Sparsity Constrained Nonlinear Optimization:
Optimality Conditions and Algorithms

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The Sparsity Constrained Problem

\[(P): \min \quad f(x) \quad \text{s.t.} \quad \|x\|_0 \leq s\]

- \(f\) - continuously differentiable function.
- \(s\) - a positive integer \((s \ll n)\).
- \(\|x\|_0 = \#\{i : x_i \neq 0\}\) - number of nonzero elements.
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Problem \((P)\) is a difficult nonconvex, noncontinuous problem.
The basic problem in CS is:

**Compressive Sensing:** Find a sparse vector $x$ satisfying the underdetermined linear system $Ax = b$ ($m \ll n$).

- Under suitable conditions on $A$, only $s \log n$ measurements are needed to recover $x$. [Donoho]
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- When noise is present it is natural to consider problem (P) with
  \[ f(x) = f_{LI}(x) \equiv \|Ax - b\|^2 \]

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- When noise is present is is natural to consider problem $(P)$ with $f(x) = f_{LI}(x) \equiv \|Ax - b\|^2$

$$\min \|Ax - b\|^2$$
$$\text{s.t. } \|x\|_0 \leq s$$

- Other formulations:

$$\min \|x\|_0$$
$$\text{s.t. } \|Ax - b\|^2 \leq \rho$$

$$\min \{\|Ax - b\|^2 + \lambda \|x\|_0\}$$
Algorithms for "solving" CS:

- **Greedy-based**: Matching Pursuit (MP) [Mallat & Zhang, 93'] and Orthogonal Matching pursuit (OMT) [Mallat 99'] (sequentially "discovering" the support).
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- **Iterative Hard Thresholding (IHT)**: [Blumensath, Davies 04’]

\[ x^{k+1} = H_s(x^k - A^T(Ax - b)) \]

\( H_s \) - hardthresholding operator.

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- Many more... (StOMP, CoSAMP) (Needell, Tropp, Starck, Wright, Elad...)
Given $m$ symmetric matrices $A_1, \ldots, A_m$, find a vector $x$ satisfying:

\[ x^T A_i x \approx c_i, \quad i = 1, \ldots, m \]

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Can be formulated as problem (P) with

$$ f(x) = f_{QU}(x) = \sum_{i=1}^{m} (x^T A_i x - c_i)^2 $$

$$ \min \quad \sum_{i=1}^{m} (x^T A_i x - c_i)^2 $$

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2nd Prototype Example - Recovery from Quadratic Meas.

Given \( m \) symmetric matrices \( \mathbf{A}_1, \ldots, \mathbf{A}_m \), find a vector \( \mathbf{x} \) satisfying:

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\]

- sub-wavelength optical imaging (Shechtman, Eldar, Szameit, Segev): SDR based.
- phase retrieval (recovery of a signal from the magnitude of its Fourier transform). Many many works (on the non-sparse version).
Main Objectives

(P): \[ \min_{x} f(x) \quad \text{s.t.} \quad \|x\|_0 \leq s \]

- Develop necessary optimality conditions for problem (P).
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- Develop necessary optimality conditions for problem (P).
- Construct algorithms aimed to find points satisfying the optimality conditions.
Part I: Optimality Conditions
**Definition** A vector \( x^* \in C_s \) is called a basic feasible (BF) vector of (P) if:

- when \( \| x^* \|_0 < s \), \( \nabla f(x^*) = 0 \);
- when \( \| x^* \|_0 = s \), \( \nabla_i f(x^*) = 0 \) for all \( i \in l_1(x^*) \).

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Result: $\mathbf{x}^*$ optimal solution of (P) $\Rightarrow \mathbf{x}^*$ basic feasible.
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Example:

- $f = f_{LI}$, $A$ is $s$-regular (any $s$ columns are linearly independent $\equiv \text{spark}(A) \geq s + 1$).
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Here each choice of a support $S \subseteq \{1, 2, \ldots, n\}$ with $|S| \leq s$ gives rise to a single BF solution:

$$x_S = (A_S^T A_S)^{-1} A_S^T b$$
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- Only a finite number of BF vectors in this setting.
2nd Optimality Condition: Stationarity

Well known optimality conditions for convex-constrained differentiable problem:

\[ \text{(M)}: \quad \min_{\mathbf{x}} \ f(\mathbf{x}) \quad \text{s.t.} \quad \mathbf{x} \in C \]

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Equivalently: \(x^*\) is a stationary point iff

\[(S_2) \quad x^* = P_C \left( x^* - \frac{1}{L} \nabla f(x^*) \right)\]

\[P_C(y) = \arg\min_{x \in C} \|x - y\|^2\] - orthogonal projection onto \(C\) (unique).
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\( (S_1) \Leftrightarrow (S_2) \) independently of \( L \).

For Problem \( P \) we can generalize \( (S_2) \) (not \( (S_1) \)), but...
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**Definition.** $\mathbf{x}^*$ is an $L$-stationary point of (P) if

$$[\text{NC}_L] \quad \mathbf{x}^* \in P_{C_s} \left( \mathbf{x}^* - \frac{1}{L} \nabla f(\mathbf{x}^*) \right).$$

$$C_s = \{ \mathbf{x} \in \mathbb{R}^n : \|\mathbf{x}\|_0 \leq s \}$$
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\[C_s = \{ x \in \mathbb{R}^n : \| x \|_0 \leq s \}\]

- \( P_{C_s} = H_s \) is the **hard thresholding** operator which is a multivalued mapping, e.g.,

\[
P_{C_2}( (2, 1, 1)^T ) = \{ (2, 1, 0)^T, (2, 0, 1)^T \}.
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A more explicit condition

**Lemma:** \( x^* \) is an \( L \)-stationary point iff

\[
|\nabla_i f(x^*)| \begin{cases} \leq LM_s(x^*) & \text{if } i \in l_0(x^*), \\ = 0 & \text{if } i \in l_1(x^*). \end{cases}
\]

\( l_0(x^*) = \{ i : x_i^* = 0 \}, M_s(x^*) \) - \( s \)-th largest absolute value component.
\( \mathbf{x}^* \) \( L \)-stationary \( \Rightarrow \) \( \mathbf{x}^* \) is BF.
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**Stationarity Level:**

If $\|x^*\|_0 < s$, then $S_L(x^*) = 0$.

If $\|x^*\|_0 = s$, then

$$SL(x^*) \equiv \max_{i \in I_0(x^*)} \frac{\nabla_i f(x^*)}{M_s(x^*)}.$$
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**Question:** for what values of $L$ is $L$-stationarity a necessary optimality condition?
We will occasionally (but not always!) make the following assumption:

**The Lipschitz Assumption.** \( \nabla f \) is Lipschitz with constant \( L(f) \) over \( \mathbb{R}^n \):

\[
\| \nabla f(x) - \nabla f(y) \| \leq L(f) \| x - y \| \quad \text{for every} \ x, y \in \mathbb{R}^n.
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- Satisfied for $f = f_{LI}$ with $L(f) = 2\lambda_{\max}(A^T A)$.
- Not satisfied for $f = f_{QU}$.
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- Not satisfied for \( f = f_{QU} \).

**Theorem.** Lipschitz assumption holds + \( L > L(f) \) \( \Rightarrow \)

\( x^* \) optimal solution \( \Rightarrow x^* \) is an \( L - \) stationary point.
Is there a method able to find an $L$-stationary point for $L > L(f)$?

Is it possible to prove that $L$-stationarity is a necessary optimality condition for some $L \leq L(f)$?

Is there a better optimality condition, relevant also when the Lipschitz assumption does not hold?
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- Is it possible to prove that $L$-stationarity is a necessary optimality condition for some $L \leq L(f)$?
- Is there a better optimality condition, relevant also when the Lipschitz assumption does not hold?

The answer to all questions is YES!!
A definition of local minimum: cannot improve the objective by making a change of at most two coordinates.

**Definition.** Let $\mathbf{x}^*$ be a feasible solution of (P). Then $\mathbf{x}^*$ is called a coordinate-wise (CW) minimum of (P) if one of the following cases hold true:

**Case I:** $\|\mathbf{x}^*\|_0 < s$ and for every $i = 1, 2, \ldots, n$ one has:

$$f(\mathbf{x}^*) = \min_{t \in \mathbb{R}} f(\mathbf{x}^* + t\mathbf{e}_i).$$

**Case II:** $\|\mathbf{x}^*\|_0 = s$ and for every $i \in I_1(\mathbf{x}^*), j = 1, 2, \ldots, n$:

$$f(\mathbf{x}^*) \leq \min_{t \in \mathbb{R}} f(\mathbf{x}^* - x_i^* \mathbf{e}_i + t\mathbf{e}_j).$$
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- $x^*$ optimal solution $\Rightarrow$ $x^*$ CW minimum.
- $x^*$ CW-minimum $\Rightarrow$ $x^*$ BF vector.
Remarks on CW-minima

- CW-minimality is a necessary optimality condition regardless of the validity of the Lipschitz assumption.
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- Easy to check CW-minimality for the linear \((f = f_{LI})\) and quadratic \((f = f_{QU})\) cases. In the latter case it amounts to solving a cubic equation.
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Easy to check CW-minimality for the linear \( f = f_{LI} \) and quadratic \( f = f_{QU} \) cases. In the latter case it amounts to solving a cubic equation.

Under the Lipschitz assumption, is there a relation between CW-minimality to \( L(f) \)-stationarity?
Under the Lipschitz assumption,

- For any $i \neq j$ there exists a $L_{i,j}(f)$ for which:

  $$\|\nabla_{i,j} f(x) - \nabla_{i,j} f(x + d)\| \leq L_{i,j}(f)\|d\|,$$

  for any $d \in \mathbb{R}^n$ satisfying $d_k = 0$ for any $k \neq i, j$. 


Local Lipschitz Constant

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- The Local Lipschitz constant is

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L_2(f) = \max_{i \neq j} L_{i,j}(f)
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- $L_2(f) \leq L(f)$.

Example: $f(x) = x^TQx + 2b^Tx$ with $Q_n = I_n + J_n$ ($I_n$ - identity, $J_n$ - all ones)
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**Example:** \( f(x) = x^T Q x + 2b^T x \) with \( Q_n = I_n + J_n \) (\( I_n \) - identity, \( J_n \) - all ones)

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L(f) = 2 \lambda_{\text{max}}(Q_n) = 2(n + 1)
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On the other hand,

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L_{i,j}(f) = 2 \lambda_{\text{max}} \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} = 6
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We got: $L(f) = 2(n + 1), L_2(f) = 6$
**Theorem.** Suppose that the Lipschitz assumption holds. If $x^*$ is a CW-minimum, then it is also an $L_2(f)$—stationary point:

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|\nabla_i f(x^*)| \begin{cases} 
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without Lip. assumption

optimal solution of (P) \\[\downarrow\]
CW-minimum of (P) \\[\downarrow\]
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with Lip. assumption

optimal solution of (P)  \downarrow  
CW-minimum of (P)  \downarrow  
$L_2(f)$—stationary  \downarrow  
BF vector of (P)
Example

\[ f(x) = x^T Q x + 2b^T x \]  
with

\[ Q = I_5 + J_5, \quad b = -(3, 2, 3, 12, 5)^T \]

10 BF vectors:

\[ x_1 = (1.3333, 0.3333, 0, 0, 0)^T, \]
\[ x_2 = (1.0000, 0, 1.0000, 0, 0)^T, \]
\[ x_3 = (-2.0000, 0, 0, 7.0000, 0)^T, \]
\[ x_4 = (0.3333, 0, 0, 0, 2.3333)^T, \]
\[ x_5 = (0, 0.3333, 1.3333, 0, 0)^T, \]
\[ x_6 = (0, -2.6667, 0, 7.3333, 0)^T, \]
\[ x_7 = (0, -0.3333, 0, 0, 2.6667)^T, \]
\[ x_8 = (0, 0, -2.0000, 7.0000, 0)^T, \]
\[ x_9 = (0, 0, 0.3333, 0, 2.3333)^T, \]
\[ x_{10} = (0, 0, 0, 6.3333, -0.6667)^T. \]
Function values and stationarity levels:

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$L_2(f) = 6$ and therefore only $x_3, x_6, x_8$ are candidates for optimal solutions.
Function values and stationarity levels:

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- $L_2(f) = 6$ and therefore only $x_3, x_6, x_8$ are candidates for optimal solutions.
- $L(f) = 12 \Rightarrow$ the previous weaker result would also imply that $x_{10}$ is a candidate.
Function values and stationarity levels:

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- $L_2(f) = 6$ and therefore only $x_3, x_6, x_8$ are candidates for optimal solutions.
- $L(f) = 12 \Rightarrow$ the previous weaker result would also imply that $x_{10}$ is a candidate.
- Only $x_6$ is a CW minima.
Previous Questions, Answers and Questions

Previous Questions:

- Is there a method able to find an $L$-stationary point for $L > L(f)$?
  YES - not yet shown

- Is it possible to prove that $L$-stationarity is a necessary optimality condition for some $L \leq L(f)$? YES

- Is there a better optimality condition, relevant also when the Lipschitz assumption does not hold? YES
Previous Questions:

- Is there a method able to find an $L$-stationary point for $L > L(f)$?  
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- Is it possible to prove that $L$-stationarity is a necessary optimality condition for some $L \leq L(f)$?  
  YES

- Is there a better optimality condition, relevant also when the Lipschitz assumption does not hold?  
  YES

New Question:

- Is there a method able to find a CW minima?  
  YES - not yet shown
Part II: Algorithms
Two types of methods:

- **Iterative Hard-Thresholding** based on $L$-stationarity.
- **Sparse-simplex methods** coordinate descent-type method based on CW-minimality.
IHT is a fixed point method for solving the $L$-stationarity condition:

\[
\left[ \text{NC}_L \right] \quad x^* \in P_{C_s} \left( x^* - \frac{1}{L} \nabla f(x^*) \right).
\]

**IHT** ($L > L(f)$)

\[
x^{k+1} = P_{C_s} \left( x^k - \frac{1}{L} \nabla f(x^k) \right).
\]
IHT is a fixed point method for solving the $L$-stationarity condition:

$$[NC_L] \quad x^* \in P_{C_s} \left( x^* - \frac{1}{L} \nabla f(x^*) \right).$$

**IHT ($L > L(f)$)**

$$x^{k+1} = P_{C_s} \left( x^k - \frac{1}{L} \nabla f(x^k) \right)$$

**Theorem.** Any accumulation point of is an $L$-stationary point ($L > L(f)$).
IHT when $f = f_{LI}$

**Theorem.** When $f = f_{LI}$, $L > L(f)$, the sequence generated by IHT method with stepsize $\frac{1}{L}$ converges.

Blumensath and Davies [04’]: convergence for $f = f_{LI}$ with $\|A\| < 1$ and stepsize $1/2$. 
**Theorem.** When \( f = f_{LI} \), \( L > L(f) \), the sequence generated by IHT method with stepsize \( \frac{1}{L} \) converges.

Blumensath and Davies [04']: convergence for \( f = f_{LI} \) with \( \|A\| < 1 \) and stepsize 1/2.

**Drawbacks**

- The method is not guaranteed to generate \( L_2(f) \)-stationary points.
- Relevant only under Lip. assumption.
- Requires knowledge on the Lipschitz constant.
- Sensitive to the choice of \( L \).
Example

\[
\min \left\{ f(x_1, x_2) = 12x_1^2 + 20x_1x_2 + 32x_2^2 : \| (x_1; x_2)^T \|_0 \leq 1 \right\}
\]

\[
L(f) = 48.3961
\]

Two BF vectors: \((0, -9/16)\) - optimal solution. \((-1/12, 0)\) - non-optimal, SL=196.
The Greedy Sparse-Simplex (GSS) Method

- Aims at finding a CW-minimum.
- does not require a knowledge (or existence) of a Lipschitz constant.
- At each iteration finds the best change in at most two coordinates (best = lowest value).
- If the Lipschitz assumption holds, it is guaranteed to find $L_2(f)$-stationary points.
The GSS Method - Description

- **Initialization:** Choose $x_0 \in C_s$.

- **General step:** ($k = 0, 1, \ldots$)
  - If $\|x^k\|_0 < s$, then compute for every $i = 1, 2, \ldots, n$
    
    $$
    t_i \in \text{argmin}_{t \in \mathbb{R}} f(x^k + te_i), f_i = \min_{t \in \mathbb{R}} f(x^k + te_i).
    $$

    Let $i_k \in \text{argmin}_{i=1,\ldots,n} f_i$. If $f_{i_k} < f(x^k)$, then set
    $$
    x^{k+1} = x^k + t_{i_k} e_{i_k}.
    $$

    Otherwise, STOP.

  - If $\|x^k\|_0 = s$, then for every $i \in l_1(x^k)$ and $j = 1, \ldots, n$ compute
    
    $$
    t_{i,j} \in \text{argmin}_{t \in \mathbb{R}} f(x^k - x_i^k e_i + te_j), f_{i,j} = \min_{t \in \mathbb{R}} f(x^k - x_i^k e_i + te_j).
    $$

    Let $(i_k, j_k) \in \text{argmin}\{f_{i,j} : i \in l_1(x^k), j = 1, \ldots, n\}$. If $f_{i_k,j_k} < f(x^k)$,
    then set
    $$
    x^{k+1} = x^k - x_{i_k}^k e_{i_k} + t_{i_k,j_k} e_{j_k}.
    $$

    Otherwise, STOP.
At each iteration the algorithm explores all possible changes of at most two variables:

- **if** $\|x^k\|_0 < s$: changes the coordinate resulting with the largest decrease.
- **if** $\|x^k\|_0 = s$: two options:
  1. changes the coordinate in the support with the largest decrease.
  2. makes the “best” swap: removes a variable from the support and adds a new variable to the support (while optimizing it).
At each iteration the algorithm explores all possible changes of at most two variables:

- if $\|x^k\|_0 < s$: changes the coordinate resulting with the largest decrease.
- if $\|x^k\|_0 = s$: two options:
  1. changes the coordinate in the support with the largest decrease.
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- $n$ 1D minimizations when $\|x\|_0 < s$.
- $sn$ 1D minimizations when $\|x\|_0 = s$. 
Theorem: Any Accumulation point of the GSS method is a CW-minimum.
Theorem: Any Accumulation point of the GSS method is a CW-minimum.

Consequently,

Corollary: Under the Lipschitz assumption, any Accumulation point of the GSS method is an $L_2(f)$-stationary point.
Matching Pursuit

Initialization: \( r^0 = b, x^0 = 0 \).
for \( k = 1 : s \)

1. \( m \in \arg\max_{i=1,...,n} \frac{|a_i^T r^k|}{\|a_i\|} \).
2. \( x^{k+1} = x^k - \frac{a_m^T r^k}{\|a_m\|^2} e_m \).
3. \( r^{k+1} = r^k - \frac{a_m^T r^k}{\|a_m\|^2} a_m \).
Matching Pursuit

Initialization: \( r^0 = b, x^0 = 0 \).

for \( k = 1 : s \)

\[ m \in \text{argmax}_{i=1,\ldots,n} \frac{|a_i^T r^k|}{\|a_i\|}. \]

\[ x^{k+1} = x^k - \frac{a_m^T r^k}{\|a_m\|^2} e_m. \]

\[ r^{k+1} = r^k - \frac{a_m^T r^k}{\|a_m\|^2} a_m \]

The MP method coincides with the GSS method when started with the zeros vector for the first \( s \) iterations, BUT

- No need to start with the zeros vector in GSS.
- GSS allows removal of variables from the support (regret...) while the MP does not.
- GSS continues also when the maximal support is achieved.
Simulation details

- $f = f_{LI}$.
- 1000 realizations of $A \in \mathbb{R}^{4 \times 5}$, $b \in \text{Range}(A)$.
- GSS was initiated with the zeros vector.
Simulation details

- \( f = f_{LI} \).
- 1000 realizations of \( A \in \mathbb{R}^{4 \times 5}, b \in \text{Range}(A) \).
- GSS was initiated with the zeros vector.

Results:

- MP found the correct support in 452 cases. GSS found the correct vector in 652 cases.
Simulation details

- $f = f_{\text{LI}}$.
- 1000 realizations of $\mathbf{A} \in \mathbb{R}^{4 \times 5}$, $\mathbf{b} \in \text{Range}(\mathbf{A})$.
- GSS was initiated with the zeros vector.

Results:

- MP found the correct support in 452 cases. GSS found the correct vector in 652 cases.
- When allowing GSS start from 5 different random initial vectors, it found the correct vector in 952 cases.
The Partial Sparse-Simplex (PSS) Method

The GSS method:
- Finds a CW-minimum, but...
- Drawback: has no index selection strategy resulting with $sn$ 1D minimizations.
The GSS method:
- Finds a CW-minimum, but...
- Drawback: has no index selection strategy resulting with \( sn \) 1D minimizations.

The partial sparse-simplex (PSS) method replaces all SWAPS with a single SWAP:

**The SWAP stage in PSS:**
- the variable leaving the support is the one with the minimal absolute value

\[
i \in \arg\min\{|x_i^k| : i \in I_1(x^k)\}
\]

- the variable entering the support is the one corresponding to the maximal absolute value partial derivative.

\[
j \in \arg\max\{|\nabla_j f(x^k)| : j \in I_0(x^k)\}
\]
Under the general setting:

**Lemma.** Any accumulation point of the PSS method is a BF-vector.
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**Lemma.** Any accumulation point of the PSS method is a BF-vector.

- We cannot prove convergence to a CW-minima, but...
The PSS method - Results

Under the general setting:

**Lemma.** Any accumulation point of the PSS method is a BF-vector.

- We cannot prove convergence to a CW-minima, but...

**Theorem.** Under the Lipschitz assumption, any accumulation point of the PSS method is an $L_2(f)$-stationary point.

- Better than IHT.
- Much less computations.
Numerical Results

- $f = f_{LI}$ with $A \in \mathbb{R}^{4 \times 5}$ (random).
- IHT with $L = 1.1L(f)$.
- IHT with $L = 2L(f)$.
- GSS
- PSS

1000 randomly generated initial vectors.

<table>
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<tr>
<th>BF vector $(i)$</th>
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<tbody>
<tr>
<td>$N_1(i)$</td>
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<td>50</td>
<td>63</td>
<td>92</td>
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<td>0</td>
<td>130</td>
<td>0</td>
<td>61</td>
<td>46</td>
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<tr>
<td>$N_2(i)$</td>
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<td>89</td>
<td>256</td>
<td>0</td>
<td>187</td>
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<td>69</td>
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<td>0</td>
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<td>0</td>
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<td>93</td>
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<td>43</td>
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</table>
Numerical Results

Quadratic equations:

\[(a_i^T x)^2 = c_i, \quad i = 1, 2, \ldots, m\]

\[\|x\|_0 \leq s\]

- \(m = 80, n = 120\).
- \(s = 3, 4, \ldots, 10\).
- 100 randomly generated initial vectors.

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<tr>
<th>s</th>
<th>(N_{PSS})</th>
<th>(N_{GSS})</th>
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THANK YOU FOR YOUR ATTENTION