Iterative Mix Thresholding Algorithm with Continuation Technique for Mix Sparse Optimization and Application

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Abstract Mix sparse structure is inherited in a wide class of practical applications, namely, the sparse structure appears as the inter-group and intra-group manners simultaneously. In this paper, we propose an iterative mix thresholding algorithm with continuation technique (IMTC) to solve the ℓ_0 regularized mix sparse optimization. The significant advantage of the IMTC is that it has a closed-form expression and low storage requirement, and it is able to promote the mix sparse structure of the solution. We prove the convergence property and the linear convergence rate of the ITMC to a local minimum; moreover, we show that the ITMC approaches an approximate true mix sparse solution within a tolerance relevant to the noise level under an assumption of restricted isometry property. We also apply the mix sparse optimization to model the differential optical absorption spectroscopy analysis with the wavelength misalignment, and numerical results indicate that the IMTC can exactly and quantitatively predict the existing materials and the factual wavelength misalignment simultaneously within 0.1 second, which meets the demand of improvement of the automatic analysis software.

Keywords mix sparse optimization, ℓ_0 regularization, iterative thresholding algorithm, continuation technique, convergence theory

1 Introduction

In past decades, sparse optimization has become one of the most popular topics in mathematical optimization and gained successful applications in various disciplines, such as compressive sensing [18], image science [4], systems biology [27, 38], and machine learning [2].

Sparse optimization is to find a sparse solution of an ill-coonditioned linear system:

$$b = Ax + \varepsilon, \tag{1.1}$$

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where $A \in \mathbb{R}^{m\times n}$ is a linear transformation matrix with $m \ll n$, $b \in \mathbb{R}^m$ is an observation vector with an unknown noise $\varepsilon \in \mathbb{R}^m$, and $x \in \mathbb{R}^n$ is the variable to be estimated. The sparsity of a vector x is defined to be the number of its nonzero components, denoted as the ℓ_0 quasi-norm $\|x\|_0$. Moreover for $0 < p \leq 1$, the ℓ_p norm of a vector x is defined by $\|x\|_p := (\sum_{i=1}^n |x_i|^p)^{\frac{1}{p}}$ and, when x is of a group structure $(x_{\mathcal{G}_1}^\top, \ldots, x_{\mathcal{G}_N}^\top)^\top$, the group $\ell_{2,p}$ norm of vector x is defined by $\|x\|_{2,p} := (\sum_{i=1}^N \|x_{\mathcal{G}_i}\|^p)^{\frac{1}{p}}$. When $p = 0$, $\|x\|_{2,0}$ is the number of non-zero groups of x.

A popular and practical technique for approaching a sparse solution of the linear system (1.1) is to solve the following convex ℓ_1 regularization problem (also named as Lasso in statistics and basis pursuit in compressive sensing):

$$\min_{x\in\mathbb{R}^n} \|Ax - b\|^2 + \tau\|x\|_1, \tag{1.2}$$

where $\tau > 0$ is the regularization parameter providing a tradeoff between data fidelity and sparsity. Benefiting from its convexity property, a great deal of attention has been attracted to explore theoretical property [5, 10, 33] and develop numerical algorithms [4, 15, 19, 48] for the ℓ_1 regularization problem (1.2).

1.1 Structured sparse optimization

Variants of the following structured (group) sparse optimization problem have been studied in the literature:

$$\min_{x\in\mathbb{R}^n} \|Ax - b\|^2 + \lambda \sum_{i=1}^N \varphi(\|x_{\mathcal{G}_i}\|) + \tau \sum_{i=1}^n \varphi(|x_i|). \tag{1.3}$$

Here $\lambda > 0$ is the group sparsity regularization parameter and $\tau > 0$ is the sparsity regularization parameter. Examples of the problem (1.3) and their structure and strength are illustrated as follows.

When $\lambda = 0$ and $\varphi(t) := t$, (1.3) is the Lasso (1.2).

When $\tau = 0$ and $\varphi(t) := t$, (1.3) is the group Lasso proposed in Yuan and Lin [49] to approach the group variable selection and multi-factor analysis-of-variance problems. Employing the $\ell_{2,1}$ penalty to characterize the group sparse structure, the $\ell_{2,1}$ regularization problem (group Lasso) processes the components in a particular group synchronously, and thus leads to the reduction of freedom degrees in the solution and meets the synergistic effect in applications. Furthermore, benefitting from these advantages, group sparse optimization has been widely applied in multi-task machine learning [2], multi-channel image reconstruction [35], and systems biology [39, 43].

When $\varphi(t) := t^p$ with $0 < p < 1$ and $\lambda = 0$ or $\tau = 0$, (1.3) is the ℓ_p- or group $\ell_{2,p}$-lower-order regularization problem, introduced by [47] and [21] respectively. The nonconvex lower-order regularization methods have been found to endow with better theoretical property and numerical performance than the convex ℓ_1 regularization methods; see also [11, 17, 21, 22, 47, 52].

When $\varphi(t) := 0$ if $t = 0$, and 1 otherwise, and $\lambda = 0$ or $\tau = 0$, (1.3) is the ℓ_0 or $\ell_{2,0}$ regularization problems explored in [7] and [36] to approach a sparse solution and a group sparse solution, respectively. In contrast with ℓ_p $(0 < p \leq 1)$ norms that penalize the larger components more heavily than the smaller ones, the ℓ_0 norm forces the unbiased penalization on all components regardless of the magnitude.

When $\varphi(t) := t$ and $\lambda > 0$, $\tau > 0$, (1.3) is the sparse group Lasso (SGL) introduced by Simon et al. [41], that blends the $\ell_{2,1}$ and ℓ_1 penalties to achieve sparse effects on the inter-group and intra-group structures. Benefitting from the mix sparse structure, the SGL has gained an increasing amount of successful applications in portfolio selection [12], genomic association study [30], and hyperspectral imaging [16].

A major challenge of the (nonconvex) lower-order regularization problems is the computational issue as it is intractable to find a global solution of a general nonconvex optimization problem. Alternatively, tremendous efforts have been devoted to the development of optimization algorithms for approaching a local minimum or a stationary point of the lower-order regularization problem, such as smoothing method [13], splitting method [28], iterative reweighted minimization method [25], penalty method [32] and difference of convex functions algorithm (DCA) [29, 36].

Besides, one of the most widely applied numerical algorithms for solving the lower-order regularization problems is the class of iterative thresholding algorithms (ITA), which are of simple formulations and low computational complexity and thus efficient for large-scale sparse optimization problems. In particular, iterative hard thresholding algorithm (IHTA) [7] and iterative half thresholding algorithm [47] were proposed to solve the ℓ_0 regularization problem and $\ell_{\frac{1}{2}}$ regularization problem, respectively. The ITA for the lower-order $\ell_{2,p}$ regularization problem was studied in [21] under a unified framework of proximal gradient method (PGM). The convergence theorem of the ITA for the lower-order regularization problems has been established under the framework of the Kurdyka-Łojasiewicz theory [1]. Moreover, various variants and extensions of IHTA have been proposed and explored in [8, 24, 31, 53] and references therein.

1.2 Aims of this paper

Inspired by the ℓ_0 regularization method and motivated by the mix sparse structure, we consider the following ℓ_0 regularized mix regularization problem:

$$\min_{x\in\mathbb{R}^n} F(x) := \|Ax - b\|^2 + \lambda\|x\|_{2,0} + \tau\|x\|_0. \tag{1.4}$$

The mix sparse optimization problem (1.4) blends the $\ell_{2,0}$ and ℓ_0 penalties, and covers the ℓ_0 regularization problem and the $\ell_{2,0}$ regularization problem as special cases when $\lambda = 0$ or $\tau = 0$, respectively.

It is worth noting that the continuation technique is a widely-applied parameter update strategy for speeding up relevant algorithms in an easily-implemented but efficient way; see, e.g., [19, 24, 46]. Inspired by the ideas of the ITA and the continuation technique, we will

propose an iterative mix thresholding algorithm with continuation technique (IMTC) to solve the mix sparse optimization problem (1.4). The IMTC consists of a gradient descent operator, a hard thresholding operator in an individual manner and a group hard thresholding operator in a group manner successively. The significant advantage of the IMTC is that it has a closed-form expression and low storage requirement, and is able to promote the mix sparse structure of the solution.

In convergence analysis, we show that the sequence generated by the IMTC globally converges to a local minimum of the mix sparse optimization problem (1.4) at a linear convergence rate under a mild condition on the stepsize; see Theorem 3.1. Moreover, under the assumption of the restricted isometry property (RIP) [10], we show that the IMTC approaches an approximate true mix sparse solution of (1.1) within a tolerance proportional to the noise level; see Theorem 3.3.

It is worth mentioning that in a closely relevant paper [44] in recent year, the authors studied the Kurdyka-Łojasiewicz property of exponent being $\frac{1}{2}$ for the ℓ_0 regularized function under some regular assumptions, which is useful to ensure the linear convergence rate of several first-order descent methods [1]. Their analysis on subdifferential of the ℓ_0 regularized function is helpful to our analysis (see Proposition 2.1), while the contributions of our paper are on distinct directions: the novel algorithmic design for the ℓ_0 regularized mix regularization problem (1.4) and its convergence to a ground true sparse solution under the RIP-type condition.

The motivation of our work also stems from applications. The differential optical absorption spectroscopy (DOAS) analysis aims to quantify the concentrations of trace gases by measuring specific absorption spectrum from optical spectrometers [37]. However, traditional DOAS analysis methods suffer three major limitations. (i) Only some specific narrow band absorption structures are used and can only quantify the concentrations of certain types of gases. (ii) Traditional DOAS analysis methods divide the identification of involved gases and the quantification of the concentrations of trace gases into two separate steps, which hinder the development of DOAS software; see [37, Chapter 8]. (iii) In the data collection process from optical spectrometers, there are two major types of noise: the additive noise due to scattering and the basis noise due to wavelength misalignment. The traditional linear least-squares method is designed to deal with the additive noise but does not consider the wavelength misalignment; see [16]. To overcome these limitations, we propose a novel mathematical method for DOAS analysis by dealing with the full spectra data and the wavelength misalignment and executing identification and quantification simultaneously. By enlarging the full spectra data pool to the one with possible candidates and possible wavelength misalignments, we cast the DOAS analysis to a mix sparse optimization problem (1.4) by virtue of the Lambert-Beer's law and the mix sparsity structure of the solution. Numerical results show that the IMTC can exactly and quantitatively predict the existing gases and the factual wavelength misalignment simultaneously within 0.1 second, which meets the demand of improvement of the DOAS automatic analysis software proposed in [37, Chapter 8].

1.3 Notations and organization

The notations adopted in this paper are described as follows. We consider the n-dimensional Euclidean space $\mathbb{R}^n$ with inner product $\langle\cdot,\cdot\rangle$ and Euclidean norm $\|\cdot\|$. As usual, the lowercase letters x, y, z are used to denote the vectors, calligraphic letters $\mathcal{I}$, $\mathcal{J}$, $\mathcal{S}$ denote the index sets. For $x \in \mathbb{R}^n$, $r \in \mathbb{R}_+$ and $n \in \mathbb{N}$, we use $\mathbb{B}(x, r)$ to denote the closed ball centered at x with radius r, and write $[n] := \{1, \ldots, n\}$. For $\mathcal{I} \subseteq [n]$, $x_{\mathcal{I}}$ and $A_{\mathcal{I}}$ denote the subvector of vector x indexed by $\mathcal{I}$ and the submatrix of matrix A with columns indexed by $\mathcal{I}$, respectively. Let $x := (x_{\mathcal{G}_1}^\top, \ldots, x_{\mathcal{G}_N}^\top)^\top$ represent the group structure, where $x_{\mathcal{G}_i} \in \mathbb{R}^{n_i}$ is the i-th group with $\sum_{i=1}^N n_i = n$. Moreover, we write $n_{\max} := \max_{i\in[N]} n_i$ and $\mathcal{G}_{\mathcal{S}} := \cup_{i\in\mathcal{S}}\mathcal{G}_i$, and use $\mathbb{I}$ and $\sharp(\cdot)$ to denote an identical matrix and the number of elements in an index set, respectively. The support function is denoted by $\mathrm{supp} : \mathbb{R}^n \to 2^{[n]}$ as

$$\mathrm{supp}(x) := \{i : x_i \neq 0\} \quad \text{for each } x \in \mathbb{R}^n.$$

This paper is organized as follows. In Section 2, we provide characterizations for subdifferentials of ℓ_0-type penalties and the local minima of (1.4). In Section 3, we propose an IMTC to solve problem (1.4) and establish its convergence theory, including the linear convergence rate to a local minimum and and the convergence to an approximate true solution. An application to DOAS analysis is presented in Section 4.

2 Characterization of local minima

The structure of local minima usually provides useful information for the theoretical study and numerical algorithms of optimization problems; see, e.g., [13, 21, 22, 47]. This section aims to explore the characterization and structure of local minima of problem (1.4), which will be useful in convergence analysis of numerical algorithms.

For this purpose, we first study the subdifferentials of $\|\cdot\|_0$ and $\|\cdot\|_{2,0}$ and their regularity property, which will be useful in characterizing the optimality condition of problem (1.4). The definitions of subdifferentials and subdifferential regularity of nonconvex functions are taken from [40, Definitions 8.3 and 7.25], respectively.

Definition 2.1. *Let $f : \mathbb{R}^n \to \bar{\mathbb{R}}$ be proper and lower semicontinuous, and $x \in \mathrm{dom}(f)$.*

(i) *The regular subdifferential of f at x is defined by*

$$\hat{\partial} f(x) := \left\{ u \in \mathbb{R}^n : \liminf_{y\neq x, y\to x} \frac{f(y) - f(x) - \langle u, y - x\rangle}{\|y - x\|} \geq 0 \right\}.$$

(ii) *The (limiting) subdifferential of f at x is defined by*

$$\partial f(x) := \left\{ u \in \mathbb{R}^n : \exists x^k \xrightarrow{f} x, u^k \in \hat{\partial} f(x^k) \text{ with } u^k \to u \right\}.$$

(iii) *The horizon subdifferential of f at x is defined by*

$$\partial^\infty f(x) := \left\{ u \in \mathbb{R}^n : \exists x^k \xrightarrow{f} x, u^k \in \hat{\partial} f(x^k), \kappa^k \downarrow 0, \ \textit{with } \kappa^k u^k \to u \right\}.$$

f is said to be subdifferentially regular at x if epi$f$ *is Clarke regular at $(x, f(x))$.*

Below we characterize the subdifferentials of $\|\cdot\|_0$ and $\|\cdot\|_{2,0}$. In the following proposition, (2.1) is taken from [26, Theorem 1] and [44, Lemma 3.2] while (2.2) adopts a line of analysis similar to (2.1) and due to the fact that $x_i \neq 0$ implies $x_{G_j} \neq 0$ with $i \in G_j$. Subdifferential formulae (2.3) and (2.4) follow from [40, Exercise 8.8(c)].

Proposition 2.1. *The functions $\|\cdot\|_0$, $\|\cdot\|_{2,0}$ and $\|\cdot\|_0 + \|\cdot\|_{2,0}$ are subdifferentially regular at each $x \in \mathbb{R}^n$. Particularly, we have*

$$\partial\|x\|_0 = \{y \in \mathbb{R}^n : y_i = 0 \textit{ for each } i \in [n] \textit{ such that } x_i \neq 0\}, \tag{2.1}$$

$$\partial\|x\|_{2,0} = \{y \in \mathbb{R}^n : y_{\mathcal{G}_i} = 0 \textit{ for each } i \in [N] \textit{ such that } \|x_{\mathcal{G}_i}\| \neq 0\}, \tag{2.2}$$

$$\partial(\|\cdot\|_{2,0} + \|\cdot\|_0)(x) = \partial\|x\|_{2,0} + \partial\|x\|_0. \tag{2.3}$$

Moreover, if $f : \mathbb{R}^n \to \mathbb{R}$ is differentiable on $\mathbb{R}^n$, then

$$\partial(f + \|\cdot\|_{2,0} + \|\cdot\|_0)(x) = \nabla f(x) + \partial\|x\|_{2,0} + \partial\|x\|_0. \tag{2.4}$$

The following theorem provides an equivalent characterization for a local minimum of problem (1.4) in terms of a global minimum of a least squares problem over the subspace associated to its support.

Theorem 2.1. *Let $x^* \in \mathbb{R}^n$ and $X := \{x \in \mathbb{R}^n : \text{supp}(x) \subseteq \text{supp}(x^*)\}$. Then x^* is a local minimum of problem* (1.4) *if and only if x^* is a global minimum of*

$$\min_{x \in X} \|Ax - b\|^2. \tag{2.5}$$

Proof. "⇒": Suppose that x^* is a local minimum of problem (1.4). By the optimality condition and the sum rule of subdifferential (2.4), we obtain

$$0 \in \partial F(x^*) = 2A^\top(Ax^* - b) + \lambda\partial\|x^*\|_{2,0} + \tau\partial\|x^*\|_0.$$

Then one has by (2.1) and (2.2) that the following optimality condition holds

$$A_i^\top(Ax^* - b) = 0 \quad \text{for each } i \in \text{supp}(x^*). \tag{2.6}$$

Note that x^* is an (relative) interior point of subspace X and that (2.6) is also the optimality condition of problem (2.5). Since (2.5) is a convex optimization problem, we conclude that x^* is a global minimum of problem (2.5), as desired.

"⇐": Suppose that x^* is a global minimum of problem (2.5). Define

$$\epsilon := \min\left\{\frac{\tau}{2\|A\|\|Ax^*-b\|}, \min_{i\in\mathrm{supp}(x^*)}|x_i^*|\right\}. \tag{2.7}$$

Then it suffices to show that, for each $x \in \mathbb{B}(x^*,\epsilon)$,

$$F(x) \geq F(x^*). \tag{2.8}$$

Fix $x \in \mathbb{B}(x^*,\epsilon)$. Without loss of generality, we assume that $\mathrm{supp}(x) \neq \mathrm{supp}(x^*)$; otherwise, (2.8) follows directly from the optimality of x^* to (2.5). Noting by (2.7) that $\epsilon \leq \min_{i\in\mathrm{supp}(x^*)}|x_i^*|$, one has $\mathrm{supp}(x) \supseteq \mathrm{supp}(x^*)$. This, together with the inconsistency of the supports $\mathrm{supp}(x) \neq \mathrm{supp}(x^*)$, implies that $\|x\|_0 \geq \|x^*\|_0 + 1$ and $\|x\|_{2,0} \geq \|x^*\|_{2,0}$. Then we obtain

$$\begin{aligned} F(x) - F(x^*) &\geq \|Ax-b\|^2 - \|Ax^*-b\|^2 + \tau \\ &= \langle x-x^*, 2A^\top(Ax^*-b)\rangle + \|A(x-x^*)\|^2 + \tau \\ &\geq -2\epsilon\|A\|\|Ax^*-b\| + \tau \\ &\geq 0 \end{aligned}$$

(thanks to (2.7)). Hence (2.8) is proved for each $x \in \mathbb{B}(x^*,\epsilon)$. The proof is complete. □

Remark 2.1. One can observe from Theorem 2.1 that the characterization of the local minimum of problem (1.4) has no relation to the $\ell_{2,0}$ term. This is because that
(i) $x_i \neq 0 \Rightarrow x_{G_j} \neq 0$ with $i \in G_j$, and $\mathrm{supp}(x) \subseteq \mathrm{supp}(x^*) \Rightarrow \mathrm{Gsupp}(x) \subseteq \mathrm{Gsupp}(x^*)$; and
(ii) $\partial(\|\cdot\|_{2,0} + \|\cdot\|_0)(x) = \partial\|x\|_{2,0} + \partial\|x\|_0 = \partial\|x\|_0$ (by (2.1) - (2.3)).

Although the characterization of the local minimum has no relation to the $\ell_{2,0}$ term, we will show in the next section that the algorithm is designed with relevant to the $\ell_{2,0}$ term and outperforms the ones with only relevant to the ℓ_0 term (see Section 4).

3 Iterative mix thresholding algorithm with continuation

Inspired by the ideas of the ITA and the continuation technique, we propose an iterative mix thresholding algorithm with the continuation technique (IMTC) to solve the mix sparse optimization problem (1.4) and establish its convergence theorem in this section. In particular, by selecting a decreasing sequence of parameter pairs $(\lambda_k,\tau_k) \downarrow (\lambda,\tau)$, the iteration of IMTC consists of a gradient descent operator (3.1), a hard thresholding operator in an individual manner (3.2) and a group hard thresholding operator in a group manner (3.3). Formally, the IMTC is presented as follows.

Algorithm 3.1. Select an initial point $x^0 \in \mathbb{R}^n$, a sequence of stepsizes $\{v_k\} \subseteq (0,+\infty)$, and a decreasing sequence of parameter pairs $(\lambda_k,\tau_k) \downarrow (\lambda,\tau)$. The sequence $\{x^k\} \subseteq \mathbb{R}^n$ are

generated via the iterations

$$y^k := x^k - 2v_k A^\top (Ax^k - b), \tag{3.1}$$

$$z^k := \mathbf{H}(y^k; \sqrt{2v_k\tau_k}), \tag{3.2}$$

$$x^{k+1}_{\mathcal{G}_i} := \mathbf{H}_{\mathcal{G}_i}\left(z^k_{\mathcal{G}_i}; \sqrt{2v_k(\lambda_k + \tau_k\|z^k_{\mathcal{G}_i}\|_0)}\right), \quad \text{for } i \in [N], \tag{3.3}$$

where $\mathbf{H} : \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^n$ and $\mathbf{H}_{\mathcal{G}_i} : \mathbb{R}^{n_i} \times \mathbb{R} \to \mathbb{R}^{n_i}$ are defined respectively by

$$\mathbf{H}(y;\alpha) := \left\{ z \in \mathbb{R}^n \middle| \begin{matrix} z_i = y_i, & \text{if } |y_i| > \alpha \\ z_i = 0, & \text{if } |y_i| \le \alpha \end{matrix} \right\}, \tag{3.4}$$

$$\mathbf{H}_{\mathcal{G}_i}(z;\beta) := \left\{ x \in \mathbb{R}^{n_i} \middle| \begin{matrix} x = z, & \text{if } \|z\| > \beta \\ x = 0, & \text{if } \|z\| \le \beta \end{matrix} \right\}. \tag{3.5}$$

It is clear that each step of the IMTC has a closed-form expression and low storage requirement; hence it is particularly attractive for large-scale problems. Moreover, the IMTC alternatively implements the hard thresholding operators in an individual manner (3.2) and in a group manner (3.3), which is able to promote the mix sparse structure of the solution.

To advance the understanding of the IMTC, we provide a reformulation of the IMTC in terms of a proximal operator. For a proper and lower semicontinuous function $f : \mathbb{R}^n \to (-\infty, +\infty]$, its proximal operator $\text{prox}_f : \mathbb{R}^n \rightrightarrows \mathbb{R}^n$ is a set-valued mapping defined by

$$\text{prox}_f(z) := \arg\min_{x\in\mathbb{R}^n} \{f(x) + \frac{1}{2}\|x - z\|^2\}.$$

We recall the closed-form expressions of proximal operators of $\tau\|\cdot\|_0$ and $\lambda\|\cdot\|_{2,0}$; see [7] and [21, Proposition 18]. One can see that the thresholding operators $\mathbf{H}$ and $\mathbf{H}_{\mathcal{G}_i}$ in Algorithm 3.1 are the analytical solutions of proximal operators of $\tau\|\cdot\|_0$ and $\lambda\|\cdot\|_{2,0}$, respectively.

Proposition 3.1. (i) *The proximal operator of $\tau\|\cdot\|_0$ has a separable formulation as*

$$(\text{prox}_{\tau\|\cdot\|_0}(z))_i = \begin{cases} z_i, & |z_i| > \sqrt{2\tau}, \\ 0 \text{ or } z_i, & |z_i| = \sqrt{2\tau}, \\ 0, & |z_i| < \sqrt{2\tau}, \end{cases} \quad \textit{for } i \in [n].$$

(ii) *The proximal operator of $\lambda\|\cdot\|_{2,0}$ has a group separable formulation as*

$$(\text{prox}_{\lambda\|\cdot\|_{2,0}}(z))_{\mathcal{G}_i} = \begin{cases} z_{\mathcal{G}_i}, & \|z_{\mathcal{G}_i}\| > \sqrt{2\lambda}, \\ 0 \text{ or } z_{\mathcal{G}_i}, & \|z_{\mathcal{G}_i}\| = \sqrt{2\lambda}, \\ 0, & \|z_{\mathcal{G}_i}\| < \sqrt{2\lambda}, \end{cases} \quad \textit{for } i \in [N].$$

It is well-known that the IHTA could be understood as an application of the PGM to solve the ℓ_0 regularization problem; see [21]. In the following proposition, we show that compounding (3.2) and (3.3) presents a closed-form expression of the proximal operator of

$\lambda\|\cdot\|_{2,0}+\tau\|\cdot\|_0$, and hence the IMTC could be understood as an application of the PGM (with the continuation technique) to solve the mix sparse optimization problem (1.4). As a consequence, for the special cases when $\lambda_k\equiv 0$ or $\tau_k\equiv 0$, the IMTC is reduced to the IHTA for the ℓ_0 regularization problem [7] or that for the $\ell_{2,0}$ regularization problem [21] with the continuation technique, respectively.

Proposition 3.2. *Let $\{x^k\}$ be a sequence generated by Algorithm 3.1. Then it holds that*

$$x^{k+1}\in \mathrm{prox}_{v_k\lambda_k\|\cdot\|_{2,0}+v_k\tau_k\|\cdot\|_0}(x^k-2v_kA^\top(Ax^k-b)) \quad \textit{for each } k\in\mathbb{N}.$$

Proof. Fix $k\in\mathbb{N}$. In view of Algorithm 3.1, it suffices to show

$$x^{k+1}\in \arg\min_{x\in\mathbb{R}^n}\{v_k\lambda_k\|x\|_{2,0}+v_k\tau_k\|x\|_0+\frac{1}{2}\|x-y^k\|^2\}. \tag{3.6}$$

Note that problem (3.6) is of a group separable structure. The solution of problem (3.6) can be achieved parallelly at each group, and thus it remains to verify the solutions of a cycle of low dimensional proximal optimization subproblems:

$$x^{k+1}_{\mathcal{G}_i}\in \arg\min_{x\in\mathbb{R}^{n_i}}\ \Psi_i(x;y^k_{\mathcal{G}_i}) \quad \text{for each } i\in[N], \tag{3.7}$$

where $\Psi_i:\mathbb{R}^{n_i}\times\mathbb{R}^{n_i}\to\mathbb{R}$ is defined by $\Psi_i(x;y):=v_k\lambda_k\|x\|^0+v_k\tau_k\|x\|_0+\frac{1}{2}\|x-y\|^2$.

Fix $i\in[N]$. To validate (3.7), we shall find the minimum of $\Psi_i(\cdot;y^k_{\mathcal{G}_i})$ over $\mathbb{R}^{n_i}\setminus\{0\}$ and then compare the obtained minimal value with $\Psi_i(0;y^k_{\mathcal{G}_i})$. For each $x\in\mathbb{R}^{n_i}\setminus\{0\}$, one has

$$\Psi_i(x;y^k_{\mathcal{G}_i})=v_k\lambda_k+v_k\tau_k\|x\|_0+\frac{1}{2}\|x-y^k_{\mathcal{G}_i}\|^2,$$

which is the objective function of the proximal operator of $v_k\tau_k\|\cdot\|_0$ (plus a constant $v_k\lambda_k$). Then by Proposition 3.1(i), we have that a minimum of $\Psi_i(\cdot;y^k_{\mathcal{G}_i})$ over $\mathbb{R}^{n_i}\setminus\{0\}$ is $z^k_{\mathcal{G}_i}=\mathbf{H}(y^k_{\mathcal{G}_i};\sqrt{2v_k\tau_k})$; see (3.2). Moreover, one has by (3.4) that

$$\Psi_i(z^k_{\mathcal{G}_i};y^k_{\mathcal{G}_i})=v_k\lambda_k+v_k\tau_k\|z^k_{\mathcal{G}_i}\|_0+\frac{1}{2}(\|y^k_{\mathcal{G}_i}\|^2-\|z^k_{\mathcal{G}_i}\|^2) \quad\text{and}\quad \Psi_i(0;y^k_{\mathcal{G}_i})=\frac{1}{2}\|y^k_{\mathcal{G}_i}\|^2.$$

Hence by comparing $\Psi_i(z^k_{\mathcal{G}_i};y^k_{\mathcal{G}_i})$ and $\Psi_i(0;y^k_{\mathcal{G}_i})$, we can verify that a minimum of $\Psi_i(\cdot;y^k_{\mathcal{G}_i})$ over $\mathbb{R}^{n_i}$ is given by (3.3). That is, (3.7) is verified, and the proof is complete. □

3.1 Convergence theorem of IMTC

This subsection aims to establish the convergence theorem of the IMTC, including the global convergence theorem and the linear convergence rate. For the remainder of this subsection, we make the following blanket assumption that

- $\{x^k\}$ is a sequence generated by Algorithm 3.1 with $\{v_k\}$ satisfying

$$0<\inf_{k\in\mathbb{N}}v_k\le\sup_{k\in\mathbb{N}}v_k<\frac{1}{2\|A\|^2}. \tag{3.8}$$

We recall that F is defined in (1.4), and define a sequence of functions $\{F_k : \mathbb{R}^n \to \mathbb{R}\}$ by

$$F_k(\cdot) := \|A \cdot -b\|^2 + \lambda_k \|\cdot\|_{2,0} + \tau_k \|\cdot\|_0. \tag{3.9}$$

By the continuation technique rule that $\{(\lambda_k, \tau_k)\}$ is a decreasing sequence of positive parameter pairs converging to (λ, τ), one easily gets that

$$F_k(x) \geq F_{k+1}(x) \geq F(x) \quad \text{for each } k \in \mathbb{N} \text{ and } x \in \mathbb{R}^n. \tag{3.10}$$

To establish the convergence theorem of the IMTC, we begin with several lemmas that describe useful properties of sequences $\{x^k\}$ and $\{F(x^k)\}$. The following lemma provides a lower bound for the absolute value of nonzero entries of $\{x^k\}$.

Lemma 3.1. (i) $|x_j^k| > \sqrt{2\tau \inf_{i\in\mathbb{N}} v_i}$ *for each* $k \in \mathbb{N}$ *and* $j \in \operatorname{supp}(x^k)$.

(ii) $\|x^{k+1} - x^k\| > \sqrt{2\tau \inf_{i\in\mathbb{N}} v_i}$ *whenever* $\operatorname{supp}(x^k) \neq \operatorname{supp}(x^{k+1})$.

Proof. (i) It directly follows from (3.2) and (3.3) in Algorithm 3.1 and (3.8).

(ii) Suppose that $\operatorname{supp}(x^k) \neq \operatorname{supp}(x^{k+1})$. Then there exists $i \in [n]$ such that (a) $x_i^k = 0$ and $x_i^{k+1} \neq 0$, or (b) $x_i^k \neq 0$ and $x_i^{k+1} = 0$. Hence by statement (i) of this lemma, we have for both cases that

$$\|x^{k+1} - x^k\| \geq |x_i^{k+1} - x_i^k| > \sqrt{2\tau \inf_{i\in\mathbb{N}} v_i}.$$

The proof is complete. □

Recall from Proposition 3.2 that x^{k+1} could be understood as an iterate generated by one PGM step for minimizing F_k (defined by (3.9)) starting at x^k. Hence the following lemma directly follows from the descent property of the PGM; see, e.g., [9, Lemma 2].

Lemma 3.2. $F_k(x^{k+1}) - F_k(x^k) \leq -\frac{1}{2}(\frac{1}{v_k} - 2\|A\|^2)\|x^{k+1} - x^k\|^2$ *for each* $k \in \mathbb{N}$.

The following lemma shows a decreasing property of $\{F_k(x^k)\}$ and the vanishing property of $\{\|x^{k+1} - x^k\|\}$.

Lemma 3.3. $\{F_k(x^k)\}$ *is decreasing and convergent, and* $\lim_{k\to\infty} \|x^{k+1} - x^k\| = 0$.

Proof. By Lemma 3.2, we have by (3.10) and (3.8) that

$$F_{k+1}(x^{k+1}) - F_k(x^k) \leq F_k(x^{k+1}) - F_k(x^k) \leq -\frac{1}{2}(\frac{1}{v_k} - 2\|A\|^2)\|x^{k+1} - x^k\|^2 \leq 0, \tag{3.11}$$

which shows that $\{F_k(x^k)\}$ is decreasing and convergent (as $\{F_k(x^k)\}$ are positive). This also indicates that

$$\sum_{k=0}^{\infty} \|x^{k+1} - x^k\|^2 \leq 2\left(\frac{1}{\sup_{i\in\mathbb{N}} v_i} - 2\|A\|^2\right)^{-1} F_0(x^0) < +\infty;$$

consequently, $\lim_{k\to\infty} \|x^{k+1} - x^k\| = 0$. The proof is complete. □

The following lemma displays a feature of the IMTC that $\{x^k\}$ shares a consistent support when k is sufficiently large, which is useful for providing a uniform decomposition of $\{x^k\}$ in convergence analysis.

Lemma 3.4. *There exists $K \in \mathbb{N}$ such that $\mathrm{supp}(x^k) = \mathrm{supp}(x^{k+1})$ for each $k \geq K$.*

Proof. By Lemma 3.3 that $\lim_{k\to\infty} \|x^{k+1} - x^k\| = 0$, there exists $K \in \mathbb{N}$ such that

$$\|x^{k+1} - x^k\|^2 < 2\tau \inf_{i\in\mathbb{N}} v_i \quad \text{for each } k \geq K. \tag{3.12}$$

Proving by contradiction, we assume that there exists $k \geq K$ such that $\mathrm{supp}(x^k) \neq \mathrm{supp}(x^{k+1})$. Then one has by Lemma 3.1(ii) that $\|x^{k+1} - x^k\|^2 > 2\tau \inf_{i\in\mathbb{N}} v_i$, which yields a contradiction with (3.12). The proof is complete. □

The following lemma shows that the IMTC enjoys a descent property of $\{F(x^k)\}$.

Lemma 3.5. *There exists $K \in \mathbb{N}$ such that*

$$F(x^{k+1}) - F(x^k) \leq -\frac{1}{2}(\frac{1}{v_k} - 2\|A\|^2)\|x^{k+1} - x^k\|^2 \quad \textit{for each } k \geq K.$$

Proof. By Lemma 3.4, there exists $K \in \mathbb{N}$ such that $\mathrm{supp}(x^k) = \mathrm{supp}(x^{k+1})$, and thus $\|x^k\|_{2,0} = \|x^{k+1}\|_{2,0}$ and $\|x^k\|_0 = \|x^{k+1}\|_0$, for each $k \geq K$. Then we obtain that

$$F(x^{k+1}) - F(x^k) = \|Ax^{k+1} - b\|^2 - \|Ax^k - b\|^2 = F_k(x^{k+1}) - F_k(x^k).$$

Consequently, the conclusion follows from Lemma 3.2. The proof is complete. □

Lemma 3.6. *The number of changes of $\mathrm{supp}(x^k)$ is at most $\lfloor \frac{(F_0(x^0)-F^*)\sup_{i\in\mathbb{N}} v_i}{\tau(1-2\|A\|^2 \sup_{i\in\mathbb{N}} v_i)\inf_{i\in\mathbb{N}} v_i} \rfloor$.*

Proof. It follows from Lemma 3.4 that $\mathrm{supp}(x^k)$ only changes for a finite number of times, assumed as C. Below we aim to estimate an upper bound of C. Suppose that $\mathrm{supp}(x^k)$ only changes at k_j+1, that is $\mathrm{supp}(x^{k_j}) \neq \mathrm{supp}(x^{k_j+1})$, for each $j \in [C]$. Then we have by Lemma 3.1(ii) that $\|x^{k_j+1} - x^{k_j}\|^2 > 2\tau \inf_{i\in\mathbb{N}} v_i$ for each $j \in [C]$. This, together with (3.11) and (3.8), implies that

$$F_{k_j}(x^{k_j}) - F_{k_j+1}(x^{k_j+1}) \geq \left(\frac{1}{\sup_{i\in\mathbb{N}} v_i} - 2\|A\|^2\right)\tau \inf_{i\in\mathbb{N}} v_i,$$

for each $j \in [C]$. Then it follows from the decreasing property of $\{F_k(x^k)\}$ in Lemma 3.3 that

$$\begin{aligned}\left(\frac{1}{\sup_{i\in\mathbb{N}} v_i} - 2\|A\|^2\right)\tau C \inf_{i\in\mathbb{N}} v_i &\leq \sum_{j=1}^{C} F_{k_j}(x^{k_j}) - F_{k_j+1}(x^{k_j+1}) \\ &\leq \sum_{k=1}^{k_C} F_k(x^k) - F_{k+1}(x^{k+1}) \\ &\leq F_0(x^0) - F^*.\end{aligned}$$

Consequently, $C \leq \lfloor \frac{(F_0(x^0)-F^*)\sup_{i\in\mathbb{N}} v_i}{\tau(1-2\|A\|^2 \sup_{i\in\mathbb{N}} v_i)\inf_{i\in\mathbb{N}} v_i} \rfloor$. The proof is complete. □

The main theorem of this subsection is presented as follows, in which we establish the global convergence of the IMTC to a local minimum of the mix sparse optimization problem (1.4) at a linear rate.

Theorem 3.1. *Let $\{x^k\}$ be a sequence generated by Algorithm 3.1 with* (3.8) *being satisfied. Then $\{x^k\}$ linearly converges to a local minimum of problem* (1.4).

Proof. We first show that $\{x^k\}$ converges to a local minimum of problem (1.4). By Proposition 3.2, we obtain that

$$x^{k+1} \in \arg\min_{x\in\mathbb{R}^n} \left\{ \lambda_k \|x\|_{2,0} + \tau_k \|x\|_0 + \frac{1}{2v_k} \|x - (x^k - 2v_k A^\top (Ax^k - b))\|^2 \right\} \tag{3.13}$$

for each $k \in \mathbb{N}$. By Lemma 3.4, there exists $K \in \mathbb{N}$ such that $\mathrm{supp}(x^k) = \mathrm{supp}(x^{k+1})$ for each $k \geq K$. Fix $k \geq K$ and define a subspace $X := \{x \in \mathbb{R}^n : \mathrm{supp}(x) \subseteq \mathrm{supp}(x^K)\}$. Then one has by the consistency of support that $x^{k+1} \in X$, and also, $\|x^{k+1}\|_{2,0} \geq \|x\|_{2,0}$ and $\|x^{k+1}\|_0 \geq \|x\|_0$ for each $x \in X$. Hence (3.13) is reduced to

$$x^{k+1} = \arg\min_{x\in X} \|x - (x^k - 2v_k A^\top (Ax^k - b))\|^2. \tag{3.14}$$

This shows that $\{x^k\}_{k=K}^\infty \subseteq X$ is a sequence generated by the projected gradient method for solving the following constrained least squares problem

$$\min_{x\in X} \|Ax - b\|^2. \tag{3.15}$$

We will show that $\{x^k\}$ converges to a global minimum of (3.15) with support being $\mathrm{supp}(x^K)$. To this end, we use X^* to denote the set of global minima of problem (3.15). Fix $k \geq K$ and write $g^k := 2A^\top(Ax^k - b)$ for the sake of simplicity. We obtain by the optimality condition of problem (3.14) that

$$\langle x^{k+1} - (x^k - v_k g^k), x - x^{k+1} \rangle \geq 0 \quad \text{for each } x \in X.$$

Fix $x \in X$. Then it follows that

$$\|x - (x^k - v_k g^k)\|^2 = \|x - x^{k+1} + x^{k+1} - (x^k - v_k g^k)\|^2 \geq \|x^{k+1} - (x^k - v_k g^k)\|^2 + \|x - x^{k+1}\|^2;$$

equivalently,

$$\|x - x^k\|^2 + 2v_k \langle x - x^k, g^k \rangle \geq \|x^{k+1} - x^k\|^2 + 2v_k \langle x^{k+1} - x^k, g^k \rangle + \|x - x^{k+1}\|^2. \tag{3.16}$$

Note by definition of g^k that

$$\langle x - x^k, g^k \rangle = \langle x - x^k, 2A^\top(Ax^k - b) \rangle = \|Ax - b\|^2 - \|Ax^k - b\|^2 - \|Ax - Ax^k\|^2.$$

Substituting this into (3.16), we derive that

$$\begin{aligned}
&\|Ax-b\|^2+\frac{1}{2v_k}\|x-x^k\|^2\\
&\geq \|Ax^{k+1}-b\|^2+\frac{1}{2v_k}\|x-x^{k+1}\|^2+\frac{1}{2v_k}\|x^{k+1}-x^k\|^2-\|Ax^{k+1}-Ax^k\|^2 \qquad (3.17)\\
&\geq \|Ax^{k+1}-b\|^2+\frac{1}{2v_k}\|x-x^{k+1}\|^2
\end{aligned}$$

(due to (3.8)). Note that $x\in X$ is arbitrary. Taking $x:=x^k$ in (3.17), one has

$$\|Ax^{k+1}-b\|^2\leq \|Ax^k-b\|^2-\frac{1}{2v_k}\|x^k-x^{k+1}\|^2,$$

i.e., $\{\|Ax^k-b\|^2\}$ is decreasing. Taking $x:=\bar{x}\in X^*$ in (3.17), we obtain

$$0\leq \|Ax^{k+1}-b\|^2-\|A\bar{x}-b\|^2\leq \frac{1}{2v_k}(\|x^k-\bar{x}\|^2-\|x^{k+1}-\bar{x}\|^2). \qquad (3.18)$$

This shows that $\{\|x^k-\bar{x}\|^2\}$ is decreasing for each $\bar{x}\in X^*$, and so, $\{x^k\}$ is bounded and must have a cluster point x^*. By the decreasing property of $\{\|Ax^k-b\|^2\}$, we inductively obtain by (3.18) and (3.8) that

$$\|Ax^k-b\|^2-\|A\bar{x}-b\|^2\leq \frac{1}{k}\sum_{i=1}^{k}(\|Ax^i-b\|^2-\|A\bar{x}-b\|^2)\leq \frac{1}{2k\inf_{i\in\mathbb{N}}v_i}\|x^0-\bar{x}\|^2$$

(by the decreasing property of $\{\|x^k-\bar{x}\|^2\}$). By letting $k\to\infty$, we have that $\|Ax^*-b\|^2=\|A\bar{x}-b\|^2$, and thus $x^*\in X^*$. Since $\{\|x^k-x^*\|^2\}$ is decreasing and x^* is a cluster point of $\{x^k\}$, then $\{x^k\}$ converges to such $x^*\in X^*$.

By Lemma 3.1(i) and since $\mathrm{supp}(x^k)=\mathrm{supp}(x^K)$, one has that $|x_j^k|>\sqrt{2\tau\inf_{i\in\mathbb{N}}v_i}$ for each $j\in\mathrm{supp}(x^K)$ and each $k\geq K$. By taking $k\to\infty$, we have that $|x_j^*|\geq\sqrt{2\tau\inf_{i\in\mathbb{N}}v_i}$ for each $j\in\mathrm{supp}(x^K)$, and consequently, $\mathrm{supp}(x^*)=\mathrm{supp}(x^K)$. This, together with Theorem 2.1, shows that x^* is a local minimum of problem (1.4); consequently, the convergence of $\{x^k\}$ to a local minimum x^* of problem (1.4) is obtained.

Next we show the linear convergence rate of $\{x^k\}$ to x^*. Since x^* is a local minimum of problem (1.4), the optimality condition (2.6) is satisfied. Moreover by Lemma 3.4, there exists $K\in\mathbb{N}$ such that

$$\mathrm{supp}(x^k)=\mathrm{supp}(x^*)\quad \text{for each } k\geq K. \qquad (3.19)$$

Fix $k\geq K$. In view of Algorithm 3.1 and by (2.6), we obtain that, for each $i\in\mathrm{supp}(x^*)$,

$$\begin{aligned}
x_i^{k+1}-x_i^* &= x_i^k-2v_kA_i^\top(Ax^k-b)-x_i^*\\
&= x_i^k-x_i^*-2v_kA_i^\top((Ax^k-b)-(Ax^*-b))\\
&= (\mathbb{I}_i-2v_kA_i^\top A)(x^k-x^*).
\end{aligned}$$

Then one has by (3.19) that

$$\begin{aligned}\|x^{k+1}-x^*\|^2 &= \sum_{i\in \mathrm{supp}(x^*)} (x_i^{k+1}-x_i^*)^2\\ &= \sum_{i\in \mathrm{supp}(x^*)} \Big((\mathbb{I}_i - 2v_k A_i^\top A)(x^k-x^*)\Big)^2\\ &\le \|\mathbb{I}-2v_kA^\top A\|^2\|x^k-x^*\|^2.\end{aligned}$$

By (3.8), there exists $\eta\in(0,1)$ such that $\|\mathbb{I}-2v_kA^\top A\|<\eta$. This, together with the above inequality, shows the linear convergence rate of $\{x^k\}$ to x^*. The proof is complete. □

The following theorem provides an upper bound for the model error at the limiting point approached by the IMTC. Recall that n_i is the size of the i-th group and $n_{\max}:=\max_{i\in[N]} n_i$.

Theorem 3.2. *Let $\{x^k\}$ be a sequence generated by Algorithm 3.1 with* (3.8) *being satisfied. Let x^* be the limiting point of $\{x^k\}$. Suppose that*

$$\psi(A):=\inf_{u\in\mathbb{R}^m}\frac{\|A^\top u\|_\infty^2}{\|u\|^2}>0^1. \tag{3.20}$$

Then

$$\|Ax^*-b\|^2\le\frac{\lambda+\tau n_{\max}}{2\psi(A)\inf_{k\in\mathbb{N}}v_k}. \tag{3.21}$$

Proof. Since x^* is the limiting point of $\{x^k\}$, in view of Algorithm 3.1 and by (3.8), there exists $v\in[\inf_{k\in\mathbb{N}}v_k,\sup_{k\in\mathbb{N}}v_k]$ such that

$$y^*_{\mathcal{G}_i}=x^*_{\mathcal{G}_i}-2vA^\top_{\mathcal{G}_i}(Ax^*-b),\ z^*_{\mathcal{G}_i}=\mathbf{H}(y^*_{\mathcal{G}_i},\sqrt{2v\tau}),\ x^*_{\mathcal{G}_i}=\mathbf{H}_{\mathcal{G}_i}\left(z^*_{\mathcal{G}_i};\sqrt{2v(\lambda+\tau\|z^*_{\mathcal{G}_i}\|_0)}\right) \tag{3.22}$$

for each $i\in[N]$. Let $\Lambda:=\{i:\|x^*_{\mathcal{G}_i}\|\neq0\}$ and Λ^c be its complement set. We first claim that

$$\|A^\top_{\mathcal{G}_i}(Ax^*-b)\|^2\le\frac{\lambda+\tau n_i}{2\inf_{k\in\mathbb{N}}v_k}\quad\text{for each } i\in\Lambda^c, \tag{3.23}$$

and

$$(A_j^\top(Ax^*-b))^2\le\frac{\tau}{2\inf_{k\in\mathbb{N}}v_k}\quad\text{for each } j\in\mathcal{G}_\Lambda\setminus\mathrm{supp}(x^*). \tag{3.24}$$

To show (3.23), we fix $i\in\Lambda^c$. This says $x^*_{\mathcal{G}_i}=0$. Consequently, we derive by the first two equalities in (3.22) and the definition of $\mathbf{H}$ in (3.4) that

$$\|2vA^\top_{\mathcal{G}_i}(Ax^*-b)\|^2=\|y^*_{\mathcal{G}_i}\|^2\le\|z^*_{\mathcal{G}_i}\|^2+2v\tau(n_i-\|z^*_{\mathcal{G}_i}\|_0), \tag{3.25}$$

and by the last equality of (3.22) and the definition of $\mathbf{H}_{\mathcal{G}_i}$ in (3.5) that

$$\|z^*_{\mathcal{G}_i}\|^2\le2v(\lambda+\tau\|z^*_{\mathcal{G}_i}\|_0).$$

[1] A verifiable sufficient condition for (3.20) is that A is of full row rank.

This, together with (3.25), deduces (3.23).

To prove (3.24), fix $j \in \mathcal{G}_i \setminus \mathrm{supp}(x^*)$ with $i \in \Lambda$. This says that $x_j^* = 0$ and $x_{\mathcal{G}_i}^* \neq 0$. Then we obtain by (3.22) that $|2vA_j^\top(Ax^* - b)| = |y_j^*| \leq \sqrt{2v\tau}$, and thus (3.24) is achieved.

By (2.6), (3.23) and (3.24), we conclude that

$$\|A^\top(Ax^* - b)\|_\infty^2 \leq \frac{\lambda + \tau n_{\max}}{2\inf_{k\in\mathbb{N}} v_k}.$$

Then we obtain by assumption (3.20) (with $Ax^* - b$ in place of u) that

$$\|Ax^* - b\|^2 \leq \frac{1}{\psi(A)}\|A^\top(Ax^* - b)\|_\infty^2 \leq \frac{\lambda + \tau n_{\max}}{2\psi(A)\inf_{k\in\mathbb{N}} v_k}.$$

The proof is complete. □

3.2 Convergence theorem under RIP

Puzzled by the nonconvex and nonsmooth structure, Theorem 3.1 only showed the convergence of the IMTC to a local minimum of problem (1.4); there is few theoretical evidence to guarantee the convergence of first-order iterative algorithms to a global minimum of nonconvex optimization problems. To partially fill this gap, we aim to establish the convergence of the IMTC to an approximate true sparse solution under an assumption of the restricted isometry property (RIP) [10].

Definition 3.1. *Let $A \in \mathbb{R}^{m\times n}$ and $s \in \mathbb{N}$. The s-restricted isometry constant δ_s is defined to be the smallest quantity such that*

$$(1 - \delta_s)\|x\|^2 \leq \|Ax\|^2 \leq (1 + \delta_s)\|x\|^2$$

for each $x \in \mathbb{R}^n$ with $\|x\|_0 \leq s$. The matrix A is said to satisfy the s-RIP with δ_s if $\delta_s < 1$.

It is clear by definition that δ_s is nondecreasing in s, that is $\delta_s \leq \delta_t$ whenever $s \leq t$. The following lemma recalls some properties of the RIP, which will be useful in convergence analysis.

Lemma 3.7. *Suppose that A satisfies s-RIP with $\delta_s < 1$. Let $x \in \mathbb{R}^n$, $\varepsilon \in \mathbb{R}^m$, $\mathcal{I}, \mathcal{J} \subseteq [n]$, and $v \in [0, \frac{1}{1-\delta_s}]$. Then the following assertions are true.*

(i) *If $\sharp(\mathcal{I} \cup \mathrm{supp}(x)) \leq s$, then $\|((\mathbb{I} - vA^\top A)x)_\mathcal{I}\| \leq (1 - v + v\delta_s)\|x\|$.*

(ii) *If $\sharp(\mathcal{I}) \leq s$, then $\|A_\mathcal{I}^\top \varepsilon\| \leq \sqrt{1 + \delta_s}\|\varepsilon\|$.*

(iii) *If $\mathcal{I} \cap \mathcal{J} = \emptyset$ and $\sharp(\mathcal{I} \cup \mathcal{J}) \leq s$, then $\|A_\mathcal{J}^\top A_\mathcal{I} x_\mathcal{I}\| \leq \delta_s\|x_\mathcal{I}\|$.*

Proof. The proof of item (i) with a general v follows an analysis similar to that of [18, Lemma 6.16] with $v = 1$ and is thus omitted. Items (ii) and (iii) are taken from [34, Propositions 3.1 and 3.2] respectively. □

A practical continuation technique is using a geometrically decreasing sequence of regularization parameters starting at a large one. In particular, using a geometrically decreasing sequence of parameter pairs with a homogeneous ratio, a variant of Algorithm 3.1 is introduced as follows.

Algorithm 3.2. Select regularization parameters $(\lambda_0, \tau_0) > 0$, $(\lambda, \tau) > 0$ and the continuation parameter $\kappa \in (0, 1)$, and set the initial point $x^0 := 0$ and the stepsize $v > 0$. For each $k \in \mathbb{N}$, if $\lambda_k < \lambda$ or $\tau_k < \tau$, then stop and output $x^* := x^k$; otherwise, determine x^{k+1} via the iterations (3.1)-(3.3), and update regularization parameters $(\lambda_{k+1}, \tau_{k+1}) := \kappa(\lambda_k, \tau_k)$.

Let $\bar{x}$ be the unique true s-sparse solution of (1.1) with support $\mathcal{S} := \mathrm{supp}(\bar{x})$ (the uniqueness is guaranteed under the RIP assumption [21]). The following theorem provides certain parameters setting (relevant to the RIP) in Algorithm 3.2 to guarantee its convergence to an approximate true sparse solution of (1.1) within a tolerance proportional to the noise magnitude. In addition, the support of the output of Algorithm 3.2 is exactly a subset of the support of the true sparse solution. We write $n_{\mathcal{S}} := \max_{i \in \mathcal{S}} n_i$.

Theorem 3.3. *Suppose that A satisfies the RIP with $\delta_{s+1}(1 + \sqrt{s} + \sqrt{S(\alpha + n_{\mathcal{S}})}) < 1$ and some $\alpha := \frac{\lambda_0}{\tau_0} > 0$, and let*

$$\eta \in \left(0, 1 - \delta_{s+1}(1 + \sqrt{s} + \sqrt{S(\alpha + n_{\mathcal{S}})})\right). \tag{3.26}$$

Set the stepsize $v \leq \frac{1}{2(1-\delta_s)}$, the regularization parameters

$$\tau_0 \geq \frac{2v\|\bar{x}\|^2}{(1 + \sqrt{s} + \sqrt{S(\alpha + n_{\mathcal{S}})})^2}, \quad \tau := \frac{2v(1+\delta_s)}{\eta^2}\|\varepsilon\|^2, \quad \frac{\lambda}{\tau} = \frac{\lambda_0}{\tau_0}, \tag{3.27}$$

and the continuation parameter

$$\kappa \in \left[\left(\frac{2v\delta_{s+1}(1 + \sqrt{s} + \sqrt{S(\alpha + n_{\mathcal{S}})})}{1 - \eta} + 1 - 2v\right)^2, 1\right). \tag{3.28}$$

Let Algorithm 3.2 with these parameters output x^*. Then it holds that

$$\mathrm{supp}(x^*) \subseteq \mathcal{S} \quad \textit{and} \quad \|x^* - \bar{x}\| \leq \frac{(1-\eta)\sqrt{1+\delta_s}}{\eta\delta_{s+1}}\|\varepsilon\|. \tag{3.29}$$

Furthermore, if $\min_{i \in \mathcal{S}} |\bar{x}_i| > \frac{(1-\eta)\sqrt{1+\delta_s}}{\eta\delta_{s+1}}\|\varepsilon\|$, then $\mathrm{supp}(x^*) = \mathcal{S}$.

Proof. By assumption of the RIP that $1 - \delta_{s+1}(1 + \sqrt{s} + \sqrt{S(\alpha + n_{\mathcal{S}})}) > 0$, one sees that η in (3.26) is well-defined. It follows from (3.26) that $\frac{2v\delta_{s+1}(1+\sqrt{s}+\sqrt{S(\alpha+n_{\mathcal{S}})})}{1-\eta} + 1 - 2v < 1$. Hence κ in (3.28) and Algorithm 3.2 with these parameters are well-defined.

To furniture the proof, we let Algorithm 3.2 generate the finite sequence $\{x^k, y^k, z^k\}_{k=0}^K$ and output $x^* = x^K$, and write

$$\rho := \frac{1-\eta}{\delta_{s+1}}, \tag{3.30}$$

and

$$r^k := x^k - \bar{x}, \quad \mathcal{S}_k := \mathrm{supp}(x^k) \tag{3.31}$$

for each $k = 0, \ldots, K$. By the homogeneous assumption of regularization parameters in (3.27) that $\frac{\lambda}{\tau} = \frac{\lambda_0}{\tau_0} = \alpha$ and the same continuation parameter κ for $\{(\lambda_k, \tau_k)\}$, we have that

$$\lambda_k = \alpha \tau_k \tag{3.32}$$

for each $k = 0, \ldots, K$, and the stopping criteria $\lambda_k < \lambda$ and $\tau_k < \tau$ happen at iterate K simultaneously. We shall show by induction that the following inclusion and estimate hold for each $k = 0, \ldots, K$:

$$\mathcal{S}_k \subseteq \mathcal{S} \quad \text{and} \quad \|r^k\| \leq \rho \sqrt{\frac{\tau_k}{2v}}. \tag{3.33}$$

By the initial selection that $x^0 := 0$, one has that $\mathcal{S}_0 = \emptyset \subseteq \mathcal{S}$. By definition of ρ in (3.30) and assumption (3.26), we obtain by assumption of τ_0 in (3.27) that

$$\rho \sqrt{\frac{\tau_0}{2v}} = \frac{1-\eta}{\delta_{s+1}} \sqrt{\frac{\tau_0}{2v}} > (1 + \sqrt{s} + \sqrt{S(\alpha + n_{\mathcal{S}})}) \sqrt{\frac{\tau_0}{2v}} \geq \|\bar{x}\| = \|r^0\|.$$

It is shown that (3.33) holds for $k = 0$.

Now suppose that (3.33) holds for iterate $k < K$. Then by (3.1) and (1.1), we have that

$$y^k = x^k - 2vA^\top (Ax^k - A\bar{x} - \varepsilon) = x^k - 2vA^\top A_{\mathcal{S}} r^k_{\mathcal{S}} + 2vA^\top \varepsilon, \tag{3.34}$$

where the second equality follows from the hypothesis $\mathcal{S}_k \subseteq \mathcal{S}$ in (3.33). Fix $i \in \mathcal{S}^c$. It follows from the hypothesis $\mathcal{S}_k \subseteq \mathcal{S}$ in (3.33) that $x^k_i = 0$, and then (3.34) is reduced to

$$|y^k_i| \leq 2v |A_i^\top A_{\mathcal{S}} r^k_{\mathcal{S}}| + 2v |A_i^\top \varepsilon|. \tag{3.35}$$

Since $\{i\} \cap \mathcal{S} = \emptyset$, we obtain by Lemma 3.7(iii) and (ii) that

$$|A_i^\top A_{\mathcal{S}} r^k_{\mathcal{S}}| \leq \delta_{s+1} \|r^k_{\mathcal{S}}\| = \delta_{s+1} \|r^k\| \quad \text{and} \quad |A_i^\top \varepsilon| \leq \sqrt{1+\delta_1} \|\varepsilon\| \leq \sqrt{1+\delta_s} \|\varepsilon\|$$

(by the nondecreasing property that $\delta_1 \leq \delta_s$). This, together with (3.35), yields that

$$|y^k_i| \leq 2v\delta_{s+1} \|r^k\| + 2v\sqrt{1+\delta_s} \|\varepsilon\|. \tag{3.36}$$

By the stopping criterion that $\tau_K < \tau$ and the definition of τ in (3.28), one can get that $\tau_k \geq \tau = \frac{2v(1+\delta_s)}{\eta^2} \|\varepsilon\|^2$, that is, $\|\varepsilon\| \leq \sqrt{\frac{\tau_k}{2v(1+\delta_s)}}\, \eta$. This, together with hypothesis (3.33), deduces

$$2v\delta_{s+1} \|r^k\| + 2v\sqrt{1+\delta_s} \|\varepsilon\| \leq \delta_{s+1} \rho \sqrt{2v\tau_k} + \eta \sqrt{2v\tau_k} = \sqrt{2v\tau_k}, \tag{3.37}$$

where the equality holds by definition of ρ in (3.30). Then (3.36) is reduced to $|y^k_i| \leq \sqrt{2v\tau_k}$. Hence it follows from (3.2) that $z^k_i = 0$ and then from (3.3) that $x^{k+1}_i = 0$; consequently, $i \in \mathcal{S}^c_{k+1}$. Since $i \in \mathcal{S}^c$ is arbitrary, we get that $\mathcal{S}^c \subseteq \mathcal{S}^c_{k+1}$, and equivalently, $\mathcal{S}_{k+1} \subseteq \mathcal{S}$.

On the other hand, we get by the inclusion $\mathcal{S}_{k+1} \subseteq \mathcal{S}$ that

$$\|x^{k+1} - \bar{x}\| = \|x^{k+1}_{\mathcal{S}} - \bar{x}_{\mathcal{S}}\| \leq \|x^{k+1}_{\mathcal{S}} - z^k_{\mathcal{S}}\| + \|z^k_{\mathcal{S}} - y^k_{\mathcal{S}}\| + \|y^k_{\mathcal{S}} - \bar{x}_{\mathcal{S}}\|. \tag{3.38}$$

We obtain by the group hard thresholding operator (3.3) that

$$\|x^{k+1}_{\mathcal{S}} - z^k_{\mathcal{S}}\| \leq \sqrt{S}\|x^{k+1} - z^k\|_{2,\infty} \leq \sqrt{2vS(\lambda_k + \tau_k n_{\mathcal{S}})} = \sqrt{2vS\tau_k(\alpha + n_{\mathcal{S}})} \tag{3.39}$$

(due to (3.32)), and by the hard thresholding operator (3.2) that

$$\|z^k_{\mathcal{S}} - y^k_{\mathcal{S}}\| \leq \sqrt{s}\|z^k - y^k\|_\infty = \sqrt{2vs\tau_k}. \tag{3.40}$$

Moreover we obtain by (3.34) that

$$\|y^k_{\mathcal{S}} - \bar{x}_{\mathcal{S}}\| = \|((\mathbb{I} - 2vA^\top A)r^k)_{\mathcal{S}} + 2vA^\top_{\mathcal{S}}\varepsilon\| \leq \|((\mathbb{I} - 2vA^\top A)r^k)_{\mathcal{S}}\| + 2v\|A^\top_{\mathcal{S}}\varepsilon\|. \tag{3.41}$$

It follows from Lemma 3.7(i) and (ii) that

$$\|((\mathbb{I} - 2vA^\top A)r^k)_{\mathcal{S}}\| \leq (1 - 2v + 2v\delta_s)\|r^k\| \quad \text{and} \quad \|A^\top_{\mathcal{S}}\varepsilon\| \leq \sqrt{1+\delta_s}\|\varepsilon\|,$$

respectively. This, together with (3.38)-(3.41), implies that

$$\|x^{k+1} - \bar{x}\| \leq (\sqrt{s} + \sqrt{S(\alpha + n_{\mathcal{S}})})\sqrt{2v\tau_k} + (1 - 2v + 2v\delta_s)\|r^k\| + 2v\sqrt{1+\delta_s}\|\varepsilon\|. \tag{3.42}$$

By the fact that $\delta_s \leq \delta_{s+1}$ and by (3.37), one has that

$$2v\delta_s\|r^k\| + 2v\sqrt{1+\delta_s}\|\varepsilon\| \leq 2v\delta_{s+1}\|r^k\| + 2v\sqrt{1+\delta_s}\|\varepsilon\| \leq \sqrt{2v\tau_k}.$$

By this and (3.33), (3.42) is reduced to

$$\|x^{k+1} - \bar{x}\| \leq \left(2v(1 + \sqrt{s} + \sqrt{S(\alpha + n_{\mathcal{S}})}) + \rho(1 - 2v)\right)\sqrt{\frac{\tau_k}{2v}}. \tag{3.43}$$

Noting by definition of ρ in (3.30) that

$$2v(1+\sqrt{s}+\sqrt{S(\alpha+n_{\mathcal{S}})})+\rho(1-2v) = \rho\left(\frac{2v\delta_{s+1}(1+\sqrt{s}+\sqrt{S(\alpha+n_{\mathcal{S}})})}{1-\eta} + 1 - 2v\right) \leq \rho\sqrt{\kappa}$$

(due to definition of κ in (3.28)), (3.43) is reduced to

$$\|x^{k+1} - \bar{x}\| \leq \rho\sqrt{\frac{\kappa\tau_k}{2v}} = \rho\sqrt{\frac{\tau_{k+1}}{2v}}$$

(by the continuation rule that $\tau_{k+1} := \kappa\tau_k$). This, together with $\mathcal{S}_{k+1} \subseteq \mathcal{S}$, shows that (3.33) holds for each iterate $k = 0, \ldots, K$. Then by (3.33) and the stopping criterion that $\tau_K < \tau$, we conclude that $\mathrm{supp}(x^*) \subseteq \mathcal{S}$ and

$$\|x^* - \bar{x}\| = \|x^K - \bar{x}\| \leq \rho\sqrt{\frac{\tau_K}{2v}} < \rho\sqrt{\frac{\tau}{2v}} = \frac{(1-\eta)\sqrt{1+\delta_s}}{\eta\delta_{s+1}}\|\varepsilon\|$$

by definitions of τ and ρ in (3.27) and (3.30). Hence (3.29) is proved.

Moreover, suppose that $\min_{i\in\mathcal{S}} |\bar{x}_i| > \frac{(1-\eta)\sqrt{1+\delta_s}}{\eta\delta_{s+1}}\|\varepsilon\|$. We prove by contradiction, assuming that $\mathrm{supp}(x^*) \neq \mathcal{S}$. This, together with $\mathrm{supp}(x^*) \subseteq \mathcal{S}$ in (3.29), indicates that there exists $i \in \mathcal{S}$ such that $x_i^* = 0$. Hence

$$\|x^* - \bar{x}\| \geq |x_i^* - \bar{x}_i| > \frac{(1-\eta)\sqrt{1+\delta_s}}{\eta\delta_{s+1}}\|\varepsilon\|,$$

which yields a contradiction with (3.29). Hence $\mathrm{supp}(x^*) = \mathcal{S}$. The proof is complete. □

Remark 3.1. (i) The RIP-type conditions used in Theorem 3.3 have been assumed in order to guarantee the convergence of several algorithms to the ground true sparse solution, such as OMP [42], primal dual active set algorithm [23], iterative difference hard-thresholding algorithm [14], optimal thresholding algorithm [53], proximal gradient algorithm [20], scaled proximal gradient algorithm [45]. It was reported in [6, 20] that the RIP-type conditions are guaranteed with high probability for a Gaussian or sub-Gaussian matrix.

(ii) For sparse optimization with a nonlinear loss function, the restricted strong convexity (RSC) and restricted strong smoothness (RSS) are assumed to guarantee the convergence of some algorithms to the ground true sparse solution; see [3, 50, 54]. The RSC and RSS are the extensions of the RIP-type conditions to nonlinear loss functions.

(iii) The restricted eigenvalue condition (REC) [5] is a weaker regularity condition than the RIP-type conditions. It was shown in [51, Theorem 5] that the convergence of the proximal majorization-minimization method to a ground true sparse solution is guaranteed under the weak REC and the additional assumptions on the Gaussian distribution of A and the interval of parameter λ. Our convergence guarantee in Theorem 3.3 assumed the strong RIP but does not require the Gaussian distribution of A.

4 Application to differential optical absorption spectroscopy

Differential optical absorption spectroscopy (DOAS) analysis is a fundamental and commonly used technique in atmospheric chemistry and computational optics [37]. The goal of DOAS is to identify the gases or materials in a mixture and quantify their concentrations by measuring the reduction over a range of wavelengths in terms of the intensity of light shined through it. When the light shines through a gas with path length L and concentration $x(\cdot)$, the light intensity will be absorbed and attenuated; Lambert-Beer's law [37, Chapter 8] relates the process of light absorption as

$$A(\omega) = \log\frac{I_0(\omega)}{I(\omega)} = \theta(\omega)\int_0^L x(l)dl \tag{4.1}$$

where ω is the wavelength, $A(\cdot)$, $I(\cdot)$ and $I_0(\cdot)$ are the absorbed, transmitted and the initial intensity of the light, respectively, and $\theta(\cdot)$ is the characteristic absorption spectra for

the absorbing gas. For simplicity, assuming that the gas is equable at the path line, the concentration is a constant x, and then Lambert-Beer's law (4.1) is reduced to

$$A(\omega) = Lx\theta(\omega). \tag{4.2}$$

When multiple absorbing gases $\mathcal{M}$ are present at the path line and the reduction of the light intensity due to scattering is considered, $x\theta(\cdot)$ can be replaced by a linear combination of the characteristic absorption spectra of involved gases plus an additive noise of light scattering, and hence Lambert-Beer's law (4.2) can be rewritten as

$$A(\omega) = L \sum_{i \in \mathcal{M}} x_i \theta_i(\omega) + \epsilon(\omega). \tag{4.3}$$

Collected the reference characteristic absorption spectra $\{\theta_i\}$ from database and measured the absorption spectra of the mixture of gases A from the optical spectrometer, the DOAS analysis aims to estimate the concentrations of gases $\{x_i\}_{i \in \mathcal{M}}$ via (4.3). Considering only the involved gases and dealing with the additive white Gaussian noise ϵ, one of the most classical and common mathematical methods for DOAS analysis is the linear least-squares method; see [37, Chapter 8].

Two issues should be considered in the improvement of the DOAS analysis technique. The first issue is the identification of involved gases $\mathcal{M}$, which was assumed to be known in advance (or identified by other methods) as in the traditional DOAS analysis technique. However, as shown in [37, Chapter 8], this prior information requirement may hinder the development and applications of DOAS automatic analysis technique. Secondly, besides the additive noise due to scattering, a challenging complication in practice is the wavelength misalignment, which is caused by the installment of the optical spectrometer and leads to the basis noise; see [16]. In particular, caused by the installment or environment of optical spectrometers, the nominal wavelengths in the measurement of $A(\omega)$ may not correspond exactly to those in the basis $\{\theta_i(\omega)\}$, but approximately aligned with a linear deformation $\{\theta_i(\omega + d(\omega))\}$. Hence, equipped with the wavelength misalignment, (4.3) is turned into

$$A(\omega) = L \sum_{i \in \mathcal{M}} x_i \theta_i(\omega + d(\omega)) + \epsilon(\omega). \tag{4.4}$$

However, the quantity of linear deformation $d(\cdot)$ is usually unknown in practice. Therefore, given the data $A(\cdot)$ and reference spectra $\{\theta_i(\cdot)\}$, the DOAS automatic analysis aims to identify the involved gases and quantify their concentrations $\{x_i\}$ and the deformation $\{d(\cdot)\}$ from the linear model (4.4).

To deal with these two issues, inspired by the ideas of variable selection and using a set of modified bases [16], we construct a dictionary by enlarging characteristic absorption spectra database $\{\theta_i\}_{i \in \mathcal{M}}$ to that of a set of possible (common but concerned) gases $\{\theta_i\}_{i \in \mathcal{P}}$ with $\mathcal{M} \subseteq \mathcal{P}$ and deforming each θ_i with a set of possible deformations $\mathcal{D}$. In particular, the deformations can be approximated by linear functions, i.e.,

$$\mathcal{D} := \{d(\omega) : d(\omega) = u\omega + v, u \in \mathcal{U}, v \in \mathcal{V}\}, \tag{4.5}$$

from two predetermined sets $\mathcal{U}$ and $\mathcal{V}$. Let Θ_j denote a matrix whose columns are the reference spectra $\{\theta_i\}_{i\in\mathcal{P}}$ of j-th deformation, i.e., $\Theta_j := [\theta_i(\omega + d_j(\omega))]_{i\in\mathcal{P}}$ for $j \in \mathcal{D}$, and let $x_{d_j} \in \mathbb{R}^{|\mathcal{P}|}$ denote the concentrations of possible gases at j-th deformation. Then with the enlarged sets of candidates $\mathcal{P}$ and deformations $\mathcal{D}$, (4.4) can be rewritten as

$$A = L\left[\Theta_1, \ldots, \Theta_{|\mathcal{D}|}\right] \begin{bmatrix} x_{d_1} \\ \vdots \\ x_{d_{|\mathcal{D}|}} \end{bmatrix} + \epsilon. \tag{4.6}$$

Note that the solution of the linear system (4.6) enjoys a mix sparse structure. Specifically, there are in general only a few gases involved in a mixture (contrast with the number of possible candidates), and the deformation for the involved gases is unique and consistent (tested in an experiment). Consequently, with the group structure $x := (x_{d_1}^\top, \ldots, x_{d_{|\mathcal{D}|}}^\top)^\top$, the ground true solution of the DOAS has 1-group sparsity (inter-group sparsity) and the nonzero group is also sparse (intra-group sparsity). Therefore, writing $n := |\mathcal{P}| \times |\mathcal{D}|$, the mix sparse optimization model for the DOAS automatic analysis with wavelength misalignment (4.6) can be formulated as

$$\min_{x\in\mathbb{R}^n} \|\Theta x - \frac{A}{L}\|^2 + \lambda\|x\|_{2,0} + \tau\|x\|_0,$$

where $\|x\|_{2,0}$ is to promote the consistent deformation, $\|x\|_0$ is to promote the sparsity of candidate selection.

For the database of numerical experiments, we choose 15 concerned materials as possible candidates (listed in Table 1) and collect their reference characteristic absorption infrared (IR) spectra $\{\theta_i\}_{i\in\mathcal{P}}$ at National Institute of Standards and Technology (NIST) Chemistry WebBook[2]. Then we construct a dictionary Θ by deforming each collected reference IR spectrum by a set of linear deformations (4.5) with $\mathcal{U} = \{-0.15 + 0.05k : k = 1, \ldots, 5\}$ and $\mathcal{V} = \{-3 + k : k = 1, \ldots, 5\}$; see Figure 1 for the reference IR spectra with some deformed examples. Therefore, there are 15 possible materials and 25 possible deformations, and each spectrum has 554 sample intensity along with wavelength; consequently, the dictionary $\Theta \in \mathbb{R}^{554\times 375}$.

In the numerical experiments, the simulation data are generated via the following process. Firstly, the dictionary Θ is constructed as mentioned above with each θ_i being normalized. Then we randomly pick several materials in $\mathcal{P}$ with their concentrations being i.i.d. Gaussian ensembles and randomly select a deformation in $\mathcal{D}$ with a uniform distribution, that is, the ground true solution $\bar{x}$ is randomly generated. With the generated Θ and $\bar{x}$, the observation data (absorption spectra) A is generated via (4.6) with ϵ being an additive Gaussian noise with the standard deviation being 0.1%. All numerical experiments are implemented in Matlab R2014a and executed on a personal desktop (Intel Core Duo i7-8550, 1.80 GHz, 8.00 GB of RAM).

[2]https://webbook.nist.gov/chemistry/

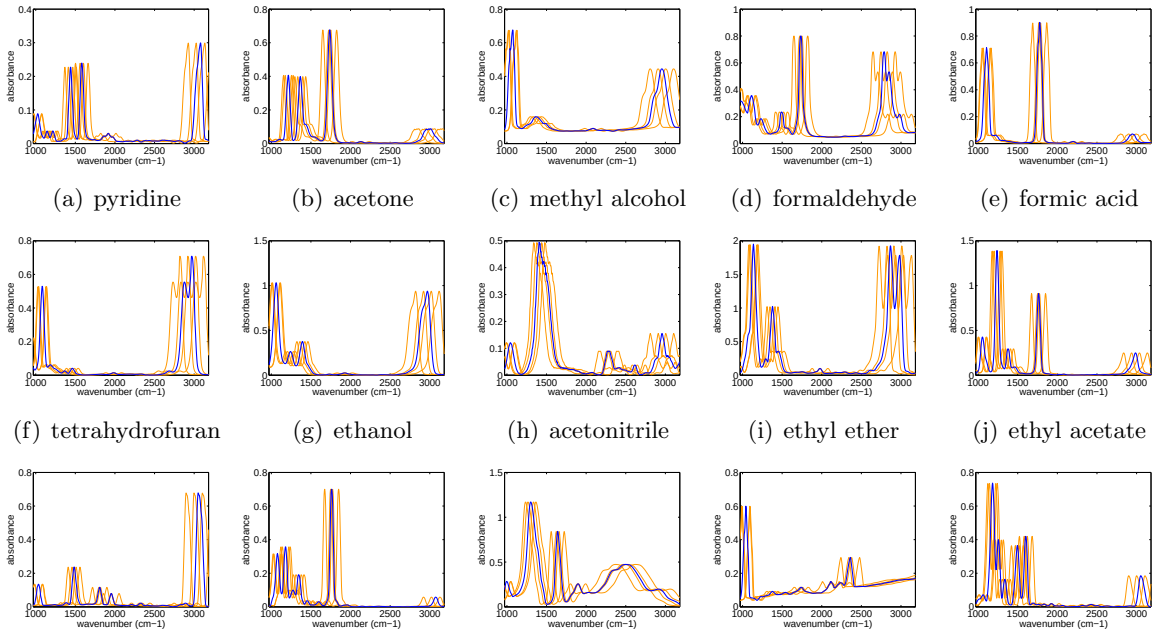
Table 1: Materials in reference dataset.

Number	Name	Formula	Number	Name	Formula
1	pyridine	C5H5N	9	ethyl ether	C4H10O
2	acetone	C3H6O	10	ethyl acetate	C4H8O2
3	methyl alcohol	CH4O	11	benzene	C6H6
4	formaldehyde	CH2O	12	benzoic acid	C7H6O2
5	formic acid	CH2O2	13	sodium bicarbonate	CHNaO3
6	tetrahydrofuran	C4H8O	14	ozone	O3
7	ethanol	C2H6O	15	phenol	C6H6O
8	acetonitrile	C2H3N			

In the implementation of the IMTC (cf. Algorithm 3.1), the initial point and parameters are selected as follows. The initial point is $x^0 := 0$, and we set the constant stepsize $v := \frac{1}{2\|\Theta\|^2}$, regularization parameters $(\lambda_0, \tau_0) := (1, 0.1)$, $(\lambda, \tau) := (10^{-4}, 10^{-5})$ and the continuation parameter $\kappa := 0.96$. Two key criteria to measure the performance of the solvers are the relative error (on observation or solution) and the true positive rate of solution (on materials or misalignment). In the numerical experiments, we compare the numerical performance on DOAS analysis of the IMTC with several state-of-the-art solvers, including the sparse solvers: OMP, ISTA, HardTA, HalfTA, the group sparse solvers: PGA ($\ell_{2,1}$), PGA ($\ell_{2,0}$), and the mix sparse solver: PGASGL.

In the first experiment, we aim to show the spectrum reconstruction, the materials identification and quantification capability of the algorithms. Figure 2 exhibits the materials and the misalignment predicted by algorithms, as well as their relative error of concentrations, and Figure 3 displays the absorbtion spectra reconstructed by the algorithms, as well as their relative error of spectra, at a random trial. It is illustrated from Figure 2 that the solutions obtained by the sparse solvers have different misalignments and thus have no physical sense; the solutions obtained by the group sparse solvers can exactly predict the misalignment but cannot predict the involved materials; and the IMTC can exactly predict the misalignment and the involved materials simultaneously (the relative error is quite small), and outperform the PGASGL. It is revealed from Figure 3 the IMTC can exactly reconstruct the absorbtion spectra and outperform other solvers.

In the second experiment, we aim to show the stability of the IMTC on predicting the materials and misalignment, comparing with other algorithms. Figure 4 plots the true positive rate (TPR) of the predicted materials and misalignment and the relative error of solutions obtained by the algorithms along with the number of involved materials (from 1 to 15) at 500 random simulations. It is demonstrated from Figures 4(a) and 4(b) that the IMTC has a much higher true positive rate than other algorithms and from Figure 4(c) that the solution of the IMTC is much more precise than the ones obtained by other algorithms. Moreover, the CPU time of the IMTC is less than 0.1 second. Therefore, the numerical results show that the IMTC can quickly, stably, exactly and quantitatively predict the existing materials and the factual wavelength misalignment simultaneously, which meets the demand of improvement of



(a) pyridine (b) acetone (c) methyl alcohol (d) formaldehyde (e) formic acid

(f) tetrahydrofuran (g) ethanol (h) acetonitrile (i) ethyl ether (j) ethyl acetate

(k) benzene (l) benzoic acid (m) bicarbonate (n) ozone (o) phenol

Figure 1: For each material, the reference spectrum is plotted in blue, while four deformed spectra are in orange.

the DOAS automatic analysis software proposed in [37, Chapter 8].

Declarations

Conflict of Interest The authors have no competing interests to declare that are relevant to the content of this article.

Data Availability Statements The datasets generated during the DOAS study are available at https://webbook.nist.gov/chemistry/.

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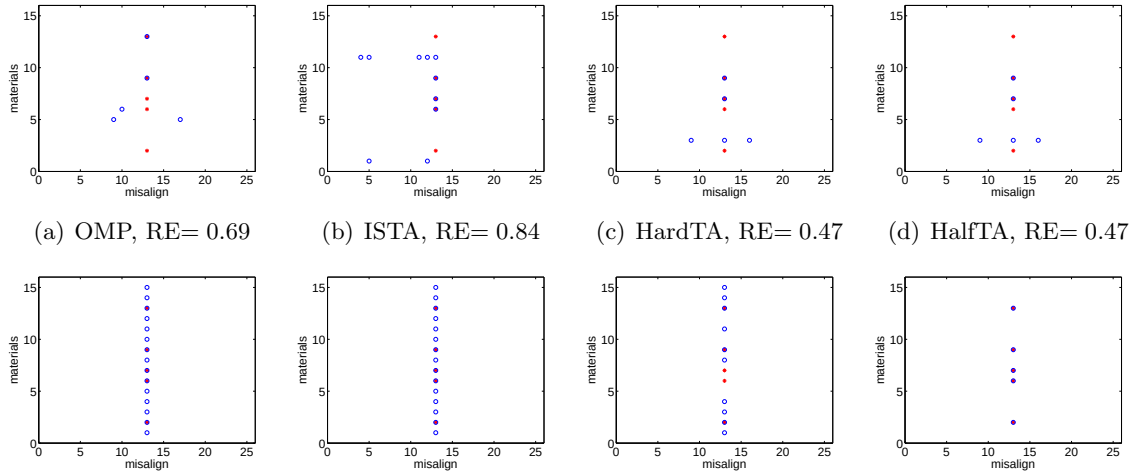
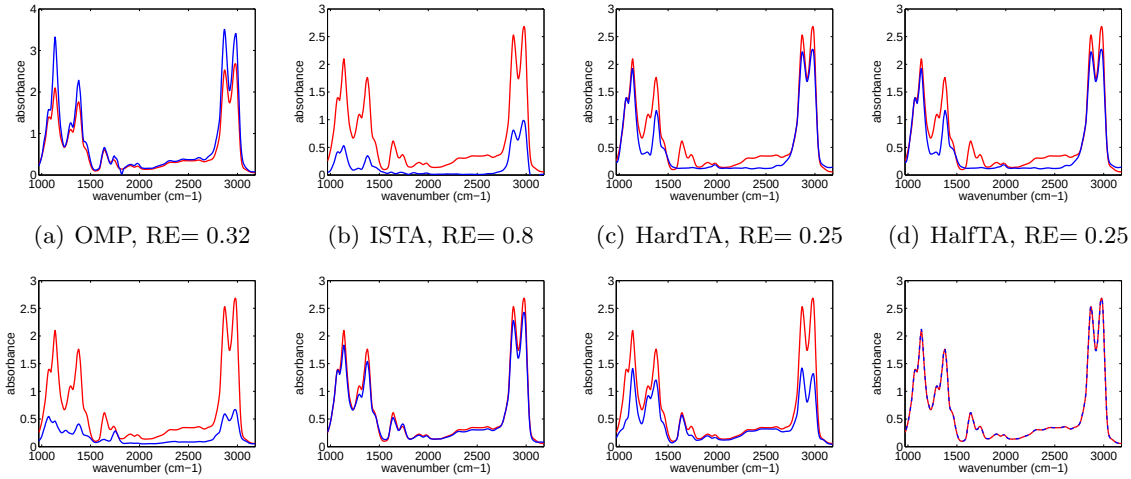


(a) OMP, RE= 0.69 (b) ISTA, RE= 0.84 (c) HardTA, RE= 0.47 (d) HalfTA, RE= 0.47

(e) PGA ($\ell_{2,1}$), RE= 0.82 (f) PGA ($\ell_{2,0}$), RE= 0.26 (g) PGASGL, RE= 0.42 (h) IMTC, RE= 0.008

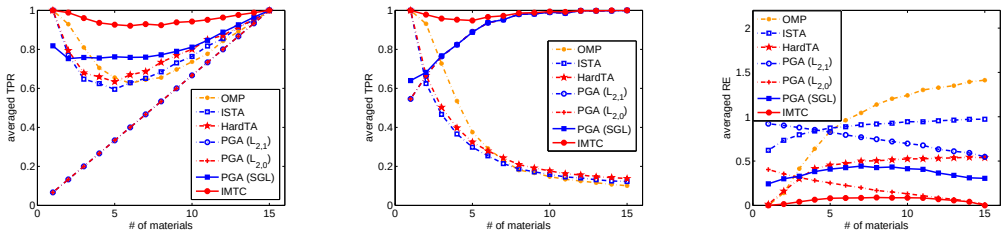
Figure 2: Identification and quantification of algorithms at a trial.



(a) OMP, RE= 0.32 (b) ISTA, RE= 0.8 (c) HardTA, RE= 0.25 (d) HalfTA, RE= 0.25

(e) PGA ($\ell_{2,1}$), RE= 0.74 (f) PGA ($\ell_{2,0}$), RE= 0.10 (g) PGASGL, RE= 0.45 (h) IMTC, RE= 0.006

Figure 3: Spectrum reconstruction of algorithms at a trial.



(a) TPR of materials (b) TPR of misalign (c) RE of prediction

Figure 4: Identification and quantification of algorithms in 500 simulations.

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