation, TR-TRDH and TR-iTRDH outperform TR-R2 on the same metric. Our detailed results are in Section 6.

Related research

Most of the literature focuses on positive-definite diagonal scaling of the proximal operator; Becker and Fadili [9] and Becker et al. [10] consider positive-definite quasi-Newton approximations of the form $H = D + VV^T$ where D is positive definite and diagonal, and a specialized procedure to solve the proximal quasi-Newton subproblems. Under their assumptions, H remains uniformly bounded. Their analysis is restricted to f and h convex and does not provide complexity bounds.

Duchi et al. [17] present the ADAGRAD algorithm, which is commonly used in online learning. ADAGRAD is a stochastic algorithm but a deterministic implementation of it would minimize a smooth objective such as f using a variant of the projected gradient algorithm, that can be seen as a special case of the proximal gradient method, using a positive diagonal gradient scaling. At iteration k, the scaling is set to $\text{diag}(G_k)^{-1/2}$ where $G_k = \sum_{j=0}^k \nabla f(x_j) \nabla f(x_j)^T$.

Scheinberg and Tang [27] also focus on positive-definite and uniformly-bounded Hessian approximations for f and h convex. Their numerical results employ a limited-memory BFGS approximation, although the latter is liable to grow unbounded [14, §8.4]. The proximal quasi-Newton subproblem is solved inexactly with a coordinate descent algorithm.

Aravkin et al. [3] propose a proximal quasi-Newton trust-region method for nonconvex f and h under weak assumptions, accompanied by a complexity analysis. They employ limited-memory BFGS or SR1 approximations and solve subproblems using the proximal-gradient method or R2. Though their analysis assumes the Hessian approximations are uniformly bounded, there are known procedures to estimate bounds on the eigenvalues of quasi-Newton approximations after an update, and those bounds can be used to skip or modify the update to keep it bounded [22].

Similarly, Baraldi and Kouri [4] present a proximal trust-region method with inexact objective and gradient evaluations, under the additional assumption that h must be convex. They show numerical results with exact Hessian when it is available, and employ iterative solvers to approximate it otherwise.

Notation

 $\mathbb B$ is the unit ball centered at the origin and defined by a norm dictated by the context, and $\Delta \mathbb B$ is the ball of radius $\Delta > 0$ centered at the origin. For fixed $x \in \mathbb R^n$, the ball of radius Δ centered at x is $x + \Delta \mathbb B$. When it is necessary to indicate that $\mathbb B$ is defined by the ℓ_p -norm, for $1 \leqslant p \leqslant +\infty$, we write $\mathbb B_p$. For $A \subseteq \mathbb R^n$, the indicator of A is $\chi(\cdot \mid A) : \mathbb R^n \to \mathbb R \cup \{+\infty\}$ defined as $\chi(x \mid A) = 0$ if $x \in A$ and $+\infty$ otherwise. If $A \neq \varnothing$, $\chi(\cdot \mid A)$ is proper. If A is closed, $\chi(\cdot \mid A)$ is lsc. For $D \in \mathbb R^{m \times n}$ with elements $\delta_{i,j}$, $|D| \in \mathbb R^{m \times n}$ has elements $|\delta_{i,j}|$. For a finite set $A \subset \mathbb N$, we denote |A| its cardinality. If f_1 and f_2 are two positive functions of $\varepsilon > 0$, we say that $f_1(\varepsilon) = O(f_2(\varepsilon))$ if there exists a constant C > 0 such that $f_1(\varepsilon) \leqslant Cf_2(\varepsilon)$ for all $\varepsilon > 0$ sufficiently small.

2 Background

The following are standard variational analysis concepts—see, e.g., [26]. Let $\phi: \mathbb{R}^n \to \overline{\mathbb{R}}$ and $\bar{x} \in \mathbb{R}^n$ where ϕ is finite. The Fréchet subdifferential of ϕ at \bar{x} is the closed convex set $\hat{\partial}\phi(\bar{x})$ of $v \in \mathbb{R}^n$ such

that

$$\liminf_{\substack{x \to \bar{x} \\ x \neq \bar{x}}} \frac{\varphi(x) - \varphi(\bar{x}) - \nu^{\mathsf{T}}(x - \bar{x})}{\|x - \bar{x}\|} \geqslant 0.$$

The limiting subdifferential of φ at \bar{x} is the closed, but not necessarily convex, set $\partial \varphi(\bar{x})$ of $\nu \in \mathbb{R}^n$ for which there exist $\{x_k\} \to \bar{x}$ and $\{\nu_k\} \to \nu$ such that $\{\varphi(x_k)\} \to \varphi(\bar{x})$ and $\nu_k \in \widehat{\partial} \varphi(x_k)$ for all k. $\widehat{\partial} \varphi(\bar{x}) \subset \partial \varphi(\bar{x})$ always holds.

The horizon subdifferential of φ at \bar{x} is the closed, but not necessarily convex, cone $\vartheta^{\infty}\varphi(\bar{x})$ of $\nu \in \mathbb{R}^n$ for which there exist $\{x_k\} \to \bar{x}$, $\{\nu_k\}$ and $\{\lambda_k\} \downarrow 0$ such that $\{\varphi(x_k)\} \to \varphi(\bar{x})$, $\nu_k \in \widehat{\vartheta}\varphi(x_k)$ for all k, and $\{\lambda_k\nu_k\} \to \nu$.

If $C \subseteq \mathbb{R}^n$ and $\bar{x} \in C$, the closed convex cone $\widehat{N}_C(\bar{x}) := \widehat{\partial} \chi(\bar{x} \mid C)$ is called the regular normal cone to C at \bar{x} . The closed cone $N_C(\bar{x}) := \partial \chi(\bar{x} \mid C) = \partial^\infty \chi(\bar{x} \mid C)$ is called the normal cone to C at \bar{x} . $\widehat{N}_C(\bar{x}) \subseteq N_C(\bar{x})$ always holds, and is an equality if C is convex.

If $\phi: \mathbb{R}^n \to \overline{\mathbb{R}}$ is proper lsc, and $C \subseteq \mathbb{R}^n$ is closed, we say that the *constraint qualification* is satisfied at $\bar{x} \in C$ for the constrained problem

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} \ \varphi(x) \quad \text{subject to } x \in C$$

if

$$\partial^{\infty} \phi(\bar{\mathbf{x}}) \cap \mathsf{N}_{\mathsf{C}}(\bar{\mathbf{x}}) = \{0\}. \tag{2}$$

As an example where (2) fails to hold, let n = 1, f(x) = 0 for all $x \in \mathbb{R}$,

$$h(x) = \begin{cases} x & \text{if } x \ge 0, \\ +\infty & \text{if } x < 0, \end{cases}$$

and C = [0, 1]. Clearly, $\bar{x} = 0$ is the only stationary point and $N_C(\bar{x}) = \{\nu \mid \nu \leq 0\}$. Let epi h denote the epigraph of h, i.e., the set $\{(x, t) \mid x \in \mathbb{R}^n, t \geqslant h(x)\}$. Because h is locally lsc about \bar{x} , [26, Theorem 8.9] yields

$$\eth^{\infty} h(\bar{x}) = \{ \nu \mid (\nu, 0) \in N_{epi\,h}(\bar{x}, h(\bar{x})) \} = \{ \nu \mid (\nu, 0) \in N_{epi\,h}(0, 0) \} = N_{C}(\bar{x}),$$

and the constraint qualification does not hold. The reason is that h and $\chi(\cdot \mid C)$ both have a jump discontinuity at \bar{x} and take the value $+\infty$ for $x < \bar{x}$, which is akin to repeating a constraint.

We say that \bar{x} is first-order stationary for (1) if $0 \in \partial(f+h+\chi(\cdot\mid [\ell,u]))(\bar{x}) = \nabla f(\bar{x}) + \partial(h+\chi(\cdot\mid [\ell,u]))(\bar{x})$. If \bar{x} is a local solution of (1), it is first-order stationary [26, Theorem 10.1]. Under (2) applied to (1), which reads $(\nabla f(\bar{x}) + \partial^{\infty} h(\bar{x})) \cap N_{[\ell,u]}(\bar{x}) = \{0\}$, the necessary optimality condition can be written equivalently as $0 \in \nabla f(\bar{x}) + \partial h(\bar{x}) + N_{[\ell,u]}(\bar{x})$ [26, Theorem 8.15]. When (1) is unconstrained or $\bar{x} \in \text{int}[\ell,u]$, the normal cone is $\{0\}$, the constraint qualification is satisfied, and the necessary condition reduces to $0 \in \nabla f(\bar{x}) + \partial h(\bar{x})$.

The proximal operator associated with h is

$$\underset{vh}{\text{prox}}(q) := \underset{x}{\text{argmin}} \ \frac{1}{2}v^{-1} \|x - q\|_{2}^{2} + h(x), \tag{3}$$

where $\nu > 0$ is a preset steplength. If h is prox-bounded and $\nu > 0$ is sufficiently small, $\text{prox}_{\nu h}(q)$ is a nonempty and closed set. It may contain multiple elements.

The proximal gradient method [21] is a generalization of the gradient method that takes the nonsmooth term into account. It generates iterates $\{x_k\}$ according to

$$x_{k+1} \in \underset{\nu_k h}{\text{prox}}(x_k - \nu_k \nabla f(x_k)). \tag{4}$$

Equivalently, and more instructively,

$$s_k \in \operatorname{argmin} \ \frac{1}{2} \nu_k^{-1} \| s + \nu_k \nabla f(x_k) \|_2^2 + h(x_k + s),$$
 (5a)

= argmin
$$\nabla f(x_k)^T s + \frac{1}{2} \nu_k^{-1} ||s||_2^2 + h(x_k + s),$$
 (5b)

$$x_{k+1} = x_k + s_k, \tag{5c}$$

where it becomes clear that the computation of s_k results from formulating a simple quadratic model

$$f(x_k) + \nabla f(x_k)^T s + \frac{1}{2} \nu_k^{-1} ||s||_2^2 \approx f(x_k + s)$$
 (6)

of the smooth term f, to which we add the nonsmooth term h.

The effectiveness of (5) comes from the observation that it is possible to determine a closed form solution s_k , or at least a specialized procedure to identify such a global minimizer, for numerous choices of h that are relevant in applications [8], without resort to a general-purpose optimization solver.

Aravkin et al. [3] devise a trust-region quasi-Newton method for (1) without explicit bound constraints in which subproblems are solved inexactly by a method closely related to (5). However, the subproblem has the additional trust-region constraint $s \in \Delta_k \mathbb{B}$:

$$s_k \in \underset{s}{\operatorname{argmin}} \ \nabla f(x_k)^{\mathsf{T}} s + \frac{1}{2} \nu_k^{-1} ||s||_2^2 + h(x_k + s) + \chi(s \mid \Delta_k \mathbb{B}),$$
 (7)

where $\Delta_k > 0$, which may be construed as changing $h(x_k + s)$ to $h(x_k + s) + \chi(s \mid \Delta_k \mathbb{B})$. Because both $s \mapsto h(x_k + s)$ and $s \mapsto \chi(s \mid \Delta \mathbb{B})$ are proper and lsc, so is their sum. In addition, because $\Delta_k \mathbb{B}$ is bounded, h no longer needs to be prox-bounded for a solution to exist. Again, a closed form solution may be found for a variety of cases of interest in applications [2, 3].

3 The indefinite proximal operator

3.1 Definition and Examples

We restrict ourselves to the case where h is separable, i.e., $h(x) = h_1(x_1) + \cdots + h_n(x_n)$, in which case the search for an element s of (6) decouples componentwise:

$$s_i \in \underset{s_i}{\operatorname{argmin}} \ g_i s_i + \frac{1}{2} v^{-1} s_i^2 + h_i (x_i + s_i),$$

where g_i is the i-th component of $\nabla f(x_k)$. If $\mathbb B$ is defined in the ℓ_∞ -norm, (7) also decouples. Without loss of generality, and accounting for the bound constraints of (1), we write it as

$$s_{i} \in \underset{s_{i}}{\operatorname{argmin}} \ g_{i}s_{i} + \frac{1}{2}\nu^{-1}s_{i}^{2} + h_{i}(x_{i} + s_{i}) + \chi(s_{i} \mid [\tilde{\ell}_{i}, \tilde{u}_{i}]),$$
 (8)

where $\tilde{\ell}_i := max(\ell_i - x_i, -\Delta)$ and $\tilde{u}_i := min(u_i - x_i, \Delta)$ are the ith components of $\tilde{\ell}$ and $\tilde{u} \in \mathbb{R}^n$, which describe the intersection of the box $[\ell, u]$ with the trust region.

Replacing the quadratic coefficient in (8) by a positive scalar $\delta_i > 0$ does not complicate the problem as it simply amounts to changing the value of ν . In the following, we contend that replacing the quadratic coefficient by $\delta_i \leq 0$ continues to allow us to derive a closed form solution in certain cases. Observe that modifying the quadratic term as described amounts to changing (6) to

$$f(x_k) + \nabla f(x_k)^T s + \frac{1}{2} s^T D_k s$$

where $D_k = diag(d_k)$, and $d_k \in \mathbb{R}^n$ has components $\delta_{k.i}$. Crucially, we wish to allow D_k to be indefinite to capture any nonconvexity of f about x_k to a certain extent. While such change may make the quadratic model nonconvex, the indicator of $[\tilde{\ell}_i, \, \tilde{u}_i]$ ensures that a finite solution exists.

Definition 1. Let $g \in \mathbb{R}^n$, $D \in \mathbb{R}^{n \times n}$ be diagonal and $C \subset \mathbb{R}^n$ be nonempty. The indefinite proximal operator of h with respect to g, D and C is

The usual proximal operator of vh at $q \in \mathbb{R}^n$ is a special case of Definition 1 in which $C = \mathbb{R}^n$, $D = v^{-1}I$, and $g = -v^{-1}q$.

Example 1. Consider $h(x) = \lambda ||x||_0$, where $\lambda > 0$, and $C := [\ell, u]$, where ℓ , $u \in \mathbb{R}^n$ with $\ell < u$ componentwise. The computation of x in (9) decouples componentwise as

$$x_i \in \operatorname*{argmin}_{x_i} g_i x_i + \tfrac{1}{2} \delta_i x_i^2 + \lambda |x_i|_0 + \chi(x_i \mid [\ell_i, \, u_i]).$$

Note that

$$g_ix_i+\tfrac{1}{2}\delta_ix_i^2+\lambda|x_i|_0=\begin{cases} 0 & \text{if } x_i=0\\ \lambda+g_ix_i+\tfrac{1}{2}\delta_ix_i^2 & \text{if } x_i\neq0. \end{cases}$$

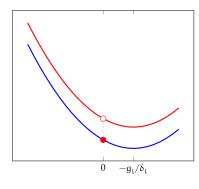
If $\delta_i = 0$, the solution set of the above problem is

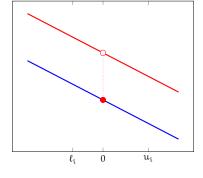
- $[\ell_i, u_i]$ if $g_i = 0$ and either $\ell_i > 0$ or $u_i < 0$;
- $argmin\{\lambda + g_ix_i \mid x_i \in M_i\}$ where M_i is the set $\{\ell_i, u_i\}$ together with 0 if $0 \in (\ell_i, u_i)$ in all other cases.

If $\delta_i \neq 0$, the solution set is $\operatorname{argmin}\{\lambda + g_i x_i + \frac{1}{2} \delta_i x_i^2 \mid x_i \in M_i\}$, where M_i is the finite set comprising ℓ_i , u_i together with

- $-g_i/\delta_i$ if $\delta_i > 0$;
- $0 \text{ if } 0 \in (\ell_i, u_i).$

See Figure 1 for an illustration of a few cases.





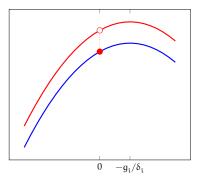


Figure 1: Illustration of Example 1 with $\delta_i > 0$ (left), $\delta_i = 0$ (center), and $\delta_i < 0$ (right). The blue curve is $g_i x_i + \frac{1}{2} \delta_i x_i^2$ while the red curve is $g_i x_i + \frac{1}{2} \delta_i x_i^2 + \lambda |x_i|_0$.

Example 2. Consider $h(x) = \lambda ||x||_1$ where $\lambda > 0$, and C as in Example 1. The computation of x in (9) decouples componentwise as

$$x_i \in \operatorname*{argmin}_{x_i} g_i x_i + \tfrac{1}{2} \delta_i x_i^2 + \lambda |x_i| + \chi(x_i \mid [\ell_i, u_i]).$$

Note that

$$g_ix_i+\tfrac{1}{2}\delta_ix_i^2+\lambda|x_i|=\begin{cases} (g_i+\lambda)x_i+\tfrac{1}{2}\delta_ix_i^2 & \text{if } x_i\geqslant 0\\ (g_i-\lambda)x_i+\tfrac{1}{2}\delta_ix_i^2 & \text{if } x_i<0. \end{cases}$$

If $\delta_i = 0$, the solution of the above problem is

- $[\ell_i, \max(0, \ell_i)]$ if $g_i = \lambda$;
- $[\min(u_i, 0), u_i]$ if $g_i = -\lambda$;
- $\operatorname{proj}(0 \mid [\ell_i, u_i]) \text{ if } 0 \leq |g_i| < \lambda;$
- $\{\ell_i\}$ if $g_i > \lambda$;
- $\{u_i\}$ if $g_i < -\lambda$.

Consider now the case where $\delta_i > 0$. The branch of quadratic for $x_i \geqslant 0$ lies above the horizontal axis if $g_i \geqslant -\lambda$, and that for $x_i < 0$ does the same if $g_i \leqslant \lambda$. Thus, if $|g_i| \leqslant \lambda$, the unique unconstrained minimizer is 0 and, by convexity, the solution of the constrained problem is $proj(0 \mid [\ell_i, u_i])$.

If $g_i > \lambda$, for the unconstrained minimizer is $\bar{x}_i := -(g_i - \lambda)/\delta_i < 0$. By convexity, the solution of the constrained problem is $proj(\bar{x}_i \mid [\ell_i, u_i])$. The situation is similar when $g_i < -\lambda$.

Consider finally the case where $\delta_i < 0$. In this case, the unique constrained minimizer is $\mathop{argmin}\{g_i x_i + \frac{1}{2} \delta_i x_i^2 + \lambda |x_i| \mid x_i \in M_i\}$ where M_i is the set containing ℓ_i and u_i together with 0 if the latter lies inside $[\ell_i, u_i]$.

Figure 2 illustrates a few representative cases.

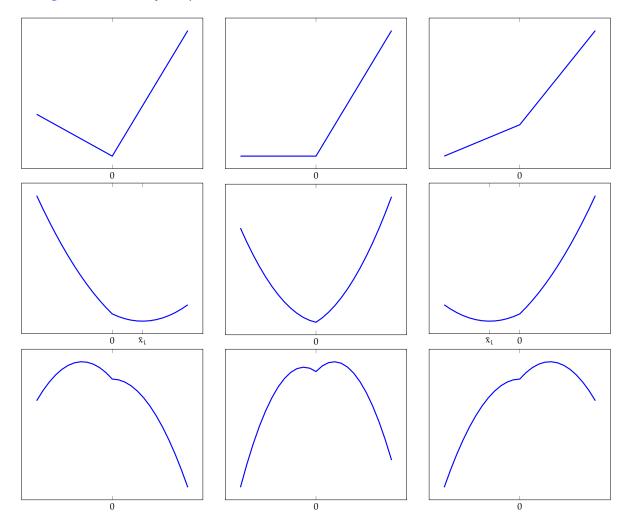


Figure 2: Illustration of Example 2. Top row: $\delta_i=0$. From left to right: $0\leqslant g_i<\lambda$, $g_i=\lambda$, and $g_i>\lambda$. Middle row: $\delta_i>0$. From left to right: $g_i<-\lambda$, $|g_i|\leqslant\lambda$, and $g_i>\lambda$. Bottom row: $\delta_i<0$. From left to right: $g_i\leqslant-\lambda$, $|g_i|<\lambda$, and $g_i>\lambda$.

3.2 Properties

At $x \in \mathbb{R}^n$ where h is finite, consider models

$$\varphi(s;x) \approx f(x+s) \tag{10a}$$

$$\psi(s;x) \approx h(x+s) \tag{10b}$$

$$m(s;x) := \varphi(s;x) + \psi(s;x). \tag{10c}$$

We make the following assumption on the models (10).

Model Assumption 3.1. For any $x \in \mathbb{R}^n$, $\varphi(\cdot; x) \in \mathbb{C}^1$, and satisfies $\varphi(0; x) = f(x)$ and $\nabla \varphi(0; x) = \nabla f(x)$. For any $x \in \mathbb{R}^n$ where h is finite, $\psi(\cdot; x)$ is proper lsc, and satisfies $\psi(0; x) = h(x)$ and $\partial \psi(0; x) = \partial h(x)$. **Proposition 1.** Let $C \subset \mathbb{R}^n$ be nonempty and compact, and let Model Assumption 3.1 be satisfied. Let (1) satisfy the constraint qualification (2) at $x \in C$. Assume $0 \in \operatorname{argmin}_s m(s; x) + \chi(x + s \mid C)$, and let the latter subproblem satisfy the constraint qualification (2) at $x \in C$. Then $x \in C$ is first-order stationary for (1).

Proof. Let $\chi_{x,C}(s) := \chi(x+s \mid C)$. Because C is compact, Model Assumption 3.1 ensures that $s \mapsto m(s;x) + \chi(x+s \mid C)$ is lsc, bounded below and that a minimizer exists. By assumption, $0 \in \nabla f(x) + \partial (\psi + \chi_{x,C})(0)$. By the constraint qualification for the subproblem and Model Assumption 3.1, $0 \in \nabla f(x) + \partial h(x) + N_C(x)$, which are the first-order optimality conditions for (1).

In the assumptions of Proposition 1, satisfaction of the constraint qualification in the subproblem is ensured if $\vartheta^{\infty}\psi(0;x) = \vartheta^{\infty}h(x)$ provided (2) is satisfied at x for (1).

4 Diagonal quasi-Newton methods

The simplest possible diagonal approximation to $\nabla^2 f(x_k)$ is $B_k := \sigma_k I$ for some scalar σ_k , where I denotes the identity. In the R2 algorithm [3, Algorithm 6.1], σ_k is chosen adaptively at each iteration based on progress. A more sophisticated strategy consists in choosing σ_k so as to best approximate $\nabla^2 f(x_k)$, in a sense to be defined, based on recently observed local information. That is the logic behind the spectral projected gradient method [11], which is easily generalized as a spectral *proximal* gradient method, and where

$$\sigma_k := s_{k-1}^\mathsf{T} y_{k-1} / s_{k-1}^\mathsf{T} s_{k-1}, \quad s_{k-1} := x_k - x_{k-1}, \quad y_{k-1} := \nabla f(x_k) - \nabla f(x_{k-1}).$$

This choice of σ_k arises from the secant equation $\sigma_k s_{k-1} = y_{k-1}$, which, in general, has no solution, but can be solved in the least-squares sense by minimizing $\|\sigma s_{k-1} - y_{k-1}\|_2$ in terms of σ .

Gilbert and Lemaréchal [19] experiment, among others, with diagonal updates of quasi-Newton approximations. However, there may be no diagonal solution B_k to the secant equation $B_k s_{k-1} = y_{k-1}$, and one must resort to a different approach to update a diagonal approximation. Dennis and Wolkowicz [15] introduce the *weak secant* equation $s_{k-1}^T B_k s_{k-1} = s_{k-1}^T y_{k-1}$ and accompanying update formulae. Nazareth [24] observes that some of those proposed updates can be constrained to update only the diagonal of B_k but that the resulting B_k no longer necessarily satisfies the weak secant equation.

Zhu et al. [30] supplement the weak secant equation by additionally requiring that B_k be diagonal, and call the resulting set of conditions the *quasi-Cauchy* conditions. In particular, the spectral gradient approximation is the only solution of the quasi-Cauchy conditions that is a multiple of I. They derive updates from variational principles resembling those used in classic quasi-Newton updates. The first update sets B_k to the unique solution of

minimize
$$\|B - B_{k-1}\|_F$$
 subject to $s_{k-1}^T B s_{k-1} = s_{k-1}^T y_{k-1}$, (11)

which is the counterpart of the Powell-symmetric-Broyden (PSB) variational problem. The solution of (11) is shown to be

$$B_{k} = B_{k-1} + \frac{s_{k-1}^{\mathsf{T}}(y_{k-1} - B_{k-1}s_{k-1})}{\operatorname{trace}(S_{k-1}^{4})} S_{k-1}^{2}, \quad S_{k-1} := \operatorname{diag}(s_{k-1}).$$
 (12)

Like the PSB update, (12) does not possess the hereditary positive-definiteness property. However, capturing negative curvature is a desirable feature in trust-region methods.

Motivated by linesearch methods, Zhu et al. [30] devise a second strategy in which they update $B_k^{1/2}$, and that results in hereditary positive definiteness. The main idea is analogous to (11) with the objective replaced with $\|B^{1/2} - B_{k-1}^{1/2}\|_F$. The update depends on the root of a scalar nonlinear equation, and is therefore more costly to perform than (12).

Andrei [1] suggests an alternative variational problem in which B_k is determined as the solution of

minimize
$$\frac{1}{2} \|B - B_{k-1}\|_F^2 + \text{trace}(B)$$
 subject to $s_{k-1}^T B s_{k-1} = s_{k-1}^T y_{k-1}$, (13)

where minimizing the trace of B tends to cluster its eigenvalues. The solution of (13) is shown to be

$$B_{k} = B_{k-1} + \frac{s_{k-1}^{\mathsf{T}}(y_{k-1} + s_{k-1} - B_{k-1}s_{k-1})}{\operatorname{trace}(S_{k-1}^{4})} S_{k-1}^{2} - I.$$
 (14)

Again, (14) does not preserve positive definiteness. Also motivated by linesearch methods, Andrei [1] employs a thresholding strategy that ensures computation of a descent direction.

Though Nazareth [24] appears to have been motivated by derivative-free methods,¹ diagonal quasi-Newton updates are good candidate approximations for use in first-order methods for regularized optimization, and we are not aware of any prior work using them.

5 The indefinite proximal gradient method

5.1 Description of the algorithm and convergence properties

For v > 0, define

$$\varphi_{cp}(s;x) := f(x) + \nabla f(x)^{\mathsf{T}} s, \tag{15a}$$

$$m(s; x, v) := \varphi_{cp}(s; x) + \frac{1}{2}v^{-1}||s||_2^2 + \psi(s; x).$$
 (15b)

Guided by Proposition 1, we compute a first step denoted s_{k,1} such that

$$s_{k,1} \in \underset{s}{\operatorname{argmin}} \ m(s; x_k, v_k) + \chi(x_k + s \mid [\ell, u] \cap (x_k + \Delta_k \mathbb{B})), \tag{16}$$

for an appropriate value of $v_k > 0$.

Let

$$m(s; x, D) := \varphi_{cp}(s; x) + \frac{1}{2}s^{T}Ds + \psi(s; x),$$
 (17)

where D is a diagonal matrix. The indefinite proximal gradient iteration with trust region for (1) is defined by changing (16) to

$$s_k \in \underset{s}{\text{argmin}} \ m(s; x_k, D_k) + \chi(x_k + s \mid [\ell, u] \cap (x_k + \Delta_k \mathbb{B})), \tag{18}$$

where D_k is diagonal, and by updating x_k and Δ_k as is customary in trust-region methods [14]. Among other possible choices, we focus on the case where D_k results from a diagonal quasi-Newton update.

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Algorithm 1 Nonsmooth trust-region algorithm with diagonal Hessian.

1: Choose constants

```
0<\eta_1\leqslant\eta_2<1,\quad 0<1/\gamma_3\leqslant\gamma_1\leqslant\gamma_2<1<\gamma_3\leqslant\gamma_4,\quad \text{and}\quad \alpha>0,\ \beta\geqslant1.
```

- 2: Choose $x_0 \in \mathbb{R}^n$ where h is finite, $\Delta_0 > 0$, compute $f(x_0) + h(x_0)$. 3: Choose $d_0 \in \mathbb{R}^n$ and set $D_0 = diag(d_0)$.
- $4: \ \text{for} \ k=0,1,\dots \, \text{do}$
- Set $\nu_k := 1/(\|\mathbf{d}_k\|_{\infty} + \alpha^{-1}\Delta_k^{-1}).$
- Define $\phi(s;x_k)$ and $\psi(s;x_k)$ according to Model Assumption 3.1. Define $m(s;x_k,\nu_k)$ as in (15) and compute $s_{k,1}$ as in (16). 6:
- 7:
- Define $m(s; x_k, D_k)$ as in (17) and compute a solution s_k of (18) with Δ_k replaced by $min(\Delta_k, \beta ||s_{k,1}||)$. 8:
- 9:

$$\rho_k := \frac{f(x_k) + h(x_k) - (f(x_k + s_k) + h(x_k + s_k))}{m(0; x_k, D_k) - m(s_k; x_k, D_k)}.$$

- If $\rho_k \geqslant \eta_1$, set $x_{k+1} = x_k + s_k$. Otherwise, set $x_{k+1} = x_k$. Choose $d_{k+1} \in \mathbb{R}^n$ and set $D_{k+1} = \text{diag}(d_{k+1})$. 10:
- 11:
- Update the trust-region radius according to 12:

$$\Delta_{k+1} \in \left\{ \begin{array}{ll} [\gamma_3 \Delta_k, \, \gamma_4 \Delta_k] & \text{if } \rho_k \geqslant \eta_2, & \text{(very successful iteration)} \\ [\gamma_2 \Delta_k, \, \Delta_k] & \text{if } \eta_1 \leqslant \rho_k < \eta_2, & \text{(successful iteration)} \\ [\gamma_1 \Delta_k, \, \gamma_2 \Delta_k] & \text{if } \rho_k < \eta_1 & \text{(unsuccessful iteration)}. \end{array} \right.$$

We summarize the entire procedure as Algorithm 1, which is a special case of [3, Algorithm 3.1].

In [3, Algorithm 3.1], convergence hinges crucially on the fact that the decrease in $\mathfrak{m}(\cdot; x_k, D_k)$ achieved by s_k is at least a fraction of the decrease in $m(\cdot; x_k, v_k)$ achieved by $s_{k,1}$, the first proximal gradient step with a well-chosen step size $v_k > 0$. At iteration k of Algorithm 1, $v_k < 1/\|\mathbf{d}_k\|_{\infty}$. Note that the choice $d_k = 0$ is allowed.

In Algorithm 1, the computation of $s_{k,1}$ serves two purposes. The first is as stopping condition by Proposition 1, and the second is to set the trust-region radius in the subproblem for s_k . This is at variance with [3, Algorithm 3.1], where, in addition, s_k is computed by continuing the proximal gradient iterations from $s_{k,1}$.

In a similar notation to that of [3], let

$$\xi_{cp}(\Delta_k; x_k, \nu_k) := f(x_k) + h(x_k) - (\varphi_{cp}(s_{k,1}; x_k) + \psi(s_{k,1}; x_k)), \tag{19a}$$

$$\xi(\Delta_{\nu}; x_{\nu}, D_{\nu}) := f(x_{\nu}) + h(x_{\nu}) - m(s_{\nu}; x_{\nu}, D_{\nu})$$
(19b)

denote the optimal model decrease for (15) and (17). The definition of (16) guarantees that

$$f(x_k) + h(x_k) = m(0; x_k, v_k) \geqslant m(s_{k,1}; x_k, v_k) = \varphi_{cp}(s_{k,1}; x_k) + \psi(s_{k,1}; x_k) + \frac{1}{2}v_k^{-1} \|s_{k,1}\|^2,$$
 (20)

which implies

$$\xi_{cp}(\Delta_k; x_k, \nu_k) \geqslant \frac{1}{2} \nu_k^{-1} \|s_{k,1}\|^2 = \frac{1}{2} (\|d_k\|_{\infty} + \alpha^{-1} \Delta_k^{-1}) \|s_{k,1}\|^2 \geqslant \frac{1}{2} \alpha^{-1} \Delta_k^{-1} \|s_{k,1}\|^2. \tag{21}$$

If $\xi_{cp}(\Delta_k; x_k, v_k) = 0$, we obtain $s_{k,1} = 0$. Proposition 1 then implies that x_k is first-order stationary provided (1) satisfies the constraint qualification at x_k and (15) satisfies it at s = 0.

To establish convergence properties of Algorithm 1, we require Aravkin et al.'s Step Assumption 3.1, recalled in the following assumption for convenience.

Step Assumption 5.1. There exists $\kappa_m > 0$ and $\kappa_{mdc} \in (0,1)$ such that for all k,

$$|f(x_k + s_k) + h(x_k + s_k) - (\phi(s_k; x_k, D_k) + \psi(s_k; x_k))| \leqslant \kappa_m ||s_k||_2^2, \tag{22a}$$

$$\xi(\Delta_k; x_k, D_k) \geqslant \kappa_{\text{mdc}} \xi_{\text{cp}}(\Delta_k; x_k; \nu_k).$$
 (22b)

 $^{^{1}}$ In the sense that the quasi-Cauchy condition only requires the gradient via $s^{T}y$.

Among other situations, (22a) is satisfied if $\{D_k\}$ is bounded, ∇f is Lipschitz continuous, and we select $\psi(s;x_k)=h(x_k+s)$. The following proposition gives a sufficient condition for which (22b) is satisfied.

Proposition 2. If

$$\|\mathbf{d}_{k}\|_{\infty} \le (\kappa_{\text{mdc}}^{-1} - 1)\alpha^{-1}\Delta_{k}^{-1},$$
 (23)

then (22b) is satisfied.

Proof. By definition of s_k ,

$$\begin{split} m(s_k; x_k, D_k) &\leqslant m(s_{k,1}; x_k, D_k) \\ &= \phi(s_{k,1}; x_k) + \tfrac{1}{2} s_{k,1}^\mathsf{T} D_k s_{k,1} + \psi(s_{k,1}; x_k) \\ &\leqslant \phi(s_{k,1}; x_k) + \tfrac{1}{2} \|d_k\|_\infty \|s_{k,1}\|^2 + \psi(s_{k,1}; x_k) \\ &= \phi(s_{k,1}; x_k) + \tfrac{1}{2} (\gamma_k^{-1} - \alpha^{-1} \Delta_k^{-1}) \|s_{k,1}\|^2 + \psi(s_{k,1}; x_k), \end{split}$$

which leads to

$$\xi(\Delta_k; x_k, D_k) \geqslant \xi_{cp}(\Delta_k; x_k, \nu_k) - \frac{1}{2}(\nu_k^{-1} - \alpha^{-1}\Delta_k^{-1}) \|s_{k,1}\|^2.$$

For (22b) to be satisfied, it is sufficient to show that

$$\xi_{cp}(\Delta_k; x_k, \nu_k) - \frac{1}{2}(\nu_k^{-1} - \alpha^{-1}\Delta_k^{-1}) \|s_{k,1}\|^2 \geqslant \kappa_{mdc} \xi_{cp}(\Delta_k; x_k, \nu_k),$$

that we rewrite as

$$(1 - \kappa_{\text{mdc}}) \xi_{\text{cp}}(\Delta_k; x_k, \nu_k) \geqslant \frac{1}{2} (\nu_k^{-1} - \alpha^{-1} \Delta_k^{-1}) \|s_{k,1}\|^2.$$
 (24)

Let $\|d_k\|_{\infty} \leqslant (\kappa_{mdc}^{-1} - 1)\alpha^{-1}\Delta_k^{-1}$, which is equivalent to $\nu_k = \frac{1}{\|d_k\|_{\infty} + \alpha^{-1}\Delta_k^{-1}} \geqslant \kappa_{mdc}\alpha\Delta_k$. Since

 $\kappa_{\text{mdc}} \in (0,1)$, we have

$$(1 - \kappa_{mdc}) \frac{1}{2} \nu_k^{-1} \geqslant \frac{1}{2} (\nu_k^{-1} - \alpha^{-1} \Delta_k^{-1}).$$

By multiplying by $\|s_{k,1}\|^2$ and recalling that $\xi_{cp}(\Delta_k; x_k, \nu_k) \geqslant \frac{1}{2}\nu_k^{-1}\|s_{k,1}\|^2$, we get

$$(1 - \kappa_{mdc}) \xi_{cp}(\Delta_k; x_k, \nu_k) \geqslant (1 - \kappa_{mdc}) \frac{1}{2} \nu_k^{-1} \|s_{k,1}\|^2 \geqslant \frac{1}{2} (\nu_k^{-1} - \alpha^{-1} \Delta_k^{-1}) \|s_{k,1}\|^2,$$

so that (24) is satisfied.

We can always choose κ_{mdc} small enough to ensure that $\|d_k\|_{\infty}$ does not have to be too close to zero if Δ_k does not grow unbounded. Whenever Algorithm 1 generates infinitely many very successful iterations, we could define a Δ_{max} from which we stop increasing Δ_k . We point out that Proposition 2 only gives a sufficient condition for (22b) to be satisfied, but it is not necessary. Therefore, for the rest of this paper, we base our analysis on (22b) rather that on (23).

Under Step Assumption 5.1, we can apply directly Aravkin et al.'s convergence properties.

Proposition 3 (3, Theorem 3.4). Let Step Assumption 5.1 be satisfied and

$$\Delta_{\text{succ}} := \frac{\kappa_{\text{mdc}}(1 - \eta_2)}{2\kappa_{\text{m}}\alpha\beta^2} > 0.$$

If x_k is not first-order stationary and $\Delta_k \leqslant \Delta_{succ}$, iteration k is very successful and $\Delta_{k+1} > \Delta_k$.

Without further assumptions, the following result also holds.

Proposition 4 (3, Theorem 3.5). Let Step Assumption 5.1 be satisfied and assume Algorithm 1 generates a finite number of successful iterations. Then $x_k = x_\star$ for all sufficiently large k. If (1) satisfies the constraint qualification at x_k and (15) satisfies it at s = 0, x_\star is first-order critical.

We continue to follow the analysis of [3] and note that $\Delta_k \geqslant \Delta_{min}$ for all $k \in \mathbb{N}$, where $\Delta_{min} := min(\Delta_0, \gamma_1 \Delta_{succ})$. Aravkin et al. [3] establish that $\xi_{cp}(\cdot; x_k, \nu_k)$ is increasing, and therefore, $\xi_{cp}(\Delta_k; x_k, \nu_k) \geqslant \xi_{cp}(\Delta_{min}; x_k, \nu_k)$. In addition, they show that $\nu_k^{-1/2} \xi_{cp}(\Delta_k; x_k, \nu_k)^{1/2}$ is an appropriate criticality measure. Let $0 < \varepsilon < 1$, and

$$\begin{split} & I(\varepsilon) := \{k \in \mathbb{N} \mid \nu_k^{-1/2} \xi_{cp}(\Delta_k; x_k, \nu_k)^{1/2} > \varepsilon\}, \\ & S(\varepsilon) := \{k \in I(\varepsilon) \mid \rho_k \geqslant \eta_1\}, \\ & U(\varepsilon) := \{k \in I(\varepsilon) \mid \rho_k < \eta_1\}, \end{split}$$

be the set of iterations, successful iterations, and unsuccessful iterations until the criticality measure drops below ϵ , respectively.

We now derive bounds on $|I(\varepsilon)|$ using the analysis of [3] specialized to Algorithm 1 under the assumption that $\{D_k\}$ is bounded. We make the following assumption.

Assumption 1. There exists $d_{max} > 0$ such that $\|d_k\|_{\infty} \leq d_{max}$ for all $k \in \mathbb{N}$.

In Algorithm 1, it is not difficult to ensure satisfaction of Assumption 1. For instance, one may prescribe a value $d_{max}>0$ and reset each d_k componentwise to $min(max(d_k,-d_{max}),d_{max})$. We point out that Assumption 1 holds if (23) in Proposition 2 is satisfied for all k, because, in this case, $\|d_k\|_{\infty}\leqslant d_{max}:=(\kappa_{mdc}^{-1}-1)\alpha^{-1}\Delta_{min}^{-1}$.

Under Assumption 1, the choice of v_k in Algorithm 1 guarantees that

$$v_k \geqslant v_{min} := 1/(d_{max} + \alpha^{-1} \Delta_{min}^{-1}) > 0.$$

The following result establishes that $|S(\epsilon)|$ is $O(\epsilon^{-2})$.

Proposition 5 (3, Lemma 3.6). Let Step Assumption 5.1 and Assumption 1 be satisfied. Assume that Algorithm 1 generates infinitely many successful iterations and that there exists $(f+h)_{low} \in \mathbb{R}$ such that $(f+h)(x_k) \ge (f+h)_{low}$ for all $k \in \mathbb{N}$. Let $\varepsilon \in (0,1)$. Then,

$$|S(\epsilon)| \leqslant \frac{(f+h)(x_0) - (f+h)_{low}}{\eta_1 \kappa_{mdc} \gamma_{min} \epsilon^2}.$$

The next result establishes that $|U(\epsilon)|$ is also $O(\epsilon^{-2})$.

Proposition 6 (3, Lemma 3.7). *Under the assumptions of Proposition 5*,

$$|U(\varepsilon)| \leqslant log_{\gamma_2}(\Delta_{min}/\Delta_0) + |S(\varepsilon)| \, |log_{\gamma_2}(\gamma_4)|.$$

The direct consequence of Propositions 5 and 6 is that $|I(\varepsilon)|$ is also $O(\varepsilon^{-2})$. Because $\varepsilon \in (0, 1)$ is arbitrary, we conclude that $\liminf \nu_k^{-1/2} \xi_{cp}(\Delta_k; x_k, \nu_k)^{1/2} = 0$.

5.2 A variant saving proximal operator computations

We present a variant of Algorithm 1 in which we set

$$v_k := 1/(\|d_k\|_{\infty} + \alpha^{-1})$$
 (25)

in line 5, we do not compute $s_{k,1}$ in line 7, and we leave Δ_k unchanged in line 8, thus saving a proximal operator computation at each iteration. Under Assumption 1, this choice of ν_k leads to a new ν_{min}

$$v_k \geqslant v_{min} := 1/(d_{max} + \alpha^{-1}) > 0.$$
 (26)

We use the criticality measure

$$v_k^{-1/2} \xi(\Delta_k; x_k, D_k)^{1/2},$$
 (27)

and modify the definition of $I(\varepsilon)$, $S(\varepsilon)$ and $U(\varepsilon)$ accordingly. To establish the same convergence properties as those of Algorithm 1, we need Step Assumption 5.1 to hold for our algorithmic variant. The following assumption summarizes our requirements.

Step Assumption 5.2. There exists $\kappa_m > 0$ and $\kappa_{mdc} \in (0,1)$ such that for all k,

$$|f(x_k + s_k) + h(x_k + s_k) - (\varphi(s_k; x_k, D_k) + \psi(s_k; x_k))| \le \kappa_m ||s_k||_2^2, \tag{28a}$$

$$\xi(\Delta_k; x_k, D_k) \geqslant \kappa_{\text{mdc}} \xi_{\text{cp}}(\Delta_k; x_k; \nu_k),$$
 (28b)

where $\nu_k = 1/(\|d_k\|_\infty + \alpha^{-1})$ in line 5 and s_k is computed without changing Δ_k in line 8 of Algorithm 1.

Even though Step Assumption 5.2 involves $\xi_{cp}(\Delta_k; x_k, \nu_k)$, we do not need to compute it in practice. Conveniently, if $\{D_k\}$ is bounded, ∇f is Lipschitz continuous, and we select $\psi(s; x_k) = h(x_k + s)$, (28a) is still satisfied. The following proposition, analogous to Proposition 2, shows that (29) is a sufficient condition for (28b) to hold.

Proposition 7. If

$$\|\mathbf{d}_{k}\|_{\infty} \leqslant (\kappa_{\text{mdc}}^{-1} - 1)\alpha^{-1},$$
 (29)

then (28b) is satisfied for Algorithm 1 with $\nu_k = 1/(\|d_k\|_\infty + \alpha^{-1})$ in line 5, $s_{k,1}$ is not computed in line 7, and Δ_k is unchanged in line 8.

Proof. The proof is identical to that of Proposition 2 if we use (25).

Whenever (28b) holds, we have

$$\nu_{k}^{-1/2} \xi(\Delta_{k}; x_{k}, \nu_{k})^{1/2} \geqslant \kappa_{\text{mdc}}^{1/2} \nu_{k}^{-1/2} \xi_{\text{cp}} (\Delta_{k}; x_{k}, \nu_{k})^{1/2} \geqslant \kappa_{\text{mdc}}^{1/2} \nu_{k}^{-1} \|s_{k,1}\|, \tag{30}$$

which ensures that $v_k^{-1/2}\xi(\Delta_k;x_k,\nu_k)^{1/2}\to 0$ implies $\|s_{k,1}\|\to 0$, and that $v_k^{-1/2}\xi(\Delta_k;x_k,\nu_k)^{1/2}$ is an appropriate criticality measure. We emphasize that there is no need to compute $s_{k,1}$ and $\xi_{cp}(\Delta_k;x_k,\nu_k)$; (30) is only used as a theoretical justification for the choice of our criticality measure.

We now establish convergence properties similar to those of Section 5.1, and follow the analysis of Cartis et al. [13, Chapter 2.3].

Proposition 8. Let Assumption 1 and Step Assumption 5.2 be satisfied. Let v_{min} be as defined in (26). If

$$\Delta_{k} \leqslant \sqrt{\frac{\nu_{\min}(1 - \eta_{2})}{\kappa_{m}}} \nu_{k}^{-1/2} \xi(\Delta_{k}; x_{k}, D_{k})^{1/2}$$
 (31)

and x_k is not first-order stationary, iteration k is very successful and $\Delta_{k+1} > \Delta_k$.

Proof. Using Step Assumption 5.2 and $||s_k|| \leq \Delta_k$, we have

$$\begin{split} |\rho_k - 1| &= \left| \frac{f(x_k + s_k) + h(x_k + s_k) - m(s_k; x_k, D_k)}{m(0; x_k, D_k) - m(s_k; x_k, D_k)} \right| \\ &\leqslant \frac{\kappa_m \|s_k\|^2}{\xi(\Delta_k; x_k, D_k)} \\ &\leqslant \frac{\kappa_m \Delta_k^2}{\xi(\Delta_k; x_k, D_k)}. \end{split}$$

Assumption 1 and (26) lead to

$$|\rho_k - 1| \leqslant \frac{\kappa_m \nu_{min}^{-1} \Delta_k^2}{\nu_k^{-1} \xi(\Delta_k; x_k, D_k)}.$$

Whenever (31) holds, we have $\rho_k \geqslant \eta_2$, implying that iteration k is very successful and $\Delta_{k+1} \geqslant \Delta_k$. \square

The following lemma is inspired by Conn et al. [14, Theorem 6.4.3] and Cartis et al. [13, Lemma 2.3.4].

Lemma 1. Let Step Assumption 5.2 be satisfied. Then, for all $k \ge 0$,

$$\Delta_{k} > \gamma_{1} \sqrt{\frac{\nu_{\min}(1 - \eta_{2})}{\kappa_{m}}} \min \left(1, \Delta_{0} \frac{\sqrt{\kappa_{m} \nu_{\min}^{-1}}}{\nu_{0}^{-1/2} \xi(\Delta_{0}; x_{0}, D_{0})^{1/2}}\right) \min_{i \in [0, k]} \nu_{i}^{-1/2} \xi(\Delta_{i}; x_{i}, D_{i})^{1/2}. \tag{32}$$

Proof. We proceed as in Cartis et al. [13, Lemma 2.3.4]. The bound certainly holds for k = 0, because

$$\Delta_0 > \gamma_1 \sqrt{1 - \eta_2} \Delta_0.$$

Now, we proceed by contradiction and assume that $k \ge 1$ is the first iteration such that (32) is not verified.

$$\begin{split} & \Delta_k \leqslant \gamma_1 \sqrt{\frac{\nu_{min}(1-\eta_2)}{\kappa_m}} \min \left(1, \Delta_0 \frac{\sqrt{\kappa_m \nu_{min}^{-1}}}{\nu_0^{-1/2} \xi(\Delta_0; x_0, D_0)^{1/2}}\right) \min_{i \in [0, k]} \nu_i^{-1/2} \xi(\Delta_i; x_i, D_i)^{1/2} \\ & \leqslant \gamma_1 \sqrt{\frac{\nu_{min}(1-\eta_2)}{\kappa_m}} \nu_{k-1}^{-1/2} \xi(\Delta_{k-1}; x_{k-1}, D_{k-1})^{1/2}. \end{split}$$

We have $\gamma_1 \Delta_{k-1} \leqslant \Delta_k$ because of the updating rules of Δ_k in Algorithm 1, which implies that

$$\Delta_{k-1} \leqslant \sqrt{\frac{\nu_{min}(1-\eta_2)}{\kappa_m}} \nu_{k-1}^{-1/2} \xi(\Delta_{k-1}; x_{k-1}, D_{k-1})^{1/2}.$$

Using Proposition 8, this results in iteration k-1 being very successful and $\Delta_k > \Delta_{k-1}$. Therefore,

$$\begin{split} \Delta_{k-1} < \Delta_k \leqslant \gamma_1 \sqrt{\frac{\nu_{min}(1-\eta_2)}{\kappa_m}} \min\left(1, \Delta_0 \frac{\sqrt{\kappa_m \nu_{min}^{-1}}}{\nu_0^{-1/2} \xi(\Delta_0; x_0, D_0)^{1/2}}\right) \min_{i \in [0, k]} \nu_i^{-1/2} \xi(\Delta_i; x_i, D_i)^{1/2} \\ \leqslant \gamma_1 \sqrt{\frac{\nu_{min}(1-\eta_2)}{\kappa_m}} \min\left(1, \Delta_0 \frac{\sqrt{\kappa_m \nu_{min}^{-1}}}{\nu_0^{-1/2} \xi(\Delta_0; x_0, D_0)^{1/2}}\right) \min_{i \in [0, k-1]} \nu_i^{-1/2} \xi(\Delta_i; x_i, D_i)^{1/2}, \end{split}$$

which is a contradiction with iteration k being the first to violate (32).

Now, we show analogous properties to Proposition 5 and Proposition 6 for our variant. **Lemma 2.** Let Step Assumption 5.2 and Assumption 1 be satisfied. Assume that Algorithm 1 with v_k as in (25) in line 5, without line 7, and with Δ_k unchanged in line 8 generates infinitely many successful iterations and that there exists $(f + h)_{low} \in \mathbb{R}$ such that $(f + h)(x_k) \ge (f + h)_{low}$ for all $k \in \mathbb{N}$. Let $\varepsilon \in (0, 1)$. Then,

$$|S(\epsilon)| \leqslant \frac{(f+h)(x_0) - (f+h)_{low}}{\eta_1 \nu_{min} \epsilon^2}.$$

Proof. For $k \in S(\epsilon)$, we have

$$\begin{split} f(x_k) + h(x_k) - f(x_k + s_k) - h(x_k + s_k) &\geqslant \eta_1(m(0; x_k, D_k) - m(s_k; x_k, D_k)) \\ &= \eta_1 \xi(\Delta_k; x_k, D_k) \\ &\geqslant \eta_1 \nu_{\min} \varepsilon^2. \end{split}$$

As $(f+h)(x_k) \ge (f+h)_{low}$, we sum the above inequalities for $k \in S(\varepsilon)$ and get

$$(f+h)(x_0) - (f+h)_{low} \geqslant \sum_{k \in S(\varepsilon)} (f+h)(x_k) - (f+h)(x_{k+1}) \geqslant |S(\varepsilon)| \eta_1 \varepsilon^2 v_{min}.$$

Lemma 3. *Under the assumptions of Lemma 2,*

$$|U(\epsilon)| = O(\epsilon^{-2}).$$

Proof. Let $k < k(\epsilon)$. Because

$$v_k^{-1/2}\xi(\Delta_k;x_k,D_k)^{1/2}>\varepsilon$$

and

$$\nu_{k(\varepsilon)}^{-1/2}\xi(\Delta_{k(\varepsilon)};x_{k(\varepsilon)},D_{k(\varepsilon)})^{1/2}\leqslant\varepsilon,$$

we have with Lemma 1

$$\begin{split} \Delta_{k(\varepsilon)-1} > & \gamma_1 \sqrt{\frac{\nu_{min}(1-\eta_2)}{\kappa_m}} \min \left(1, \Delta_0 \frac{\sqrt{\kappa_m \nu_{min}^{-1}}}{\nu_0^{-1/2} \xi(\Delta_0; x_0, D_0)^{1/2}} \right) \min_{i \in [0, k]} \nu_i^{-1} \xi(\Delta_i; x_i, D_i) \\ > & \gamma_1 \sqrt{\frac{\nu_{min}(1-\eta_2)}{\kappa_m}} \min \left(1, \Delta_0 \frac{\sqrt{\kappa_m \nu_{min}^{-1}}}{\nu_0^{-1/2} \xi(\Delta_0; x_0, D_0)^{1/2}} \right) \varepsilon. \end{split}$$

For each successful iteration, $\Delta_{k+1} \leqslant \gamma_4 \Delta_k$, and for each unsuccessful iteration, $\Delta_{k+1} \leqslant \gamma_2 \Delta_k$, which implies

$$\Delta_{k(\epsilon)-1} \leqslant \Delta_0 \gamma_2^{|U(\epsilon)|} \gamma_4^{|S(\epsilon)|}.$$

By taking the natural logarithm of the above inequality, we have

$$\begin{split} |U(\varepsilon)|\log(\gamma_2) + |S(\varepsilon)|\log(\gamma_4) &\geqslant \log(\Delta_{k(\varepsilon)-1}/\Delta_0) \\ &\geqslant \log\left(\gamma_1\sqrt{\frac{\nu_{min}(1-\eta_2)}{\kappa_m}}\min\left(\Delta_0^{-1}, \frac{\sqrt{\kappa_m\nu_{min}^{-1}}}{\nu_0^{-1/2}\xi(\Delta_0; x_0, D_0)^{1/2}}\right)\varepsilon\right), \end{split}$$

so that, using the previous inequalities and Lemma 2

$$\begin{split} |U(\varepsilon)| &\leqslant log_{\gamma_2} \left(\gamma_1 \sqrt{\frac{\nu_{min}(1-\eta_2)}{\kappa_m}} \min \left(\Delta_0^{-1}, \frac{\sqrt{\kappa_m \nu_{min}^{-1}}}{\nu_0^{-1/2} \xi(\Delta_0; x_0, D_0)^{1/2}} \right) \varepsilon \right) + |S(\varepsilon)|| \log_{\gamma_2}(\gamma_4)| \\ &\leqslant O(|log_{\gamma_2}(\varepsilon)|) + O(\varepsilon^{-2}) \\ &= O(\varepsilon^{-2}). \end{split}$$

Lemma 2 and Lemma 3 also indicate that $I(\varepsilon)$ is $O(\varepsilon^{-2})$, and $\liminf \nu_k^{-1/2} \xi(\Delta_k; x_k, D_k)^{1/2} = 0$. With (28b) in Step Assumption 5.2, we also have $\liminf \nu_k^{-1/2} \xi_{cp}(\Delta_k; x_k, \nu_k)^{1/2} = 0$.

Finally, we emphasize the changes made in this section to Algorithm 1:

- in line 5, $\nu_k = 1/(\|d_k\|_\infty + \alpha^{-1}\Delta_k^{-1})$ became $\nu_k = 1/(\|d_k\|_\infty + \alpha^{-1})$,
- line 7 of Algorithm 1 was removed,
- Δ_k was left unchanged in line 8 of Algorithm 1,

• we used $v_k^{-1/2}\xi(\Delta_k;x_k,D_k)^{1/2}$ as a criticality measure, instead of $v_k^{-1/2}\xi_{cp}(\Delta_k;x_k,\nu_k)$, however, when (28a) holds, (30) indicates that if the new criticality measure is small, then the criticality measure of Section 5.1 is also small,

- in Proposition 8, there is no $\Delta_{\min} > 0$ independent of k as in Proposition 3,
- under the assumptions of Lemma 2, which are similar to those of Proposition 5, the complexity bound is still in $O(\epsilon^{-2})$, and $\liminf v_k^{-1/2} \xi(\Delta_k; x_k, D_k)^{1/2} = \liminf v_k^{-1/2} \xi_{cp}(\Delta_k; x_k, v_k)^{1/2} = 0$.

6 Implementation and numerical experiments

Our Julia implementation of Algorithm 1 is available from our RegularizedOptimization package [5] under the name TRDH. The latter can be used to solve (1) directly, or as subproblem solver in TR [3, Algorithm 3.1], instead of R2 [3, Algorithm 6.1]. Below, we use the notation TR-R2 and TR-TRDH to denote the application of TR to solve (1) with R2 or TRDH as subproblem solver, respectively.

In our experiments, TR uses either an LSR1 or an LBFGS quasi-Newton Hessian approximation with memory 5, as implemented in the LinearOperators package [25]. The same package implements diagonal quasi-Newton operators in TRDH using the spectral update, the PSB update (12), and the update of Andrei [1] (14) with the modification that we scaled the weak secant equations as

$$\tilde{\mathbf{s}}_{k-1}^{\mathsf{T}} \mathbf{B} \tilde{\mathbf{s}}_{k-1} = \tilde{\mathbf{s}}_{k-1}^{\mathsf{T}} \tilde{\mathbf{y}}_{k-1} \tag{34}$$

in (11) and (13), where $\tilde{s}_{k-1}:=s_{k-1}/\|s_{k-1}\|_2$, and $\tilde{y}_{k-1}:=y_{k-1}/\|s_{k-1}\|_2$, in order to alleviate numerical issues as s_{k-1} approaches zero.

The indefinite proximal operators of Example 1 and Example 2 are implemented as part of the ShiftedProximalOperators package [7].

When using TRDH as the main solver, we initialize $D_0 := \nu_0^{-1}I$ for $\nu_0 > 0$ given below. When using TR-TRDH with a spectral diagonal quasi-Newton approximation, denoted TR-TRDH-Spec, we set the initial diagonal Hessian approximation in TRDH at iteration k of TR to $D_{k,0} := \nu_k^{-1}I$ (as we would initialize R2 in TR-R2). When using TR-TRDH with the PSB or the Andrei quasi-Newton approximations, denoted TR-TRDH-PSB and TR-TRDH-Andrei, respectively, we set $D_{k,0} := diag(B_k)$, where B_k is the quasi-Newton Hessian approximation at iteration k of TR.

We set $\psi(s;x_k):=h(x_k+s)$. We initialize $\nu_0=1$ for R2 and TRDH used by themselves. The stopping criteria that we used for TR, TRDH and R2 (as subproblem solvers or main solvers) are based on $\xi_{cp}(\Delta_k;x_k,\nu_k)^{1/2}$. We set $\Delta_0=1$ for TR and for TRDH used as main solver. For TR-TRDH, at iteration k of TR, the initial value of the TRDH trust-region radius is $\Delta_{k,0}=\min(\Delta_k,\beta\|s_{k,1}\|)$ / 10, where Δ_k is the TR trust-region radius at iteration k, and $s_{k,1}$ is the first step of the k-th TR subproblem. In other words, the initial TRDH trust-region radius to solve the k-th TR subproblem is a tenth of the trust-region radius of this k-th subproblem.

For all solvers, the outer iterations terminate as soon as

$$\nu_{k}^{-1/2} \xi_{cp}(\Delta_{k}; x_{k}, \nu_{k})^{1/2} < \varepsilon_{\alpha} + \varepsilon_{r} \nu_{0}^{-1/2} \xi_{cp}(\Delta_{0}; x_{0}, \nu_{0})^{1/2}, \tag{35}$$

where $\varepsilon_{\alpha}>0$ and $\varepsilon_{r}>0$ are an absolute and a relative tolerance. A round of inner iterations in TR terminates as soon as the stationarity measure of the inner solver satisfies (35), with $\tilde{\varepsilon}_{\alpha}=10^{-5}$ for the first TR iteration, otherwise $\tilde{\varepsilon}_{\alpha}=\max(\varepsilon_{\alpha,i},\min(10^{-2},\nu_{k}^{-1/2}\xi_{cp}(\Delta_{k};x_{k},\nu_{k})^{1/2}))$, and $\tilde{\varepsilon}_{r}=\varepsilon_{r,i}$, where $\varepsilon_{\alpha,i}>0$ and $\varepsilon_{r,i}>0$ are some absolute and relative inner tolerances, and $s_{k,1}$ is the first iterate of the solution of the trust-region subproblem. In the experiments below, we use $\varepsilon_{\alpha,i}=10^{-3}$ and $\varepsilon_{r,i}=10^{-6}$, except in Section 6.1, where we use $\varepsilon_{\alpha,i}=10^{-5}$.

Additionally, we test the variant presented in Section 5.2, which is denoted "iTRDH" (indefinite trust-region with diagonal Hessian approximations) in our results. When in use, the stopping criterion is based on $v_k^{-1/2}\xi(\Delta_k;x_k,D_k)^{1/2}$, instead of $v_k^{-1/2}\xi_{cp}(\Delta_k;x_k,v_k)^{1/2}$.

In our results, we report

- the final f(x);
- the final $h(x)/\lambda$;
- the final stationarity measure $\sqrt{\xi/\nu}$;
- $\|x x_{\star}\|_{2}$, where x_{\star} is the exact solution, if it is available;
- the number of smooth objective evaluations # f;
- the number of gradient evaluations # ∇f ;
- the number of proximal operator evaluations # prox;
- the elapsed time t in seconds.

Because our implementations are not yet perfectly optimized in terms of memory allocations, we neglect the elapsed time in our interpretations, and only report it in the tables as an indicator for the reader.

In our test cases, available from the RegularizedProblems package [6], the computational cost of evaluating the gradient is significantly higher than a proximal evaluation or an objective evaluation. In all cases, except in case of failure, all solvers find similar final solutions, and we only show one for illustration.

6.1 Basis pursuit denoise (BPDN)

Our first test case is the basis pursuit denoise (BPDN) problem [16, 28]. The stopping tolerances ϵ_a and ϵ_r are set to 10^{-5} . In this subsection only, when using TR, we set $\epsilon_{a,i}=10^{-5}$ in order to have accurate subproblem solves, which leads to performing fewer gradient evaluations without sacrificing too many proximal evaluations. Let m=200, n=512, $b=Ax_\star+\epsilon$, where $\epsilon\sim \mathcal{N}(0,0.01)$, $A\in\mathbb{R}^{m\times n}$ has orthonormal rows, and x_\star is a vector of zeros, except for 10 of its components that are set to ± 1 . We solve

$$\min_{x} \sum_{k=0}^{\infty} \|Ax - b\|_{2}^{2} + h(x), \tag{36}$$

where $h(x) = \lambda ||x||_0$. As in [3], we use $\lambda = 0.1 ||A^T b||_{\infty}$.

Table 1: BPDN (36) statistics with $h = \lambda \| \cdot \|_0$. All variants of TR use an LSR1 Hessian approximation, and are given a maximum of 100 inner iterations. The optimal objective value is $f(\mathbf{x}_*) = 9.90 e - 03$.

	-()	- () (2	7= /					
solver	f(x)	$h(x)/\lambda$	$\sqrt{\xi/\nu}$	$\ \mathbf{x} - \mathbf{x}_{\star}\ _2$	#f	#∇ f	#prox	t (s)
R2	9.44e-03	10	$4.4e{-03}$	4.7e - 02	30	31	30	8.0e-03
TRDH-Spec	9.44e - 03	10	4.0e - 03	4.7e - 02	9	9	17	1.7e - 02
iTRDH-Spec	9.44e - 03	10	3.4e - 03	4.7e - 02	10	9	9	4.0e - 03
TRDH-PSB	9.44e - 03	10	3.7e - 03	4.7e - 02	18	15	35	$1.1e{-02}$
iTRDH-PSB	9.44e - 03	10	2.6e - 03	4.7e - 02	20	16	19	5.0e - 03
TRDH-Andrei	9.44e - 03	10	4.5e - 03	4.7e - 02	48	29	95	1.0e - 02
iTRDH-Andrei	9.44e - 03	10	3.7e - 03	4.7e - 02	59	35	58	3.1e - 02
TR-R2	9.44e - 03	10	1.7e - 05	4.7e - 02	23	23	40	1.8e - 02
TR-TRDH-PSB	9.44e - 03	10	1.6e - 05	4.7e - 02	21	21	58	6.9e - 02
TR-iTRDH-PSB	9.44e - 03	10	1.6e - 05	4.7e - 02	21	21	39	2.5e - 02
TR-TRDH-Andrei	9.44e - 03	10	1.6e - 05	4.7e - 02	20	20	127	2.5e - 02
TR-iTRDH-Andrei	9.44e - 03	10	1.4e - 05	4.7e - 02	20	20	100	3.0e - 02
TR-TRDH-Spec	9.44e - 03	10	1.9e - 05	4.7e - 02	21	21	46	1.8e - 02
TR-iTRDH-Spec	9.44e-03	10	1.9e - 05	4.7e - 02	21	21	33	1.8e-02

Figure 3 shows the solution of (36) with TRDH-Spec. Table 1 reports the statistics for the different solvers and shows that TRDH-Spec and TRDH-PSB perform fewer objective and gradient evaluations than R2. TRDH-Andrei performs worse that R2 on this problem. As expected, the "iTRDH" variants require fewer proximal operator evaluations. They result in similar numbers of objective and gradient

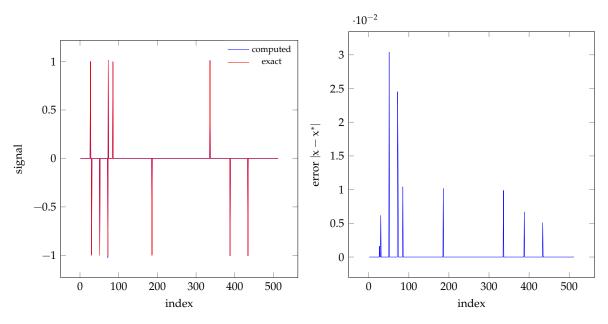


Figure 3: Solution of (36) (left), and error (right) with TRDH-Spec.

evaluations in the cases of TRDH-Spec and TRDH-PSB, but require more evaluations in the case of TRDH-Andrei.

All TR-TRDH and TR-iTRDH solvers perform fewer objective and gradient evaluations than TR-R2.

We now solve the constrained variant

$$\underset{x}{\text{minimize }} \frac{1}{2} \|Ax - b\|_2^2 + h(x) \quad \text{subject to } x \geqslant 0, \tag{37}$$

where each element in x_{\star} is either 0 or 1.

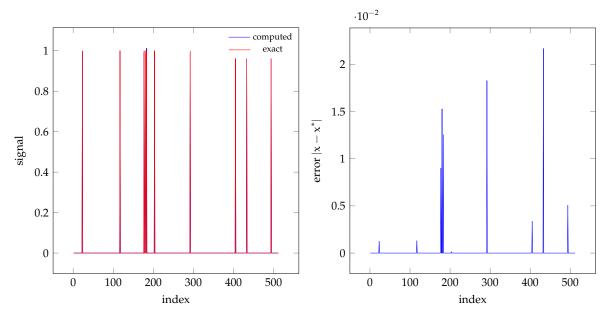


Figure 4: Solution of (37) (left), and error (right) with TR-TRDH-Spec.

Table 2: Constrained BPDN (37) statistics with $h=\lambda\|\cdot\|_0$. All variants of TR use an LSR1 Hessian approximation, and are given a maximum of 100 inner iterations. The optimal objective value is $f(x_\star)=8.98\varepsilon-03$.

solver	f(x)	$h(x)/\lambda$	$\sqrt{\xi/\nu}$	$\ \mathbf{x} - \mathbf{x}_{\star}\ _{2}$	#f	#∇ f	#prox	t (s)
R2	8.70e-03	10	3.9e-03	3.6e-02	27	28	27	1.9e-02
TRDH-Spec	8.70e - 03	10	3.6e - 03	3.6e - 02	8	8	15	$4.0e{-03}$
iTRDH-Spec	8.70e - 03	10	3.0e - 03	3.6e - 02	9	8	8	2.0e - 03
TRDH-PSB	8.70e - 03	10	3.6e - 03	3.6e - 02	11	11	21	3.0e - 03
iTRDH-PSB	8.70e - 03	10	3.7e - 03	3.6e - 02	12	11	11	3.0e - 03
TRDH-Andrei	8.70e - 03	10	4.3e - 03	3.6e - 02	48	29	95	$1.6e{-02}$
iTRDH-Andrei	8.70e - 03	10	4.0e - 03	3.6e - 02	59	35	58	2.0e-02
TR-R2	8.70e - 03	10	1.9e - 05	3.6e - 02	20	20	32	1.2e-02
TR-TRDH-PSB	8.70e - 03	10	2.1e - 05	3.6e - 02	19	19	50	1.8e - 02
TR-iTRDH-PSB	8.70e - 03	10	2.1e - 05	3.6e - 02	19	19	34	2.5e - 02
TR-TRDH-Andrei	8.70e - 03	10	1.9e - 05	3.6e - 02	20	20	63	$1.8e{-02}$
TR-iTRDH-Andrei	8.70e - 03	10	1.5e - 05	3.6e - 02	20	20	51	7.0e - 03
TR-TRDH-Spec	8.70e - 03	10	2.0e - 05	3.6e - 02	19	19	28	1.0e-02
TR-iTRDH-Spec	8.70e - 03	10	2.0e - 05	3.6e - 02	19	19	23	1.2e-02

Figure 4 shows the solution of (37) with TRDH-Spec, and Table 2 reports the statistics for the different solvers. We observe that TRDH-Spec, iTRDH-Spec, TRDH-PSB and iTRDH-PSB used as main solvers outperform R2 in terms of number of objective and gradient evaluations. TR-TRDH and TR-iTRDH perform similarly to TR-R2.

6.2 Sparse nonnegative matrix factorization (NNMF)

Our next test case is a variant of the NNMF problem of Kim and Park [20]. Let $A \in \mathbb{R}^{m \times n}$ have nonnegative entries, where each row represents a feature and each column represents an observation. We wish to factorize $A \approx WH$ by separating A into $k < \min(\mathfrak{m}, \mathfrak{n})$ clusters, where $W \in \mathbb{R}^{m \times k}$, $H \in \mathbb{R}^{k \times n}$ both have nonnegative entries and H is sparse. The problem is stated as

$$\underset{W,H}{\text{minimize}} \, \frac{1}{2} \|A - WH\|_F^2 + h(H) \quad \text{subject to } W, H \geqslant 0, \tag{38}$$

where $h(H) = \lambda \| \operatorname{vec} H \|_0$ and vec stacks the columns of a matrix to form a vector. In our experiments, each observation is generated using a mixture of Gaussians. Negative elements in the matrix A generated are reset to zero.

Table 3: NNMF (38) statistics with $h=\lambda\|\cdot\|_0$. All variants of TR use an LSR1 Hessian approximation, and are given a maximum of 100 inner iterations.

solver	f(x)	$h(x)/\lambda$	$\sqrt{\xi/\nu}$	#f	#∇ f	# prox	t (s)
R2	2.84e+03	0	2.2e-04	2	2	2	0.0e+00
TRDH-Spec	1.25e + 02	50	7.7e - 02	47	29	93	5.0e - 03
iTRDH-Spec	1.25e + 02	50	6.5e - 02	48	29	47	4.0e - 03
TRDH-PSB	1.70e + 02	62	5.7e + 00	501	352	1000	5.6e - 02
iTRDH-PSB	1.70e + 02	62	8.4e + 00	501	352	500	5.5e - 02
TRDH-Andrei	2.73e + 02	54	5.9e + 00	501	283	1000	5.9e - 02
iTRDH-Andrei	2.73e + 02	54	7.0e + 00	501	283	500	5.6e - 02
TR-R2	1.25e + 02	50	5.0e - 03	212	115	4983	2.4e - 01
TR-TRDH-PSB	1.25e + 02	50	7.2e - 03	197	104	9826	7.3e - 01
TR-iTRDH-PSB	1.25e + 02	50	6.4e - 03	129	71	3759	4.8e - 01
TR-TRDH-Andrei	1.25e + 02	50	2.9e - 03	170	91	8746	6.1e - 01
TR-iTRDH-Andrei	1.25e + 02	50	6.8e - 03	152	83	4809	6.1e - 01
TR-TRDH-Spec	1.25e + 02	50	$4.8e{-03}$	126	69	4793	3.6e - 01
TR-iTRDH-Spec	1.25e + 02	50	3.6e-03	162	82	2503	3.5e-01

We set m=100, n=50, k=5, $\lambda=10^{-1}$. The stopping tolerances ε_{α} and ε_{r} are set to 10^{-5} . Figure 5 shows the solution of (38) with TR-TRDH-PSB. The statistics are reported in Table 3. We observe that R2 is trapped in a spurious stationary point, and that all TRDH and iTRDH solvers

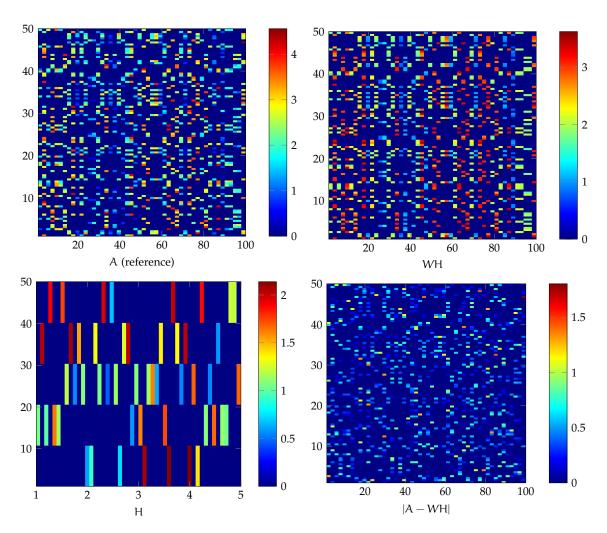


Figure 5: Solution of (38) with TR-TRDH-PSB.

except TRDH-Spec and iTRDH-Spec reach their maximum number of iterations. All solvers using TR perform well with fewer objective and gradient evaluations than TR-R2. The number of proximal operator calls is lower for all TR-iTRDH variants.

6.3 Nonlinear support vector machine (SVM)

We now consider the nonlinear SVM described by [2] to classify digits of the MNIST dataset as either 1 or 7—the other digits are removed. Let m be the number of images and n the vectorized image size. The problem reads

$$\underset{x}{\text{minimize }} \frac{1}{2} \| \mathbf{1} - \tanh(\mathbf{b} \odot (\mathbf{A}^{\mathsf{T}} \mathbf{x})) \|^2 + h(\mathbf{x}), \tag{39}$$

where $A \in \mathbb{R}^{m \times n}$ is the data matrix, b is the vector of labels with values ± 1 for all its components, \odot denotes the elementwise product between two vectors, and $h(x) = \lambda \|x\|_1$. We use n = 784, m = 13007 in the training set, m = 2163 in the testing set, $\lambda = 0.1$ and we initialize the problem at x = e, the vector of ones. We set the absolute and relative stopping tolerances ε_{α} and ε_{r} to 10^{-4} .

The solution map of (39) representing the most important pixels to classify the images between 1 and 7 is shown in Figure 6 for the solver TR-TRDH-Spec, along with a few sample digits. We observe that the mid-height pixels are selected as the most important ones, which is consistent with the fact that the images show the digits sideways. The statistics are reported in Table 4, and

show that TRDH-PSB, iTRDH-PSB, TRDH-Andrei and iTRDH-Andrei as main solvers exceed the maximum number of iterations. R2, TRDH-Spec and iTRDH-Spec are the most efficient and perform similar number of objective and gradient evaluations, with R2 terminating with a slightly higher criticality measure. TR-TRDH-PSB, TR-iTRDH-Andrei and TR-TRDH-Spec perform fewer objective and gradient evaluations, but more proximal operator evaluations than TR-R2.

Table 4: SVM (39) statistics with $h=\lambda\|\cdot\|_1$. All variants of TR use an LBFGS Hessian approximation, and are given a maximum of 100 inner iterations. The train and test accuracies are the percentage of images correctly classified, computed by counting the number of elements of the residual $1-\tanh(b\odot(A^Tx))$ that are lower than 1 for the train and test problems respectively.

solver	f(x)	$h(x)/\lambda$	$\sqrt{\xi/\nu}$	(Train, Test)	#f	#∇ f	# prox	t (s)
R2	2.18e+02	2.4e + 03	1.2e-01	(99.3, 98.8)	265	199	265	3.7e+00
TRDH-Spec	2.18e + 02	2.4e + 03	5.9e - 02	(99.3, 98.9)	306	191	611	4.4e + 00
iTRDH-Spec	2.18e + 02	2.4e + 03	5.9e - 02	(99.3, 98.9)	307	191	306	3.9e + 00
TRDH-PSB	2.38e + 02	2.4e + 03	4.5e - 01	(99.1, 98.8)	1001	686	2000	1.3e + 01
iTRDH-PSB	2.38e + 02	2.4e + 03	4.3e - 01	(99.1, 98.8)	1001	686	1000	1.3e + 01
TRDH-Andrei	3.00e+02	2.9e + 03	1.2e + 00	(99.1, 99.0)	1001	418	2000	9.1e+00
iTRDH-Andrei	3.00e + 02	2.9e + 03	2.7e + 00	(99.1, 99.0)	1001	418	1000	8.8e + 00
TR-R2	2.18e + 02	2.4e + 03	4.7e - 03	(99.3, 98.8)	361	361	1512	5.3e + 00
TR-TRDH-PSB	2.18e + 02	2.4e + 03	4.7e - 03	(99.3, 98.8)	316	316	3882	6.5e + 00
TR-iTRDH-PSB	2.18e + 02	2.4e + 03	4.7e - 03	(99.3, 98.8)	377	377	2242	7.8e + 00
TR-TRDH-Andrei	2.18e + 02	2.4e + 03	4.7e - 03	(99.3, 98.9)	396	396	27155	1.4e + 01
TR-iTRDH-Andrei	2.18e + 02	2.4e + 03	4.5e - 03	(99.3, 98.9)	283	283	11418	1.2e + 01
TR-TRDH-Spec	2.18e + 02	2.4e + 03	4.7e - 03	(99.3, 98.8)	333	333	3390	7.5e + 00
TR-iTRDH-Spec	2.18e + 02	2.4e + 03	4.7e - 03	(99.3, 98.8)	472	472	1791	9.3e+00

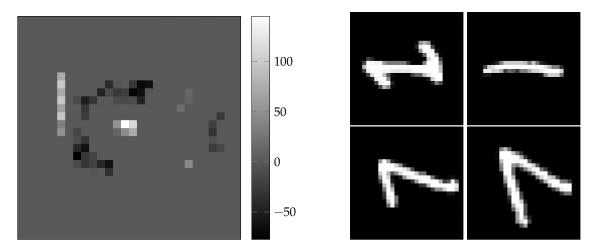


Figure 6: Solution map of (39) with TR-TRDH-Spec (left), and sample 1's (right, top row) and 7's (right, bottom row) rotated digits from the MNIST dataset.

6.4 FitzHugh-Nagumo inverse problem

Let $v(x) = (v_1(x), \dots, v_{n+1}(x))$ and $w(x) = (w_1(x), \dots, w_{n+1}(x))$ be sampled values of V(t; x) and W(t; x) for $x \in \mathbb{R}^5$ satisfying the FitzHugh [18] and Nagumo et al. [23] model for neuron activation

$$\frac{dV}{dt} = (V - V^3/3 - W + x_1)x_2^{-1}, \quad \frac{dW}{dt} = x_2(x_3V - x_4W + x_5). \tag{40}$$

The samples are generated using a discretization of the time interval $t \in [0, 20]$ with initial conditions (V(0), W(0)) = (2, 0). We define a target solution that corresponds to a simulation of the van der Pol [29] oscillator by generating solutions $(\bar{v}(x), \bar{w}(x))$ of (40) with $\bar{x} = (0, 0.2, 1, 0, 0)$, and we solve

$$\underset{x}{\text{minimize }} \frac{1}{2} \| (v(x) - \bar{v}(\bar{x}), w(x) - \bar{w}(\bar{x})) \|_{2}^{2} + h(x), \tag{41}$$

where $h(x) = \lambda \|x\|_0$ with n=100. The stopping tolerances ε_α and ε_r are set to 10^{-4} . We report the statistics of the solution of (41) with $\lambda=10$ in Table 5. TRDH as main solver results in many objective and gradient evaluations compared to TR. Moreover, TR-TRDH-PSB, TR-iTRDH-PSB, TR-TRDH-Andrei and TR-iTRDH-Andrei perform fewer objective and gradient evaluations than TR-R2. TR-TRDH-Spec is the least efficient.

Table 5: FH (41) statistics with $h = \lambda \| \cdot \|_0$. All variants of TR use an LBFGS Hessian approximation, and are given a maximum of 200 inner iterations. The optimal objective value is $f(\mathbf{x}_{\star}) = 1.03e + 00$.

solver	f(x)	$h(x)/\lambda$	$\sqrt{\xi/\nu}$	$\ \mathbf{x} - \mathbf{x}_{\star}\ _{2}$	#f	#∇ f	#prox	t (s)
TRDH-Spec	3.21e+01	5	7.0e+00	9.8e-01	501	351	1000	2.1e+00
iTRDH-Spec	3.21e + 01	5	5.9e + 00	$9.8e{-01}$	501	351	500	2.5e + 00
TRDH-PSB	1.12e + 00	2	2.7e + 00	$1.3e{-01}$	501	401	1000	4.7e + 00
iTRDH-PSB	1.12e + 00	2	2.4e + 00	$1.3e{-01}$	501	401	500	4.7e + 00
TRDH-Andrei	1.15e + 00	2	1.6e + 00	$1.5e{-01}$	501	372	1000	4.2e + 00
iTRDH-Andrei	1.15e + 00	2	2.8e + 00	$1.5e{-01}$	501	372	500	5.3e + 00
TR-R2	1.02e + 00	2	5.0e - 03	6.3e - 03	327	236	36274	6.7e + 00
TR-TRDH-PSB	1.02e + 00	2	5.7e - 03	6.1e - 03	183	149	56042	3.8e + 00
TR-iTRDH-PSB	1.02e + 00	2	6.3e - 03	6.2e - 03	211	179	33452	3.7e + 00
TR-TRDH-Andrei	1.02e + 00	2	5.6e - 03	6.5e - 03	185	138	49311	2.9e + 00
TR-iTRDH-Andrei	1.02e + 00	2	6.4e - 03	6.1e - 03	168	151	23655	2.9e + 00
TR-TRDH-Spec	1.04e + 00	2	1.0e + 00	7.3e - 02	501	428	109750	9.0e + 00
TR-iTRDH-Spec	1.02e+00	2	4.6e-03	1.1e-02	383	337	40354	6.1e+00

The left half of Table 6 reports the final solution identified by each solver. The solution of (41) with TR-TRDH-PSB and the sampled values of V and W are displayed in Figure 7. We do not show results with R2 because it encountered numerical issues when solving the problem.

Table 6: FH (41) (left) and constrained FH (42) (right) solutions identified by the solvers tested. The unconstrained solution is (0,0.2,1,0,0).

	\mathbf{x}_1	x_2	x_3	χ_4	x_5	\mathbf{x}_1	x_2	x_3	χ_4	x_5
TRDH-Spec	0.32	0.43	0.83	0.77	0.44	0.00	0.50	0.54	0.00	0.00
iTRDH-Spec	0.32	0.43	0.83	0.77	0.44	0.00	0.50	0.54	0.00	0.00
TRDH-PSB	0.00	0.24	0.87	0.00	0.00	0.00	0.50	0.54	0.00	0.00
iTRDH-PSB	0.00	0.24	0.87	0.00	0.00	0.00	0.50	0.54	0.00	0.00
TRDH-Andrei	0.00	0.25	0.86	0.00	0.00	0.00	0.50	0.54	0.00	0.00
iTRDH-Andrei	0.00	0.25	0.86	0.00	0.00	0.00	0.50	0.54	0.00	0.00
TR-R2	0.00	0.20	1.01	0.00	0.00	0.00	0.50	0.54	0.00	0.00
TR-TRDH-PSB	0.00	0.20	1.01	0.00	0.00	0.00	0.50	0.54	0.00	0.00
TR-iTRDH-PSB	0.00	0.20	1.01	0.00	0.00	0.00	0.50	0.54	0.00	0.00
TR-TRDH-Andrei	0.00	0.20	1.01	0.00	0.00	0.00	0.50	0.54	0.00	0.00
TR-iTRDH-Andrei	0.00	0.20	1.01	0.00	0.00	0.00	0.50	0.54	0.00	0.00
TR-TRDH-Spec	0.00	0.18	1.07	0.00	0.00	0.00	0.50	0.54	0.00	0.00
TR-iTRDH-Spec	0.00	0.20	1.01	0.00	0.00	0.00	0.50	0.54	0.00	0.00

We also solve the constrained variant

$$\underset{x}{\text{minimize}} \ \tfrac{1}{2} \| (v(x) - \bar{v}(\bar{x}), w(x) - \bar{w}(\bar{x})) \|_2^2 + h(x), \quad \text{subject to } x_2 \geqslant 0.5, \tag{42}$$

and we keep all parameters the same, except for λ that we set to 40 to further enforce sparsity.

The right half of Table 6 reports the solution and Table 7 the statistics of the solve of (42) with the tested solvers. Note that all solvers identify the same solution. We observe that all TR-TRDH and TR-iTRDH solvers perform fewer objective and gradient evaluations than TR-R2. However, TR-R2 has the lowest number of proximal operator calls out of all solvers using TR. The right plot of Figure 7 shows that the W part of the solution of (42) with TR-TRDH-PSB does not match the data as tightly as that of (41) in the left half of Figure 7. That is a consequence of enforcing $x_2 \ge 0.5$, since the unconstrained solution verifies $x_2 = 0.2$.

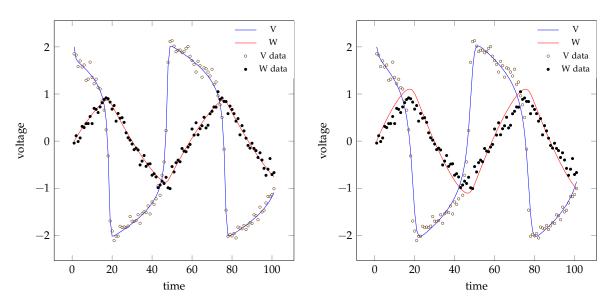


Figure 7: Solution of (41) (left) and of (42) (right) with TR-TRDH-PSB and sampled values of V and W.

Table 7: Constrained FH (42) statistics with $h = \lambda \| \cdot \|_1$. All variants of TR use an LBFGS Hessian approximation, and are given a maximum of 200 inner iterations.

solver	f(x)	$h(x)/\lambda$	ξ	$\ \mathbf{x}-\mathbf{x}_{\star}\ _2$	#f	#∇f	#prox	t (s)
TRDH-Spec	4.43e + 00	1.0e+00	1.2e-02	5.5e-01	327	226	653	2.6e+00
iTRDH-Spec	4.43e + 00	1.0e + 00	$1.1e{-02}$	5.5e - 01	328	226	327	2.4e + 00
TRDH-PSB	4.43e + 00	1.0e + 00	8.2e - 03	5.5e - 01	331	237	661	2.6e + 00
iTRDH-PSB	4.43e + 00	1.0e + 00	7.7e - 03	5.5e - 01	332	237	331	2.2e + 00
TRDH-Andrei	4.43e + 00	1.0e + 00	7.1e - 03	5.5e - 01	223	155	445	1.4e + 00
iTRDH-Andrei	4.43e + 00	1.0e + 00	7.1e - 03	5.5e - 01	224	155	223	1.6e + 00
TR-R2	4.43e + 00	1.0e + 00	4.9e - 03	5.5e - 01	47	31	3057	$4.4e{-01}$
TR-TRDH-PSB	4.43e + 00	1.0e + 00	2.7e - 04	5.5e - 01	38	29	6725	$3.1e{-01}$
TR-iTRDH-PSB	4.43e + 00	1.0e + 00	7.9e - 05	5.5e - 01	36	27	3326	3.3e - 01
TR-TRDH-Andrei	4.43e + 00	1.0e + 00	8.7e - 05	5.5e - 01	39	30	7438	3.8e - 01
TR-iTRDH-Andrei	4.43e + 00	1.0e + 00	1.6e - 03	5.5e - 01	36	27	3117	3.4e - 01
TR-TRDH-Spec	4.43e + 00	1.0e + 00	4.1e - 03	5.5e - 01	36	27	5467	3.9e - 01
TR-iTRDH-Spec	4.43e + 00	1.0e + 00	1.8e - 03	5.5e - 01	38	25	3347	2.5e - 01

7 Discussion and future work

The ℓ_0 - and ℓ_1 -norm regularizers are standard choices to promote sparsity. It is possible to derive the iprox of other useful separable regularizers, including ℓ_p pseudonorms to the p-th power, i.e.,

$$h(x) = ||x||_p^p = \sum_{i=1}^n |x_i|^p \quad (0$$

and those are also useful to promote sparsity [12]. Much remains to be done, however, including deriving the iprox of relevant non-separable regularizers, and studying other diagonal Hessian approximations than the ones considered above, including new diagonal quasi-Cauchy updates.

TRDH performs well on the problems tested and is promising, but we were surprised to see the spectral gradient update often perform better than more sophisticated diagonal quasi-Newton updates, especially when using TRDH as main solver. Future research should seek to provide an explanation for that observation. In several instances, the variant of TRDH denoted "iTRDH" performs better than the basic version, which indicates that both algorithms are relevant.

Finally, other solvers would likely benefit from using TRDH as a subproblem solver, including the methods for least-squares f of Aravkin et al. [2].

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