IHT dies hard: Provable accelerated Iterative Hard Thresholding

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Abstract

We study -both in theory and practice- the use of momentum motions in classic iterative hard thresholding (IHT) methods. By simply modifying plain IHT, we investigate its convergence behavior on convex optimization criteria with non-convex constraints, under standard assumptions. In diverse scenaria, we observe that acceleration in IHT leads to significant improvements, compared to state of the art projected gradient descent and Frank-Wolfe variants. As a byproduct of our inspection, we study the impact of selecting the momentum parameter: similar to convex settings, two modes of behavior are observed -"rippling" and linear-depending on the level of momentum.

1 Introduction

It is a well-known fact in convex optimization that momentum techniques provably result into significant gains w.r.t. convergence rate. Since 1983, when Nesterov proposed his *optimal gradient methods* [I], these techniques have been used in diverse machine learning and signal processing tasks. Lately, the use of momentum has re-gained popularity in non-convex settings, thanks to their improved performance in structured practical scenaria: from empirical risk minimization (ERM) to training neural networks.

Here, we mainly focus on structured constrained ERM optimization problems:

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} \quad f(x) \quad \text{subject to} \quad x \in \mathcal{C}, \tag{1}$$

that involve convex objectives f and simple structured, but non-convex, constraints \mathcal{C} , that can be described using a set of atoms, as in [2, 3]; see also Section [2.1].

Proceedings of the 21^{st} International Conference on Artificial Intelligence and Statistics (AISTATS) 2018, Lanzarote, Spain. PMLR: Volume 84. Copyright 2018 by the author(s).

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Practical algorithms for (1) are convexified projected gradient descent schemes 3, non-convex iterative hard thresholding (IHT) variants 4 and Frank-Wolfe (FW) methods 5. Convex methods can accommodate acceleration due to [1, 6] and come with rigorous theoretical guarantees; but, higher computational complexity might be observed in practice (depending on the nature of \mathcal{C}); further, their configuration could be harder and/or non-intuitive. FW variants 7, 8 simplify the handling of constraints, but the successive construction of estimates –by adding singleton atoms to the putative solution—could slow down convergence. Non-convex methods, such as IHT 9, 10, could be the methods of choice in practice, but only few schemes justify their behavior in theory. Even more importantly, IHT schemes that utilize acceleration inferably are lacking. We defer the discussion on related work to Section 5.

In this work, we study the use of acceleration in IHT settings and supply additional information about open questions regarding the convergence and practicality of such methods on real problems. The current paper provides evidence that "IHT dies hard":

- Accelerated IHT comes with theoretical guarantees for the general minimization problem [1]. While recent results [11] focus on plain IHT, there are no results on Accelerated IHT, apart from [12] on specific cases of [1] and under stricter assumptions. The main assumptions made here are the existence of an exact projection operation over the structure set \mathcal{C} , as well as standard regularity conditions on the objective function.
- Regarding the effect of the momentum on the convergence behavior, our study justifies that similar
 –to convex settings– behavior is observed in practice for accelerated IHT: two modes of convergence exist ("rippling" and linear), depending on the level of momentum used per iteration.
- We include extensive experimental results with real datasets and highlight the pros and cons of using IHT variants over state of the art for structured ERM problems.

Our framework applies in numerous structured applications, and one of its primary merits is its flexibility.

2 Problem statement

2.1 Low-dimensional structures

Following the notation in [3], let \mathcal{A} denote a set of atoms; *i.e.*, simple building units of general "signals". E.g., we write $x \in \mathbb{R}^n$ as $x = \sum_i w_i a_i$, where w_i are weights and $a_i \in \mathbb{R}^n$ atoms from \mathcal{A} .

Given \mathcal{A} , let the "norm" function $\|x\|_{0,\mathcal{A}}$ return the minimum number of superposed atoms that result into x. Note that $\|\cdot\|_{0,\mathcal{A}}$ is a non-convex entity for the most interesting \mathcal{A} cases. Also, define the support function $\sup_{\mathcal{A}}(x)$ as the function that returns the indices of active atoms in x. Associated with $\|\cdot\|_{0,\mathcal{A}}$ is the projection operation over the set \mathcal{A} :

$$\Pi_{k,\mathcal{A}}(x) \in \underset{y:\|y\|_{0,\mathcal{A}} \le k}{\arg\min} \frac{1}{2} \|x - y\|_2^2.$$

To motivate our discussion, we summarize some well-known sets \mathcal{A} used in machine learning problems; for a more complete description see [13].

 \mathcal{A} represents plain sparsity: Let $\mathcal{A} = \{a_i \in \mathbb{R}^n \mid a_i \equiv \pm e_i, \forall i \in [n]\}$, where e_i denotes the canonical basis vector. In this case, k-sparse "signals" $x \in \mathbb{R}^n$ can be represented as a linear combination of k atoms in \mathcal{A} : $x = \sum_{i \in \mathcal{I}} w_i a_i$, for $|\mathcal{I}| \leq k$ and $w_i \in \mathbb{R}_+$. The "norm" function is the standard ℓ_0 -"norm" and $\Pi_{k,\mathcal{A}}(x)$ finds the k-largest in magnitude entries of x.

A represents block sparsity [I4]: Let $\{G_1, G_2, \ldots, G_M\}$ be a collection of M non-overlapping group indices such that $\bigcup_{i=1}^M G_i = [n]$. With a slight abuse of notation, $\mathcal{A} = \{a_i \in \mathbb{R}^n \mid a_i \equiv \bigcup_{j:j \in G_i} e_j\}$ is the collection of grouped indices, according to $\{G_1, G_2, \ldots, G_M\}$. Then, k-sparse block "signals" $x \in \mathbb{R}^n$ can be expressed as a weighted linear combination of k group atoms in \mathcal{A} . The "norm" function is the extension of ℓ_0 -"norm" over group structures, and $\Pi_{k,\mathcal{A}}(x)$ finds the k most significant groups (i.e., groups with largest energy).

 \mathcal{A} denotes low rankness: Let $\mathcal{A} = \{a_i \in \mathbb{R}^{m \times n} \mid a_i = u_i v_i^\top, \|u_i\|_2 = \|v_i\|_2 = 1\}$ be the set of rank-one matrices. Here, sparsity corresponds to low-rankness. The "norm" function corresponds to the notion of rankness; $\Pi_{k,\mathcal{A}}(x)$ finds the best k-rank approximation.

2.2 Loss function f

Let $f: \mathbb{R}^n \to \mathbb{R}$ be a differentiable convex loss function. We consider applications that can be described by restricted strongly convex and smooth functions f.

Definition 1. Let f be convex and differentiable. f is

 α -restricted strongly convex over $\mathcal{C} \subseteq \mathbb{R}^n$ if:

$$f(y) \ge f(x) + \langle \nabla f(x), y - x \rangle + \frac{\alpha}{2} ||x - y||_2^2, \forall x, y \in \mathcal{C}.$$
 (2)

Definition 2. Let f be a convex and differentiable. f is β -restricted smooth over $C \subseteq \mathbb{R}^n$ if:

$$f(y) \le f(x) + \langle \nabla f(x), y - x \rangle + \frac{\beta}{2} ||x - y||_2^2, \ \forall x, y \in \mathcal{C}.$$
 (3)

Combined with the above, C could be the set of rk-sparse vectors, rk-sparse block "signals", etc, for some integer r > 0.

2.3 Optimization criterion

Given f and a low-dimensional structure \mathcal{A} , we focus on the following optimization problem:

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} \quad f(x) \quad \text{subject to} \quad ||x||_{0,\mathcal{A}} \le k.$$
 (4)

Here, $k \in \mathbb{Z}_+$ denotes the level of "succinctness". Examples include (i) sparse and model-based sparse linear regression, (ii) low-rank learning problems, and (iii) model-based, ℓ_2 -norm regularized logistic regression tasks; see also Section [6].

3 Accelerated IHT variant

We follow the path of IHT methods. These are first-order gradient methods, that perform per-iteration a non-convex projection over the constraint set \mathcal{A} . With math terms, this leads to:

$$x_{i+1} = \prod_{k,\mathcal{A}} (x_i - \mu_i \nabla f(x_i)), \text{ where } \mu_i \in \mathbb{R}.$$

While the merits of plain IHT, as described above, are widely known for simple sets \mathcal{A} and specific functions f (cf., [0], [1], [1]), momentum-based acceleration techniques in IHT have not received significant attention in more generic ML settings. Here, we study a simple momentum-variant of IHT, previously proposed in [16], [12], that satisfies the following recursions:

$$x_{i+1} = \Pi_{k,\mathcal{A}} \left(u_i - \mu_i \nabla_{\mathcal{T}_i} f(u_i) \right),$$

and

$$u_{i+1} = x_{i+1} + \tau \cdot (x_{i+1} - x_i). \tag{5}$$

Here, $\nabla_{\mathcal{T}_i} f(\cdot)$ denotes restriction of the gradient on the subspace spanned by set \mathcal{T} ; more details below. τ is the momentum step size, used to properly weight previous estimates with the current one, based on $\boxed{17}$.

¹Nesterov's acceleration is an improved version of Polyak's classical momentum [18] schemes. Understanding when and how hard thresholding operations still work for the whole family of momentum algorithms is open for future research direction.

Despite the simplicity of (5), to the best of our knowledge, there are no convergence guarantees for generic f, neither any characterization of its performance w.r.t. au values. Nevertheless, its superior performance has been observed under various settings and configurations 16, 19, 12.

In this paper, we study this accelerated IHT variant, as described in Algorithm 1. This algorithm was originally presented in [16, 12]. However, [16, 12] covers only a special case (i.e., squared loss) of our setting, and the theory there is restricted, and further needs justification (e.g., the role of τ in the convergence behavior is not studied). For simplicity, we will focus on the case of sparsity; same notions can be extended to more complicated sets A.

Some notation first: given gradient $\nabla f(x) \in \mathbb{R}^n$, and given a subset of [n], say $\mathcal{T} \subseteq [n]$, $\nabla_{\mathcal{T}} f(x) \in \mathbb{R}^n$ has entries from $\nabla f(x)$, only indexed by \mathcal{T}^2 \mathcal{T}^c represents the complement of $[n] \setminus \mathcal{T}$.

Algorithm 1 Accelerated IHT algorithm

- 1: **Input:** Tolerance η , T, α , $\beta > 0$, model \mathcal{A} , $k \in \mathbb{Z}_+$.
- 2: **Initialize:** $x_0, u_0 \leftarrow 0, \mathcal{U}_0 \leftarrow \{\emptyset\}$. Set $\xi = 1 \frac{\alpha}{\beta}$; select τ s.t. $|\tau| \leq \frac{1-\varphi\xi^{1/2}}{\varphi\xi^{1/2}}$, where $\varphi = \frac{1+\sqrt{5}}{2}$.
- 4: $\mathcal{T}_i \leftarrow \text{supp}_{\mathcal{A}} \left(\Pi_{k,\mathcal{A}} \left(\nabla_{\mathcal{U}_i^c} f(u_i) \right) \right) \cup \mathcal{U}_i$
- 5: $\bar{u}_i = u_i \frac{1}{\beta} \nabla_{\mathcal{T}_i} f(u_i)$
- 6: $x_{i+1} = \prod_{k,\mathcal{A}} (\bar{u}_i)^{\dagger}$ 7: $u_{i+1} = x_{i+1} + \tau (x_{i+1} x_i)$ where $\mathcal{U}_{i+1} \leftarrow$ $\operatorname{supp}_{\mathcal{A}}(u_{i+1})$
- 8: **until** $||x_i x_{i-1}|| \le \eta ||x_i||$ or after T iterations.
- 9: † Optional: Debias step on x_{i+1} , restricted on the support $\operatorname{supp}_{\mathcal{A}}(x_{i+1})$.

Algorithm 1 maintains and updates an estimate of the optimum at every iteration. It does so by maintaining two sequences of variables: x_i 's that represent our putative estimates per iteration, and u_i 's that model the effect of "friction" (memory) in the iterates. The first step in each iteration is active support expansion: we expand support set \mathcal{U}_i of u_i , by finding the indices of katoms of the largest entries in the gradient in the complement of \mathcal{U}_i . This step results into set \mathcal{T}_i and makes sure that per iteration we enrich the active support by "exploring" enough outside of it. The following two steps perform the recursion in (5), restricted on \mathcal{T}_i ; i.e., we perform a gradient step, followed by a projection onto \mathcal{A} ; finally, we update the auxiliary sequence u by using previous estimates as momentum. The iterations

terminate once certain condition holds.

Some observations: Set \mathcal{T}_i has cardinality at most 3k; x_i estimates are always k-sparse; intermediate "signal" u_i has cardinality at most 2k, as the superposition of two k-sparse "signals".

Theoretical study

Our study³ starts with the description of the dynamics involved per iteration (Lemma 1), followed by the conditions and eligible parameters that lead to convergence. Proofs are deferred to the Appendix.

Lemma 1 (Iteration invariant). Consider the nonconvex optimization problem in (4), for given structure A, associated with $\Pi_{k,A}(\cdot)$, and loss function f, satisfying restricted strong convexity and smoothness properties over 4k sparse "signals", with parameters α and β , respectively. Let x^* be the minimizer of f, with $\|x^*\|_{0,\mathcal{A}} = k$ and $f(x^*) \leq f(y)$, for any $y \in \mathbb{R}^n$ such that $||y||_{0,\mathcal{A}} \leq 3k$. Assuming $x_0 = 0$, Algorithm satisfies $\forall \tau$ the following linear system at the i-th

$$\begin{bmatrix} \|x_{i+1} - x^{\star}\|_2 \\ \|x_i - x^{\star}\|_2 \end{bmatrix} \leq \underbrace{ \begin{bmatrix} \left(1 - \frac{\alpha}{\beta}\right) \cdot |1 + \tau| & \left(1 - \frac{\alpha}{\beta}\right) \cdot |\tau| \\ 1 & 0 \end{bmatrix}}_{:=A} \cdot \underbrace{ \begin{bmatrix} \|x_i - x^{\star}\|_2 \\ \|x_{i-1} - x^{\star}\|_2 \end{bmatrix}}_{} \cdot \underbrace{ \begin{bmatrix} \|x_i - x^{\star}\|_2 \\ \|x_{i-1} - x^{\star}\|_2 \end{bmatrix}}_{} \cdot \underbrace{ \begin{bmatrix} \|x_i - x^{\star}\|_2 \\ \|x_{i-1} - x^{\star}\|_2 \end{bmatrix}}_{} \cdot \underbrace{ \begin{bmatrix} \|x_i - x^{\star}\|_2 \\ \|x_{i-1} - x^{\star}\|_2 \end{bmatrix}}_{} \cdot \underbrace{ \begin{bmatrix} \|x_i - x^{\star}\|_2 \\ \|x_{i-1} - x^{\star}\|_2 \end{bmatrix}}_{} \cdot \underbrace{ \begin{bmatrix} \|x_i - x^{\star}\|_2 \\ \|x_{i-1} - x^{\star}\|_2 \end{bmatrix}}_{} \cdot \underbrace{ \begin{bmatrix} \|x_i - x^{\star}\|_2 \\ \|x_{i-1} - x^{\star}\|_2 \end{bmatrix}}_{} \cdot \underbrace{ \begin{bmatrix} \|x_i - x^{\star}\|_2 \\ \|x_{i-1} - x^{\star}\|_2 \end{bmatrix}}_{} \cdot \underbrace{ \begin{bmatrix} \|x_i - x^{\star}\|_2 \\ \|x_{i-1} - x^{\star}\|_2 \end{bmatrix}}_{} \cdot \underbrace{ \begin{bmatrix} \|x_i - x^{\star}\|_2 \\ \|x_{i-1} - x^{\star}\|_2 \end{bmatrix}}_{} \cdot \underbrace{ \begin{bmatrix} \|x_i - x^{\star}\|_2 \\ \|x_{i-1} - x^{\star}\|_2 \end{bmatrix}}_{} \cdot \underbrace{ \begin{bmatrix} \|x_i - x^{\star}\|_2 \\ \|x_{i-1} - x^{\star}\|_2 \end{bmatrix}}_{} \cdot \underbrace{ \begin{bmatrix} \|x_i - x^{\star}\|_2 \\ \|x_{i-1} - x^{\star}\|_2 \end{bmatrix}}_{} \cdot \underbrace{ \begin{bmatrix} \|x_i - x^{\star}\|_2 \\ \|x_{i-1} - x^{\star}\|_2 \end{bmatrix}}_{} \cdot \underbrace{ \begin{bmatrix} \|x_i - x^{\star}\|_2 \\ \|x_{i-1} - x^{\star}\|_2 \end{bmatrix}}_{} \cdot \underbrace{ \begin{bmatrix} \|x_i - x^{\star}\|_2 \\ \|x_{i-1} - x^{\star}\|_2 \end{bmatrix}}_{} \cdot \underbrace{ \begin{bmatrix} \|x_i - x^{\star}\|_2 \\ \|x_{i-1} - x^{\star}\|_2 \end{bmatrix}}_{} \cdot \underbrace{ \begin{bmatrix} \|x_i - x^{\star}\|_2 \\ \|x_i - x^{\star}\|_2 \end{bmatrix}}_{} \cdot \underbrace{ \begin{bmatrix} \|x_i - x^{\star}\|_2 \\ \|x_i - x^{\star}\|_2 \end{bmatrix}}_{} \cdot \underbrace{ \begin{bmatrix} \|x_i - x^{\star}\|_2 \\ \|x_i - x^{\star}\|_2 \end{bmatrix}}_{} \cdot \underbrace{ \begin{bmatrix} \|x_i - x^{\star}\|_2 \\ \|x_i - x^{\star}\|_2 \end{bmatrix}}_{} \cdot \underbrace{ \begin{bmatrix} \|x_i - x^{\star}\|_2 \\ \|x_i - x^{\star}\|_2 \end{bmatrix}}_{} \cdot \underbrace{ \begin{bmatrix} \|x_i - x^{\star}\|_2 \\ \|x_i - x^{\star}\|_2 \end{bmatrix}}_{} \cdot \underbrace{ \begin{bmatrix} \|x_i - x^{\star}\|_2 \\ \|x_i - x^{\star}\|_2 \end{bmatrix}}_{} \cdot \underbrace{ \begin{bmatrix} \|x_i - x^{\star}\|_2 \\ \|x_i - x^{\star}\|_2 \end{bmatrix}}_{} \cdot \underbrace{ \begin{bmatrix} \|x_i - x^{\star}\|_2 \\ \|x_i - x^{\star}\|_2 \end{bmatrix}}_{} \cdot \underbrace{ \begin{bmatrix} \|x_i - x^{\star}\|_2 \\ \|x_i - x^{\star}\|_2 \end{bmatrix}}_{} \cdot \underbrace{ \begin{bmatrix} \|x_i - x^{\star}\|_2 \\ \|x_i - x^{\star}\|_2 \end{bmatrix}}_{} \cdot \underbrace{ \begin{bmatrix} \|x_i - x^{\star}\|_2 \\ \|x_i - x^{\star}\|_2 \end{bmatrix}}_{} \cdot \underbrace{ \begin{bmatrix} \|x_i - x^{\star}\|_2 \\ \|x_i - x^{\star}\|_2 \end{bmatrix}}_{} \cdot \underbrace{ \begin{bmatrix} \|x_i - x^{\star}\|_2 \\ \|x_i - x^{\star}\|_2 \end{bmatrix}}_{} \cdot \underbrace{ \begin{bmatrix} \|x_i - x^{\star}\|_2 \\ \|x_i - x^{\star}\|_2 \end{bmatrix}}_{} \cdot \underbrace{ \begin{bmatrix} \|x_i - x^{\star}\|_2 \end{bmatrix}}_{} \cdot \underbrace{ \begin{bmatrix}$$

Proof ideas involved: The proof is composed mostly of algebraic manipulations. For exact projection $\Pi_{k,\mathcal{A}}(\cdot)$ and due to the optimality of the step $x_{i+1} = \prod_{k,\mathcal{A}} (\bar{u}_i)$, we observe that $||x_{i+1} - x^*||_2^2 \le 2 \langle x_{i+1} - x^*, \bar{u}_i - x^* \rangle$. Using Definitions 1.2, we prove a version of Lemma 2 in 20 over non-convex constraint sets, using optimality conditions over low-dimensional structures [21]. These steps are admissible due to the restriction of the active subspace to the set \mathcal{T}_i per iteration: most operations -i.e., inner products, Euclidean distances, etc-involved in the proof are applied on "signals" comprised of at most 4k atoms. After algebraic "massaging", this leads to the two-step recursion:

$$||x_{i+1} - x^*||_2 \le \left(1 - \frac{\alpha}{\beta}\right) \cdot |1 + \tau| \cdot ||x_i - x^*||_2 + \left(1 - \frac{\alpha}{\beta}\right) \cdot |\tau| \cdot ||x_{i-1} - x^*||_2.$$

Finally, we convert this second-order linear system into a two-dimensional first-order system, that produces the desired recursion. See Appendix A for a detailed proof.

²Here, we abuse a bit the notation for the case of low rank structure A: in that case $\nabla_{\mathcal{T}} f(x) \in \mathbb{R}^{m \times n}$ denotes the part of $\nabla f(x)$ that "lives" in the subspace spanned by the atoms in \mathcal{T} .

³Our focus is to study optimization guarantees (convergence), not statistical ones (required number of measurements, etc). Our aim is the investigation of accelerated IHT and under which conditions it leads to convergence; not its one-to-one comparison with plain IHT schemes.

A specific case of the above analysis was presented in $\boxed{12}$; however, the theory specifically applies only to the matrix sensing case over low-rank matrices, using the RIP property. Here, we generalize these results for generic (restricted) strongly convex and smooth functions f, where different theoretical tools apply. Our analysis moves beyond this point, as we show next, in contrast to $\boxed{12}$. Further we investigate a variable τ selection, instead of a constant selection, as in $\boxed{12}$.

Remark 1. The assumption $f(x^*) \leq f(y)$, for any $y \in \mathbb{R}^n$ such that $\|y\|_{0,\mathcal{A}} \leq 3k$, is trivially satisfied by any noiseless norm-based objective; i.e., for $b = \Phi x^*$ and $f(x) = \frac{1}{2} \|b - \Phi x\|_2^2$, $f(x^*) = 0$ for linear regression or $b = \mathcal{M}(X^*)$ and $f(X) = \frac{1}{2} \|b - \mathcal{M}(X)\|_2^2$, $f(X^*) = 0$ for low rank recovery problems. We note that this assumption does not restrict our analysis just to the noiseless setting. It states that x^* has the minimum function value f, among all vectors that are at most 3k-sparse. E.g., any dense vector, that might be a solution also due to noise, does not affect this requirement. We conjecture that it is an artifact of our proof technique.

Lemma I just states the iteration invariant of Algorithm I it does not guarantee convergence. To do so, we need to state some interesting properties of A. The proof is elementary and is omitted.

Lemma 2. Let A be the 2×2 matrix, as defined above, parameterized by constants $0 < \alpha < \beta$, and user-defined parameter τ . Denote $\xi := 1 - \alpha/\beta$. The characteristic polynomial of A is defined as:

$$\lambda^2 - \text{Tr}(A) \cdot \lambda + \det(A) = 0$$

where λ represent the eigenvalue(s) of A. Define $\Delta := \operatorname{Tr}(A)^2 - 4 \cdot \det(A) = \xi^2 \cdot (1+\tau)^2 + 4\xi \cdot |\tau|$. Then, the eigenvalues of A satisfy the expression: $\lambda = \frac{\xi \cdot |1+\tau| \pm \sqrt{\Delta}}{2}$. Depending on the values of α, β, τ :

- A has a unique eigenvalue $\lambda = \frac{\xi \cdot |1+\tau|}{2}$, if $\Delta = 0$. This happens when $\alpha = \beta$ and is not considered in this paper (we assume functions f with curvature).
- A has two complex eigenvalues; this happens when
 Δ < 0. By construction, this case does not happen
 in our scenaria, since β > α.
- For all other cases, A has two distinct real eigenvalues, satisfying $\lambda_{1,2} = \frac{\xi \cdot |1+\tau|}{2} \pm \frac{\sqrt{\xi^2 \cdot (1+\tau) + 4\xi \cdot |\tau|}}{2}$.

Define $y(i+1) = \begin{bmatrix} \|x_{i+1} - x^{\star}\|_2 \\ \|x_i - x^{\star}\|_2 \end{bmatrix}$; then, the linear system in Lemma $\boxed{1}$ for the i-th iteration becomes $y(i+1) \leq A \cdot y(i)$. A has only non-negative values; we can unfold this linear system over T iterations such that

$$y(T) \leq A^T \cdot y(0)$$
.

Here, we make the convention that $x_{-1} = x_0 = 0$, such that $y(0) = \begin{bmatrix} \|x_0 - x^*\|_2 \\ \|x_{-1} - x^*\|_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix} \cdot \|x^*\|_2$. The following lemma describes how one can compute a power

of a 2×2 matrix A, A^i , through the eigenvalues $\lambda_{1,2}$ (real and distinct eigenvalues); the proof is provided in Section \mathbb{C} . To the best of our knowledge, there is no detailed proof on this lemma in the literature.

Lemma 3 ([22]). Let A be a 2×2 matrix with real eigenvalues $\lambda_{1,2}$. Then, the following expression holds, when $\lambda_1 \neq \lambda_2$:

$$A^{i} = \frac{\lambda_1^{i} - \lambda_2^{i}}{\lambda_1 - \lambda_2} \cdot A - \lambda_1 \lambda_2 \cdot \frac{\lambda_1^{i-1} - \lambda_2^{i-1}}{\lambda_1 - \lambda_2} \cdot I$$

where λ_i denotes the i-th eigenvalue of A in order.

Then, the main recursion takes the following form:

$$y(T) \le \frac{\lambda_1^T - \lambda_2^T}{\lambda_1 - \lambda_2} \cdot A \cdot y(0) - \lambda_1 \lambda_2 \frac{\lambda_1^{T-1} - \lambda_2^{T-1}}{\lambda_1 - \lambda_2} \cdot y(0).$$

$$\tag{6}$$

Observe that, in order to achieve convergence (i.e., the RHS convergences to zero), eigenvalues play a crucial role: Both A and y(0) are constant quantities, and only how fast the quantities $\lambda_1^T - \lambda_2^T$ and $\lambda_1^{T-1} - \lambda_2^{T-1}$ "shrink" matter most.

Given that eigenvalues appear in the above expressions in some power (i.e., $\lambda_{1,2}^T$ and $\lambda_{1,2}^{T-1}$), we require $|\lambda_{1,2}| < 1$ for convergence. To achieve $|\lambda_{1,2}| < 1$, we have:

$$|\lambda_{1,2}| = \left| \frac{\xi \cdot |1+\tau|}{2} \pm \sqrt{\frac{\xi^2 (1+\tau)^2}{4} + \xi \cdot |\tau|} \right|$$

$$\leq \left| \frac{\xi \cdot |1+\tau|}{2} \right| + \left| \sqrt{\frac{\xi^2 (1+\tau)^2}{4} + \xi \cdot |\tau|} \right|$$

$$\stackrel{(i)}{\leq} \frac{\xi \cdot |1+\tau|}{2} + \frac{1}{2} \sqrt{\xi (1+|\tau|)^2 + 4\xi (1+|\tau|)^2}$$

$$\stackrel{(i)}{\leq} \frac{\xi^{\frac{1}{2}} (1+|\tau|)}{2} + \frac{\sqrt{5}}{2} \xi^{\frac{1}{2}} (1+|\tau|)$$

$$= \varphi \cdot \xi^{\frac{1}{2}} (1+|\tau|)$$

where (i) is due to $\xi < 1$, and $\varphi = (1 + \sqrt{5})/2$ denotes the golden ratio. Thus, upper bounding the RHS to ensure $|\lambda_{1,2}| < 1$ implies $|\tau| < \frac{1-\varphi \cdot \xi^{1/2}}{\varphi \cdot \xi^{1/2}}$.

Using the assumption $|\lambda_{1,2}| < 1$ for $|\tau| < \frac{1-\varphi \cdot \xi^{1/2}}{\varphi \cdot \xi^{1/2}}$, (6) further transforms to:

$$y(T) \leq \frac{\lambda_{1}^{T} - \lambda_{2}^{T}}{\lambda_{1} - \lambda_{2}} \cdot A \cdot y(0) - \lambda_{1} \lambda_{2} \frac{\lambda_{1}^{T-1} - \lambda_{2}^{T-1}}{\lambda_{1} - \lambda_{2}} \cdot y(0)$$

$$\stackrel{(i)}{\leq} \frac{|\lambda_{1}|^{T} + |\lambda_{2}|^{T}}{|\lambda_{1}| - |\lambda_{2}|} \cdot A \cdot y(0)$$

$$+ |\lambda_{1} \lambda_{2}| \cdot \frac{|\lambda_{1}|^{T-1} + |\lambda_{2}|^{T-1}}{|\lambda_{1}| - |\lambda_{2}|} \cdot y(0)$$

$$\stackrel{(ii)}{\leq} \frac{2|\lambda_{1}|^{T}}{|\lambda_{1}| - |\lambda_{2}|} \cdot A \cdot y(0) + |\lambda_{1}| \cdot \frac{2|\lambda_{1}|^{T-1}}{|\lambda_{1}| - |\lambda_{2}|} \cdot y(0)$$

where (i) is due to $A \cdot y(0)$ and y(0) being positive quantities, and (ii) is due to $1 > |\lambda_1| > |\lambda_2|$. Focusing on the first entry of y(T) and substituting the first row of A and y(0), we obtain the following inequality:

$$||x_T - x^*||_2 \le \frac{4 \cdot |\lambda_1|^T}{|\lambda_1| - |\lambda_2|} \cdot \left(1 - \frac{\alpha}{\beta}\right) \cdot |1 + 2\tau| \cdot ||x^*||_2.$$
(7)

This suggests that, as long as $|\lambda_{1,2}| < 1$, the RHS "shrinks" exponentially with rate $|\lambda_1|^T$, but also depends (inverse proportionally) on the spectral gap $|\lambda_1| - |\lambda_2|$. The above lead to the following convergence result:

Theorem 1. Consider the non-convex optimization problem in [4], for given structure \mathcal{A} , associated with $\Pi_{k,\mathcal{A}}(\cdot)$, and loss function f, satisfying restricted strong convexity and smoothness properties over 4k sparse "signals", with parameters α and β , respectively. Under the same assumptions with Lemma [1], Algorithm [1] returns a ε -approximate solution, such that $\|x_T - x^*\|_2 \leq \varepsilon$, within $O\left(\log \frac{1-\alpha/\beta}{\varepsilon \cdot (|\lambda_1|-|\lambda_2|)}\right)$ iterations (linear convergence rate).

Proof. We get this result by forcing the RHS of (7) be less than $\varepsilon > 0$. *I.e.*,

$$\frac{4 \cdot |\lambda_1|^T}{|\lambda_1| - |\lambda_2|} \cdot \left(1 - \frac{\alpha}{\beta}\right) \cdot |1 + 2\tau| \cdot ||x^*||_2 \le \varepsilon \Rightarrow (8)$$

$$|\lambda_1|^T \le \frac{\varepsilon \cdot (|\lambda_1| - |\lambda_2|)}{4 \cdot (1 - \frac{\alpha}{\beta})|1 + 2\tau| \cdot ||x^*||_2} \Rightarrow (9)$$

$$T \ge \left\lceil \frac{\log \frac{4 \cdot (1 - \frac{\alpha}{\beta})|1 + 2\tau| \cdot ||x^{\star}||_{2}}{\varepsilon \cdot (|\lambda_{1}| - |\lambda_{2}|)}}{\log |\lambda_{1}|} \right\rceil \tag{10}$$

This completes the proof.

5 Related work

Optimization schemes over low-dimensional structured models have a long history; due to lack of space, we refer the reader to [23] for an overview of discrete and convex approaches. We note that there are both projected and proximal non-convex approaches that fit under our generic model, where no acceleration is assumed. E.g., see [4], [24], [15], [14]; our present work fills this gap. For non-convex proximal steps see [25] and references therein; again no acceleration is considered. Below, we focus on accelerated optimization variants, as well as Frank-Wolfe methods.

Related work on accelerated IHT variants. Accelerated IHT algorithms for sparse recovery were first introduced in [26, 19, 16]. In [26], the authors provide a double overrelaxation thresholding scheme [27] in order

to accelerate their projected gradient descent variant for sparse linear regression; however, no theoretical guarantees are provided. In 19, Blumensath accelerates standard IHT methods for the same problem 9, 28 using the double overrelaxation technique in 26. His result contains theoretical proof of linear convergence, under the assumption that the overrelaxation step is used only when the objective function decreases. However, this approach provides no guarantees that we might skip the acceleration term often, which leads back to the non-accelerated IHT version; see also 27 for a similar approach on EM algorithms. 29 describe a family of IHT variants, based on the conjugate gradient method 30, that includes under its umbrella methods like in [31], [32], with the option to perform acceleration steps; however, no theoretical justification for convergence is provided when acceleration motions are used. [16, 12] contain hard-thresholding variants, based on Nesterov's ideas [17]; in [12], the authors provide convergence rate proofs for accelerated IHT when the objective is just least-squares; no generalization to convex f is provided, neither a study on varied values of τ . 33 includes a first attempt towards using adaptive τ : his approach focuses on the least-squares objective. where a closed for solution for optimal τ is found 16. However, similar to [19], it is not guaranteed whether and how often the momentum is used, neither how to set up τ in more generic objectives; see also Section D in the appendix. From a convex perspective, where the non-convex constraints are substituted by their convex relaxations (either in constrained or proximal setting), the work in 34 and 35 is relevant to the current work: based on two-step methods for linear systems [36], [34] extends these ideas to non-smooth (but convex) regularized linear systems, where f is a least-squares term for image denoising purposes; see also 35. Similar to 33, 19, 34 considers variants of accelerated convex gradient descent that guarantee monotonic decrease of function values per iteration.

⁴The guarantees in these settings are restricted to finding a good stationary point.

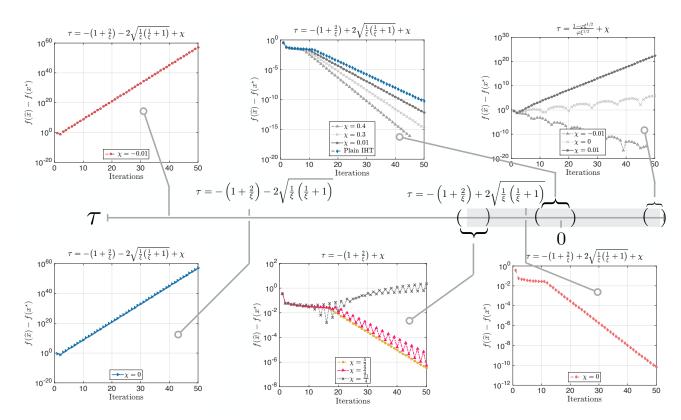


Figure 1: Behavior of accelerated IHT method, applied on a toy example for sparse linear regression. Consider \mathcal{A} as the plain sparsity model, and let x^* be a k-sparse "signal" in \mathbb{R}^{10} for k=2, drawn from multivariate normal distribution. Also, $\|x^*\|_2 = 1$. Let $b = \Phi x^*$, with $\Phi \in \mathbb{R}^{6 \times 10}$ drawn entrywise i.i.d. from a normal distribution. Let \mathcal{I} be an index set of k columns in Φ ; there are $\binom{n}{k}$ possible such subsets. By Definitions 1/2 we estimate α and β as the $\lambda_{\min}(\Phi_{\mathcal{I}}^{\top}\Phi_{\mathcal{I}})$ and $\lambda_{\max}(\Phi_{\mathcal{I}}^{\top}\Phi_{\mathcal{I}})$, where $\Phi_{\mathcal{I}}$ is the submatrix of Φ , indexed by \mathcal{I} . Here, $\alpha \approx 0.22$ and $\beta \approx 1.78$, which leads to $\xi = 1 - \alpha/\beta \approx 0.87$. We plot $f(\hat{x}) - f(x^*)$ vs. iteration count, where $f(x) = \frac{1}{2} \|b - \Phi x\|_2^2$. Gray shaded area on τ horizontal line corresponds to the range $|\tau| \leq (1 - \varphi \xi^{1/2})/(\varphi \xi^{1/2})$. (Left panel, top and bottom row). Accelerated IHT diverges for negative τ , outside the τ shaded area. (Middle panel, bottom row). "Rippling" behavior for τ values close to the lower bound of converging τ . (Middle panel, top row). Convergence behavior for accelerated IHT for various τ values and its comparison to plain IHT ($\tau = 0$). (Right panel, top row). Similar "rippling" behavior as τ approaches close to the upper bound of the shaded area; divergence is observed when τ goes beyond the shaded area (observe that, for τ values at the border of the shaded area, Algorithm 1 still diverges and this is due to the approximation of ξ).

discontinuous constraints—for instance the subset of k-sparse sets. In the case of $\boxed{44}$, our work differs in that it explores better the low-dimensional constraint sets—however, we require f to be convex. More relevant to this work is $\boxed{45}$: the authors consider non-convex proximal objective and apply ideas from $\boxed{35}$ that lead to either monotone (skipping momentum steps) or non-monotone function value decrease behavior; further, the theoretical guarantees are based on different tools than ours. We identify that such research questions could be directions for future work.

Related work on dynamical systems and numerical analysis. Multi-step schemes originate from explicit finite differences discretization of dynamical systems; e.g., the so-called Heavy-ball method 18 origins from

the discretization of the friction dynamical system $\ddot{x}(t) + \gamma \dot{x}(t) + \nabla f(x(t)) = 0$, where $\gamma > 0$ plays the role of friction. Recent developments on this subject can be found in [46]; see also references therein. From a different perspective, Scieur et al. [47] use multi-step methods from numerical analysis to discretize the gradient flow equation. We believe that extending these ideas in non-convex domains (e.g., when non-convex constraints are included) is of potential interest for better understanding when and why momentum methods work in practical structured scenaria.

Related work on Frank-Wolfe variants: The Frank-Wolfe (FW) algorithm [5], [7] is an iterative projection-free convex scheme for constrained minimization. Frank-Wolfe often has *cheap* per iteration cost by solv-

ing a constrained linear program in each iteration. The classical analysis by 5 presents sublinear convergence for general functions. For strongly convex functions, FW admits linear convergence if the optimum does not lie on the boundary of the constraint set; in that case, the algorithm still has sublinear convergence rate. To address the boundary issue. [48] allows to move away from one of the already selected atoms, where linear convergence rate can be achieved 8. Similarly, the pairwise variant introduced by 49 also has a linear convergent rate. This variant adjusts the weights of two of already selected atoms. 50 present a different perspective by showing linear convergence of classical FW over strongly convex sets and general functions. While several variants and sufficient conditions exist that admit linear convergence rates, the use of momentum for Frank-Wolfe, to the best of our knowledge is unexplored.

6 Experiments

We conducted simulations for different problems to verify our predictions. In all experiments, we use constant $\tau=1/4$ as a potential universal momentum parameter. Our experiments are proof of concept and demonstrate that accelerated projected gradient descent over nonconvex structured sets can, not only offer high-quality recovery in practical settings, but offer much more scalable routines, compared to state-of-the-art. Here, we present only a subset of our experimental findings and we encourage readers to go over the experimental results in the Appendix E.

6.1 Sparse linear regression setting

For sparse linear regression, next we consider two simulated problems settings: (i) with i.i.d. regressors, and (ii) with correlated regressors.

Sparse linear regression under the i.i.d. Gaussian setting: In this case, we consider a similar problem setting with \square , where $x^* \in \mathbb{R}^n$ is the unknown normalized k-sparse vector, observed through the underdetermined set of linear equations: $b = \Phi x^*$. $\Phi \in \mathbb{R}^{m \times n}$ is drawn randomly from a normal distribution. We consider the standard least squares objective $f(x) = \frac{1}{2} \|b - \Phi x\|_2^2$ and the plain sparsity model \mathcal{A} where $\|x\|_{0,\mathcal{A}} \equiv \|x\|_0$.

We compare Algorithm [1] (abbreviated as AccIHT in plots) with two FW variants (see [8] for FW and pairFW) Further, according to [8], pairFW performs better than awayFW for this problem case, as well as the plain IHT algorithm. In this experiment, we

use step sizes $1/\widehat{\beta}$ for Algorithm 1 and IHT, where $\widehat{\beta} = \lambda_{\max}(\Phi^{\top}\Phi)$. For the FW variants, we follow the setup in 1 and set as the constraint set the λ -scaled ℓ_1 -norm ball, where $\lambda = 40$. In the FW code, we further "debias" the selected set of atoms per iteration, by performing fully corrective steps over putative solution (i.e., solve least-squares objective restricted over the active atom set) 16, 14. We observed that such steps are necessary in our setting, in order FW to be competitive with Algorithm 1 and IHT. For IHT and Algorithm 1 we set input k either exactly or use the ℓ_1 -norm phase transition plots 1, where the input parameter for sparsity k is overshooted. See also Section k for more information. We compare the above algorithms w.r.t. function values decrease and running times.

Figure 2 depicts the summary of results we observed for the case $n = 2 \cdot 10^5$, m = 7500 and k = 500. For IHT and accelerated IHT, we also consider the case where the input parameter for sparsity is set to k = 2441 > k. The graphs indicate that the accelerated hard thresholding technique can be much more efficient and scalable than the rest of the algorithms, while at the same time being at least as good in support/"signal" recovery performance. For instance, while Algorithm 1 is only $1.2 \times$ faster than IHT, when k is known exactly, Algorithm $\boxed{1}$ is more resilient at overshooting k: in that case, IHT could take $> 2 \times$ time to get to the same level of accuracy. At the same time, Algorithm detects much faster the correct support, compared to plain IHT. Compared to FW methods (right plot), Algorithm Π is at least $10 \times$ faster than FW variants.

As stated before, we only focus on the optimization efficiency of the algorithms, not their statistical efficiency. That being said, we consider settings that are above the phase retrieval curve [], and here we make no comparisons and claims regarding the number of samples required to complete the sparse linear regression task. We leave such work for an extended version of this work.

Sparse linear regression with correlated regressors: In this section, we test Algorithm $\boxed{1}$ for support recovery, generalization and training loss performance in the sparse linear regression, under a different data generation setting. We generate the data as follows. We generate the feature matrix 800×200 design matrix Φ according to a first order auto-regressive process with correlation = 0.4. This ensures features are correlated with each other, which further makes feature selection a non-trivial task. We normalize the feature matrix so that each feature has ℓ_2 -norm equal to one. We generate an arbitrary weight vector x^* with $\|x^*\|_0 = 20$ and $\|x^*\|_2 = 1$. The response vector b is then computed as $y = \Phi x^* + \varepsilon$, where ε is guassian iid noise that is generated to ensure that the

⁵Phase transition results and comparisons to standard algorithms such as CoSaMP (restricted to squared loss) can be found in [16], and thus omitted.

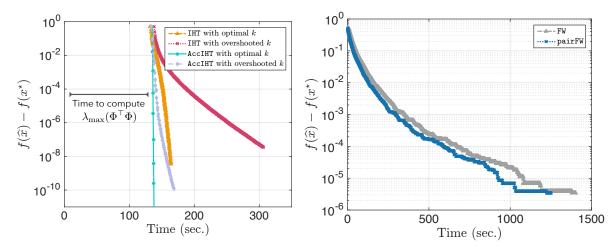


Figure 2: Time spent vs. function values gap $f(\widehat{x}) - f(x^*)$. AccIHT corresponds to Algorithm Beware in left plot the time spent to approximate step size, via computing $\lambda_{\max}(\Phi^{\top}\Phi)$.

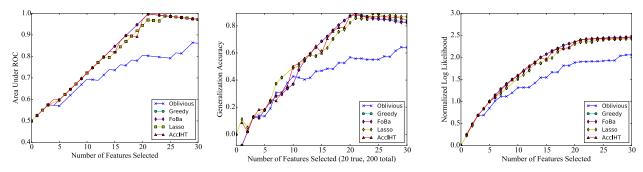


Figure 3: Empirical evaluation. Algorithm 1 achieves strong performance on true support recovery (left), generalization on test data (middle), and on training data fit (right)

signal-to-noise ratio is 10. Finally, the generated data is randomly split 50-50 into training and test sets.

We compare against Lasso [52], oblivious greedy selection (Oblivious [53]), forward greedy selection (Greedy [53]), and forward backward selection (FoBa [54]). The metrics we use to compare on are the generalization accuracy (R^2 coefficient determination performance on test set), recovery of true support (AUC metric on predicted support vs. true support), and training data fit (log likelihood on the training set). The results are presented in Figure [3], and shows Algorithm [1] performs very competitively: it is almost always better or equal to other methods across different sparsity levels.

7 Overview and future directions

The use of hard-thresholding operations is widely known. In this work, we study acceleration techniques in simple hard-thresholding gradient procedures and characterize their performance; to the best of our knowledge, this is the first work to provide theoretical support for these type of algorithms. Our preliminary results show evidence that machine learning problems can be efficiently solved using our accelerated non-convex variant, which is at least competitive with state of the art and comes with convergence guarantees.

Our approach shows linear convergence; however, in theory, the acceleration achieved has dependence on the condition number of the problem not better than plain IHT. This leaves open the question on what types of conditions are sufficient to guarantee the better acceleration of momentum in such non-convex settings?

Apart from the future directions "scattered" in the main text, another possible direction lies at the intersection of dynamical systems and numerical analysis with optimization. Recent developments on this subject can be found in [46] and [47]. We believe that extending these ideas in non-convex domains is interesting to better understand when and why momentum methods work in practical structured scenaria.

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