

# NODE-SCREENING TESTS FOR THE $\ell_0$ -PENALIZED LEAST-SQUARES PROBLEM

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## ABSTRACT

We present a novel screening methodology to safely discard irrelevant nodes within a generic branch-and-bound (BnB) algorithm solving the  $\ell_0$ -penalized least-squares problem. Our contribution is a set of two simple tests to detect sets of feasible vectors that cannot yield optimal solutions. This allows to prune nodes of the BnB search tree, thus reducing the overall optimization time. One cornerstone of our contribution is a *nesting property* between tests at different nodes that allows to implement them with a low computational cost. Our work leverages the concept of safe screening, well known for sparsity-inducing convex problems, and some recent advances in this field for  $\ell_0$ -penalized regression problems.

**Index Terms**— Sparse approximation, Mixed-integer problems, Branch and bound, Safe screening.

## 1. INTRODUCTION

Finding a sparse representation is a fundamental problem in the field of statistics, machine learning and inverse problems. It consists in decomposing some input vector  $\mathbf{y} \in \mathbb{R}^m$  as a linear combination of a few columns (dubbed *atoms*) of a dictionary  $\mathbf{A} \in \mathbb{R}^{m \times n}$ . This task can be addressed by solving

$$\min_{\mathbf{x} \in \mathbb{R}^n} \frac{1}{2} \|\mathbf{y} - \mathbf{A}\mathbf{x}\|_2^2 + \lambda \|\mathbf{x}\|_0 \quad (1)$$

where  $\|\mathbf{x}\|_0$  counts the number of nonzero entries in  $\mathbf{x}$  and  $\lambda > 0$  is a tuning parameter. Unfortunately, problem (1) has proven to be NP-hard in the general case [1, Th. 3]. This has led researchers to develop sub-optimal procedures to approximate its solution and address large-scale problems. Among the most popular, one can mention greedy algorithms [2, Sec. 3.2 and Ch. 4], methodologies based on convex relaxation [3, 4] and majorization-minimization algorithms [5].

Sub-optimal procedures are unfortunately only guaranteed to solve (1) under restrictive conditions that are rarely met in practice. On the other hand, there has been recently a

surge of interest for methods solving (1) exactly, see [6–10] to name a few. Many approaches leverage the fact that finding

$$\begin{aligned} p^* &= \min_{\mathbf{x} \in \mathbb{R}^n} \frac{1}{2} \|\mathbf{y} - \mathbf{A}\mathbf{x}\|_2^2 + \lambda \|\mathbf{x}\|_0 \\ \text{s.t. } &\|\mathbf{x}\|_\infty \leq M \end{aligned} \quad (P)$$

is equivalent to solve (1), provided that  $M$  is chosen large enough. Interestingly, (P) can be reformulated as a mixed-integer program (MIP) by introducing binary variables encoding the nullity of the entries of  $\mathbf{x}$ , see *e.g.*, [7]. Besides, (P) has been shown to be solvable for moderate-size problems by both commercial solvers [9] and tailored BnB algorithms [10].

In a recent paper, Atamtürk and Gómez extended the notion of safe screening introduced by El Ghaoui *et al.* in [11] from sparsity-promoting convex problems to non-convex  $\ell_0$ -penalized problems. In particular, they introduced a new methodology that allows to detect (some of) the positions of zero and non-zero entries in the minimizers of a particular  $\ell_0$ -penalized problem [12]. Their methodology is used as a preprocessing step of any algorithmic procedure and allows to reduce the problem dimensionality.

In this paper, we make one step forward in the development of numerical methods addressing large-scale  $\ell_0$ -penalized problems by proposing *node-screening* rules that allow to prune *nodes* within the BnB search tree. In contrast to [12], we emphasize the existence of a *nesting property* between screening tests at different nodes. This enables to (potentially) fix *multiple* entries to either zero or non-zero at any step of the optimization process with a marginal cost.

Our exposition is organized as follows. Sec. 2 gathers the main notations used in the paper. In Sec. 3, we describe a BnB algorithm tailored to (P). Sec. 4 presents our new node-screening tests and explains how to implement them efficiently within the BnB process. In Sec. 5, we assess the performance of our method on synthetic data. Due to space limitation, the proofs of our results are omitted here but can be found in our companion paper [13, App. A].

The research presented in this paper is reproducible. Code and data are available at <https://gitlab.insa-rennes.fr/Theo.Guyard/bnb-screening>.

## 2. NOTATIONS

We use the following notational conventions throughout the paper. Boldface uppercase (e.g.,  $\mathbf{A}$ ) and lowercase (e.g.,  $\mathbf{x}$ ) letters respectively represent matrices and vectors.  $\mathbf{0}$  denotes the all-zeros vector. Since the dimension will usually be clear from the context, it is omitted in the notation. The  $i$ th column of a matrix  $\mathbf{A}$  is denoted  $\mathbf{a}_i$ . Similarly, the  $i$ th entry of a vector  $\mathbf{x}$  is denoted  $x_i$ . Calligraphic letters (e.g.,  $\mathcal{S}$ ) are used to denote sets and the notation  $|\cdot|$  refers to their cardinality. If  $\mathcal{S} \subseteq \{1, \dots, n\}$  and  $\mathbf{x} \in \mathbb{R}^n$ ,  $\mathbf{x}_{\mathcal{S}}$  denotes the restriction of  $\mathbf{x}$  to its elements indexed by  $\mathcal{S}$ . Similarly,  $\mathbf{A}_{\mathcal{S}}$  corresponds to the restriction of  $\mathbf{A} \in \mathbb{R}^{m \times n}$  to its columns indexed by  $\mathcal{S}$ .

## 3. BRANCH-AND-BOUND PROCEDURES

Branch-and-bound procedures refer to an algorithmic solution to address MIPs, among others [14]. It consists in implicitly enumerating all feasible solutions and applying pruning rules to discard irrelevant candidates. When particularized to problem  $(P)$ , it can be interpreted as a search tree where a new decision regarding the nullity of an entry of the variable  $\mathbf{x}$  is taken at each node as illustrated in Fig. 1a. Formally, we define a node as a triplet  $\nu = (\mathcal{S}_0, \mathcal{S}_1, \bar{\mathcal{S}})$  where: *i*)  $\mathcal{S}_0$  and  $\mathcal{S}_1$  contain the indices of the entries of  $\mathbf{x}$  which are forced to be zero and non-zero, respectively; *ii*)  $\bar{\mathcal{S}}$  gathers all the entries of  $\mathbf{x}$  for which no decision has been taken at this stage of the decision tree.

The BnB algorithm reads as follows: starting from node  $\nu = (\emptyset, \emptyset, \{1, \dots, n\})$ , the method alternates between processing the current node (*bounding* step) and selecting a new node (*branching* step). The algorithm identifies the global minimum in a finite number of steps with a worst-case complexity equal to an exhaustive search. In practice, its efficiency depends on both the ability to process nodes quickly and the number of nodes processed. We review below specific choices for these two steps tailored to problem  $(P)$ .

### 3.1. Bounding step

When processing node  $\nu = (\mathcal{S}_0, \mathcal{S}_1, \bar{\mathcal{S}})$ , we prospect if any  $\mathbf{x}$  with zeros on  $\mathcal{S}_0$  and non-zero values on  $\mathcal{S}_1$  can yield a global minimizer of  $(P)$ . To that end, we look for the smallest objective value achieved by feasible candidates with respect to these constraints, *i.e.*, the value of

$$p_l^\nu = \min_{\mathbf{x} \in \mathbb{R}^n} \frac{1}{2} \|\mathbf{y} - \mathbf{A}\mathbf{x}\|_2^2 + \lambda \|\mathbf{x}_{\bar{\mathcal{S}}}\|_0 + \lambda |\mathcal{S}_1| \quad (P^\nu)$$

s.t.  $\|\mathbf{x}\|_\infty \leq M$  and  $\mathbf{x}_{\mathcal{S}_0} = \mathbf{0}$ .

One verifies that  $p^\nu \geq p^*$  since all minimizers of  $(P^\nu)$  are also feasible for  $(P)$ . Moreover, equality holds whenever the constraints given by  $\mathcal{S}_0$  and  $\mathcal{S}_1$  match the configuration of one of the minimizers of  $(P)$ .

If  $p^\nu > p^*$ , the node  $\nu$  can be pruned from the tree since no vector  $\mathbf{x}$  verifying the constraints defined at this node (and

therefore at any sub-nodes) can yield an optimal solution. Unfortunately, the latter pruning rule is of poor practical interest since  $p^*$  is not available. Moreover evaluating  $p^\nu$  when  $\bar{\mathcal{S}} \neq \emptyset$  is also a combinatorial problem. To circumvent these problems, a relaxed version of the rule is devised: let  $p_l^\nu$  and  $p_u$  be respectively lower and upper bounds on  $p^\nu$  and  $p^*$ . Then, a sufficient condition to prune node  $\nu$  reads  $p_l^\nu > p_u$ .

To obtain  $p_l^\nu$ , a standard approach [15] is to consider the following relaxation of  $(P^\nu)$ :

$$p_l^\nu = \min_{\mathbf{x} \in \mathbb{R}^n} \frac{1}{2} \|\mathbf{y} - \mathbf{A}\mathbf{x}\|_2^2 + \frac{\lambda}{M} \|\mathbf{x}_{\bar{\mathcal{S}}}\|_1 + \lambda |\mathcal{S}_1| \quad (P_l^\nu)$$

s.t.  $\|\mathbf{x}\|_\infty \leq M$  and  $\mathbf{x}_{\mathcal{S}_0} = \mathbf{0}$

where the  $\ell_0$ -penalty term has been replaced by an  $\ell_1$ -norm. We emphasize that  $p_l^\nu \leq p^\nu$  since  $M^{-1} \|\mathbf{x}_{\bar{\mathcal{S}}}\|_1 \leq \|\mathbf{x}_{\bar{\mathcal{S}}}\|_0$  for all feasible vectors  $\mathbf{x}$ . Interestingly,  $(P_l^\nu)$  is a constrained LASSO problem [16] and can be solved (to machine precision) in polynomial time by using one of the many methods suitable for this class of problems [17, 18].

The upper bound  $p_u$  can be obtained by keeping track of the best known objective value of  $(P)$  during the BnB process. More precisely, we construct a feasible solution of  $(P^\nu)$  at each node to obtain a potentially better upper bound  $p_u^\nu$ . The best known upper bound is then updated as  $p_u \leftarrow \min(p_u, p_u^\nu)$ . During the BnB procedure,  $p_u$  converges toward  $p^*$  and relaxations are strengthened as new variables are fixed, allowing to prune nodes more effectively.

### 3.2. Branching step

If node  $\nu = (\mathcal{S}_0, \mathcal{S}_1, \bar{\mathcal{S}})$  has not been pruned during the bounding step, the tree exploration goes on. An index  $i \in \bar{\mathcal{S}}$  is selected according to some *branching rule* and two direct sub-nodes are created below  $\nu$  by imposing either “ $x_i = 0$ ” or “ $x_i \neq 0$ ”. Finally, when all nodes have been explored or pruned, the BnB algorithm stops and any candidate yielding the best upper bound  $p_u$  is a minimizer of  $(P)$ .

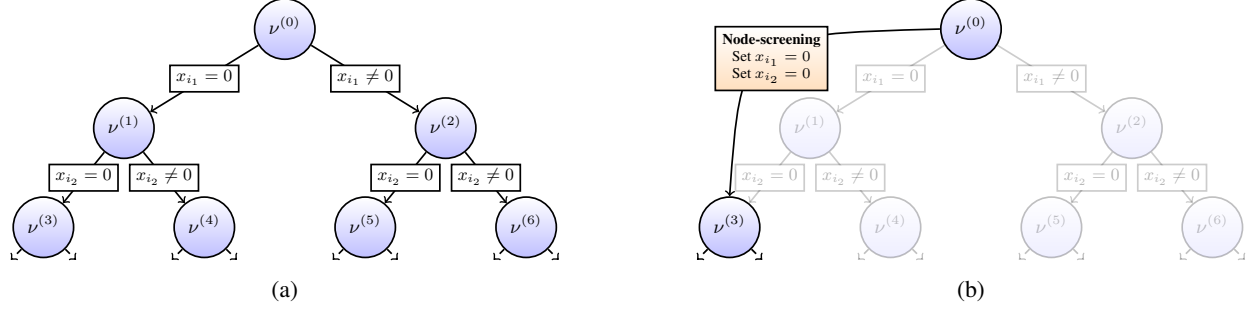
## 4. NODE-SCREENING TESTS

In this section, we present our new node-screening tests. They aim to identify, with marginal cost, nodes of the search tree that *cannot* yield a global minimum of  $(P)$ .

### 4.1. Dual properties

The crux of our procedure is a connection between the Fenchel dual problem of  $(P_l^\nu)$  at two consecutive nodes. Prior to expose this result, let us define for all  $\mathbf{u} \in \mathbb{R}^m$  and  $i \in \{1, \dots, n\}$  three families of *pivot values* as

$$\begin{aligned} \gamma_i(\mathbf{u}) &\triangleq M(|\mathbf{a}_i^T \mathbf{u}| - \frac{\lambda}{M}) \\ \gamma_i^0(\mathbf{u}) &\triangleq M[|\mathbf{a}_i^T \mathbf{u}| - \frac{\lambda}{M}]_+ \\ \gamma_i^1(\mathbf{u}) &\triangleq M[\frac{\lambda}{M} - |\mathbf{a}_i^T \mathbf{u}|]_+ \end{aligned} \quad (2)$$



**Fig. 1:** First nodes of the BnB tree. The root node  $\nu^{(0)}$  corresponds to problem  $(P)$  and each sub-node corresponds to a sub-problem  $(P^\nu)$  with different fixed variables. (a) Standard implementation of a BnB where all nodes are processed. (b) Impact of applying node-screening tests on the BnB search tree: at node  $\nu^{(0)}$ , test (6b) is passed for entries  $i_1$  and  $i_2$ ; one can thus directly switch to the sub-node including constraints “ $x_{i_1} = 0$ ” and “ $x_{i_2} = 0$ ”, namely  $\nu^{(3)}$ . The shaded nodes need not be explored.

where  $[z]_+ \triangleq \max(0, z)$  for all scalars  $z$ . We now express the Fenchel dual of  $(P_l^\nu)$  with respect to these quantities.

**Proposition 1.** *The Fenchel dual of  $(P_l^\nu)$  is given by*

$$d_l^\nu = \max_{\mathbf{u} \in \mathbb{R}^m} D_l^\nu(\mathbf{u}) \triangleq \frac{1}{2} \|\mathbf{y}\|_2^2 - \frac{1}{2} \|\mathbf{y} - \mathbf{u}\|_2^2 - \sum_{i \in \bar{S}} \gamma_i^0(\mathbf{u}) - \sum_{i \in S_1} \gamma_i(\mathbf{u}) \quad (D_l^\nu)$$

and strong duality holds for  $(P_l^\nu)$ -( $D_l^\nu$ ), i.e.,  $p_l^\nu = d_l^\nu$ . Moreover, if  $(\mathbf{x}_l^*, \mathbf{u}_l^*)$  is a couple of primal-dual solutions, one has

$$\mathbf{u}_l^* = \mathbf{y} - \mathbf{A}\mathbf{x}_l^*. \quad (3)$$

Hence, at a given node  $\nu$ , the dual objective of  $(P_l^\nu)$  is the sum of a term common to all nodes and some well-chosen pivot values. Interestingly, the dual objective function at two consecutive nodes only differs from one pivot value as shown in the following result:

**Corollary 1.** *Let  $\nu = (S_0, S_1, \bar{S})$  and  $\ell \in \bar{S}$ , then  $\forall \mathbf{u} \in \mathbb{R}^m$ ,*

$$D_l^{\nu \cup \{x_\ell=0\}}(\mathbf{u}) = D_l^\nu(\mathbf{u}) + \gamma_\ell^0(\mathbf{u}) \quad (4a)$$

$$D_l^{\nu \cup \{x_\ell \neq 0\}}(\mathbf{u}) = D_l^\nu(\mathbf{u}) + \gamma_\ell^1(\mathbf{u}) \quad (4b)$$

where  $\nu \cup \{x_\ell = 0\}$  and  $\nu \cup \{x_\ell \neq 0\}$  denote the two direct sub-nodes of  $\nu$  where index  $\ell$  has been swapped from  $\bar{S}$  to  $S_0$  or  $S_1$ , respectively.

#### 4.2. Node-screening tests

We now expose our proposed screening strategy to identify nodes of the tree that provably cannot yield a global minimizer of  $(P)$ . Let  $\nu$  be a node and  $p_u$  an upper bound on  $p^*$ . We have by strong duality between  $(P_l^\nu)$ -( $D_l^\nu$ ) that

$$\forall \mathbf{u} \in \mathbb{R}^m, \quad D_l^\nu(\mathbf{u}) \leq d_l^\nu = p_l^\nu \leq p^\nu. \quad (5)$$

Hence, combining (5) with Cor. 1 leads to the next result:

**Proposition 2.** *Let  $\ell \in \bar{S}$  be some index. Then,  $\forall \mathbf{u} \in \mathbb{R}^m$ ,*

$$D_l^\nu(\mathbf{u}) + \gamma_\ell^0(\mathbf{u}) > p_u \implies p^{\nu \cup \{x_\ell=0\}} > p^* \quad (6a)$$

$$D_l^\nu(\mathbf{u}) + \gamma_\ell^1(\mathbf{u}) > p_u \implies p^{\nu \cup \{x_\ell \neq 0\}} > p^*. \quad (6b)$$

Stated otherwise, Prop. 2 describes a simple procedure to identify some sub-nodes of  $\nu$  that cannot yield an optimal solution of  $(P)$ . In particular, if both (6a) and (6b) pass for a given index, no feasible vector with respect to the constraints defined at  $\nu$  is a minimizer of  $(P)$  and  $\nu$  can therefore be pruned.

Our proposed procedure differs from the pruning methodology described in Sec. 3 in several aspects. Performing a test only requires the evaluation of one single inner product. They can therefore be implemented at marginal cost compared to the overall cost of the bounding step. Very importantly, they also inherit from the following *nesting property*:

**Corollary 2.** *Let  $\nu = (S_0, S_1, \bar{S})$  be a node. Then, if test (6a) or (6b) passes for index  $\ell \in \bar{S}$ , then it also passes for any sub-node  $\nu' = (S'_0, S'_1, \bar{S}')$  of  $\nu$  such that  $\ell \in \bar{S}'$ .*

In particular, Cor. 2 has the following consequence. Assume that two distinct indexes  $\ell$  and  $\ell'$  pass test (6a) at node  $\nu$ . Then index  $\ell'$  will also pass (6a) at node  $\nu \cup \{x_\ell \neq 0\}$ . The same consequence holds for test (6b) and node  $\nu \cup \{x_\ell = 0\}$ . In other words, if several node-screening tests pass at a given node, one can *simultaneously* prune several sub-nodes of  $\nu$ , as illustrated in Fig. 1b. This is in contrast with the bounding procedure described in Sec. 3 which has to process each sub-node individually before applying any potential pruning operation.

#### 4.3. Implementation considerations

Implementing node-screening tests described by Prop. 2 requires the knowledge of an upper bound  $p_u$  of  $p^*$  and a suitable  $\mathbf{u} \in \mathbb{R}^m$ , i.e., as close as possible to the maximizer of  $(D_l^\nu)$ . The value of  $p_u$  can be obtained at no additional

cost since the standard implementation of BnB already requires storing such valid upper bounds on  $p^*$ . To obtain a relevant candidate for  $\mathbf{u}$ , we suggest the following procedure: assuming the method used to solve  $(P_l^\nu)$  generates a sequence of iterates  $\{\mathbf{x}^{(t)}\}_{t \in \mathbb{N}}$  that converges to a global minimizer, we set

$$\forall t \in \mathbb{N}, \quad \mathbf{u}^{(t)} = \mathbf{y} - \mathbf{A}\mathbf{x}^{(t)}. \quad (7)$$

This choice enjoys two desirable properties. First, the sequence  $\{\mathbf{u}^{(t)}\}_{t \in \mathbb{N}}$  converges toward a maximizer of  $(D_l^\nu)$  as a consequence of the optimality condition (3). Second, both  $\mathbf{u}^{(t)}$  and  $\mathbf{A}^\top \mathbf{u}^{(t)}$  are already evaluated by most solvers as they correspond to the residual error and the (negative) gradient of the least-squares term of the objective function, respectively. Thus, the computational cost of evaluating the screening tests at all undecided entries is marginal as compared to the cost needed to address  $(P_l^\nu)$ . The latter choice for  $\mathbf{u}^{(t)}$  suggests performing node-screening tests *during* the bounding step. Hence, when some entries passes the test at node  $\nu$ , the BnB algorithm immediately switches to some sub-node, without solving  $(P_l^\nu)$  at high precision.

## 5. NUMERICAL RESULTS

We finally report simulation results illustrating the relevance of the node-screening methodology on two different setups.

### 5.1. Experimental setups

For each trial, we generate a new realization of  $\mathbf{A} \in \mathbb{R}^{m \times n}$  and  $\mathbf{y} \in \mathbb{R}^m$  as follows. In the *Gaussian* setup, we set  $(m, n) = (500, 1000)$  and the entries of  $\mathbf{A}$  are i.i.d. realizations of a normal distribution. In the *Tœplitz* setup, we set  $(m, n) = (500, 300)$  and the first column of  $\mathbf{A}$  contains a sampled sinc function. The other columns are obtained by shifting the entries in a row-wise fashion so that  $\mathbf{A}$  inherits from a Tœplitz structure. In both setups, the columns of  $\mathbf{A}$  are normalized to one. To obtain  $\mathbf{y}$ , we first sample a  $k$ -sparse vector  $\mathbf{x}^0 \in \mathbb{R}^n$  with uniformly distributed non-zero entries. Each non-zero entry is set to  $s(1 + |a|)$ , where  $s \in \{-1, +1\}$  is a random sign and  $a$  is a realization of the normal distribution. In our experiment, we chose  $k \in \{5, 7, 9\}$ . Finally, the observation is constructed as  $\mathbf{y} = \mathbf{A}\mathbf{x}^0 + \epsilon$  where the entries of  $\epsilon$  are i.i.d. realizations of a centered Gaussian distribution with standard deviation  $\sigma = \|\mathbf{A}\mathbf{x}^0\|_2 / \sqrt{10m}$ . Such a design leads to a SNR of 10dB in average [19]. We tune  $\lambda$  statistically as in [20], i.e., by setting  $\lambda = 2\sigma^2 \log(n/k - 1)$ . Finally, we empirically set  $M = 1.5\|\mathbf{A}^\top \mathbf{y}\|_\infty$  as advised in [10].

We compare three methods that address  $(P)$ : *i*) `Direct`, that uses CPLEX [9], a state-of-the-art commercial MIP solver; *ii*) `BnB`, the algorithm presented in [10], which is (up to our knowledge) the fastest BnB algorithm tailored to  $(P)$ ; *iii*) `BnB+scr` which corresponds to `BnB` enhanced with the node-screening methodology presented in Sec. 4. Note that

both `BnB` and `BnB+scr` leverage an efficient implementation of the Active-Set algorithm [21, Sec. 16.5] to solve  $(P_l^\nu)$  and the branching rule described in [10, Sec. 2.2].

Experiments are run on a MacOS with an i7 CPU, clocked at 2.2 GHz and with 8Go of RAM. We restrict calculations on a single core to avoid bias due to parallelization capabilities. The Academic Version 20.1 of CPLEX is used and both `BnB` and `BnB+scr` are implemented in Julia v1.5 [22]. Results are averaged over 100 instances of problem  $(P)$ .

### 5.2. Method comparison

Table 1 compares the average number of nodes treated (i.e., the number of relaxations  $(P_l^\nu)$  solved at machine precision) and the optimization time for the three methods and all simulation setups. One observes that `BnB+scr` outperforms the two other methods on all scenarios and all figures of merit. We also note that, compared to `BnB`, the reduction in the optimization time is more significant than the reduction in the number of processed nodes. A thorough examination of our results indicates that the bounding step is performed all the faster as many variables are set to zero in  $(P_l^\nu)$ . Our node-screening methodology allows to reach quickly nodes where the bounding step is performed with a lower computational cost.

As a final remark, we mention that `Direct` relies on an efficient C++ implementation while `BnB` and `BnB+scr` are implemented in Julia. As C++ usually runs faster than Julia, there is still room for improvements in the comparison of `BnB` and `BnB+scr` with `Direct`.

	$k$	Direct			BnB			BnB+scr		
		N	T	F	N	T	F	N	T	F
Gaussian	5	96	25.9	0	70	1.5	0	<b>56</b>	<b>0.7</b>	<b>0</b>
	7	292	60.8	0	180	5.1	0	<b>152</b>	<b>3.0</b>	<b>0</b>
	9	781	102.6	10	483	15.6	0	<b>412</b>	<b>9.8</b>	<b>0</b>
Tœplitz	5	1,424	10.2	0	965	6.4	0	<b>725</b>	<b>4.2</b>	<b>0</b>
	7	17,647	106.5	0	10,461	79.3	0	<b>7,881</b>	<b>52.2</b>	<b>0</b>
	9	80,694	353.4	50	47,828	346.4	48	<b>41,166</b>	<b>267.0</b>	<b>40</b>

**Table 1:** Number of nodes explored (N), optimization time in seconds (T) and number of instances not solved within  $10^3$  seconds (F).

## 6. CONCLUSION

In this paper, we presented a novel node-screening methodology aiming to accelerate the resolution of the  $\ell_0$ -penalized least-squares problem with a branch-and-bound solver. Our contribution leverages a nesting property between the node-screening tests at two consecutive nodes. Our method leads to significant improvements in terms of number of nodes explored and optimization time on two simulated datasets.

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