AMATH 840: Advanced Numerical Methods for Computational and Data Science

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Part 1: Sparse Optimization and Compressive Sensing 1.2: ℓ_0 -Optimization Methods

Winter 2024

Problem: Given $A \in \mathbb{C}^{m \times n}$ and $\mathbf{y} \in \mathbb{C}^m$. Find

$$\mathbf{w} \in \mathbb{C}^n$$
 such that $\mathbf{y} = A\mathbf{w}$ and $\|\mathbf{w}\|_0 \leq s$.

We will go over three important algorithms:

- Orthogonal Matching Pursuit (OMP)
- Iterative Hard Thresholding (IHT)
- Hard Thresholding Pursuit (HTP)

We use the same numbers of Theorems, Lemmas, Propositions from Chapter 3 in "A Mathematical Introduction to Compressive Sensing", by S. Foucart and H. Rauhut.

Orthogonal Matching Pursuit (OMP)

Iterative Hard Thresholding (IHT)

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Orthogonal Matching Pursuit (OMP)

Problem: Given $A \in \mathbb{C}^{m \times n}$ and $\mathbf{y} \in \mathbb{C}^m$. Find

$$\mathbf{w} \in \mathbb{C}^n$$
 such that $\mathbf{y} = A\mathbf{w}$ and $\|\mathbf{w}\|_0 \leq s$.

Main Idea of OMP: Initialize $S^0 = \emptyset \subseteq [n] := \{1, 2, \dots, n\}.$

• Add one index to a target support $S^k \subseteq [n]$ at each iteration, $S^{k+1} = S^k \cup \{j_{k+1}\}$, so that

$$\min_{\sup p(z) \subseteq \mathcal{S}^{k+1}} \|\mathbf{y} - A\mathbf{z}\|_2 \le \min_{\sup p(z) \subseteq \mathcal{S}^k} \|\mathbf{y} - A\mathbf{z}\|_2$$

• Update a target vector **w**^{k+1}:

$$\mathbf{w}^{k+1} := \operatorname*{argmin}_{\sup p(z) \subseteq \mathcal{S}^{k+1}} \|y - Az\|_2.$$

In the next few slides, we will derive the steps of OMP.

Lemma 3.3. Given $A = [\mathbf{a}_1 \, \mathbf{a}_2 \dots \mathbf{a}_n] \in \mathbb{C}^{m \times n}$ such that $\|\mathbf{a}_k\|_2 = 1$, $\forall k$. Given $S \subseteq [n]$ and $j \in [n]$. If $\mathbf{w} := \operatorname{argmin}\{\|\mathbf{y} - A\mathbf{z}\|_2 : \operatorname{supp}(\mathbf{z}) \subseteq S \cup \{j\}\},\$ then $\|\mathbf{y} - A\mathbf{w}\|_2^2 \le \|\mathbf{y} - A\mathbf{v}\|_2^2 - |(A^*(\mathbf{y} - A\mathbf{v}))_j|^2,\$ for all $\mathbf{v} \in \mathbb{C}^n$ s.t. $\operatorname{supp}(\mathbf{v}) \subseteq S.$

 $\Rightarrow \text{OMP Algorithm: Choose } j = \arg \max_{j \in [n]} |(A^*(\mathbf{y} - A\mathbf{v}))_j|.$

Proof.

See the Appendix.

Orthogonal Matching Pursuit

For $z \in \mathbb{C}^n$ and $S \subseteq [n]$, denote $v_S := v|_S \in \mathbb{C}^{|S|}$, the restriction of v onto the index set S.

Lemma 3.4. Given an index set $S \subseteq [n]$. If $\mathbf{v} := \underset{\mathbf{z} \in \mathbb{C}^n}{\operatorname{argmin}} \{ \|\mathbf{y} - A\mathbf{z}\|_2, \operatorname{supp}(\mathbf{z}) \subseteq S \},$ then $A_S^* \mathbf{y} = A_S^* A_S \mathbf{v}_S, \quad \text{i.e.}, \quad (A^* (\mathbf{y} - A\mathbf{v}))_S = 0.$

 \Rightarrow OMP algorithm:

$$\begin{split} \mathbf{w}^{k+1} &:= \operatorname*{argmin}_{\operatorname{supp}(\mathbf{z}) \subseteq S^{k+1}} \|\mathbf{y} - A\mathbf{z}\|_2 \\ \mathbf{w}^{k+1}_{S^{k+1}} &= A^{\dagger}_{S^{k+1}}\mathbf{y}. \end{split}$$

Orthogonal Matching Pursuit

Input: Measurement matrix $A \in \mathbb{C}^{m \times n}$ with ℓ_2 -normalized columns, measurement vector $\mathbf{y} \in \mathbb{C}^m$, sparsity level *s* or tolerance ε .

Initialization: $S^0 = \emptyset$, $w^0 = 0$.

Iteration: Repeat until Stopping Criterion is met.

 $\begin{aligned} j_{k+1} &:= \arg \max_{j \in [n]} \{ | (A^* (\mathbf{y} - A\mathbf{w}^k))_j | \} \\ \mathcal{S}^{k+1} &:= \mathcal{S}^k \cup \{ j_{k+1} \} \\ \text{Find } \mathbf{w}^{k+1} \text{ s.t } A^*_{\mathcal{S}^{k+1}} \mathbf{y} = A^*_{\mathcal{S}^{k+1}} A_{\mathcal{S}^{k+1}} \mathbf{w}^{k+1}_{\mathcal{S}^{k+1}} \end{aligned}$

Output: The sparse vector $\mathbf{w}^{\#}$.

OMP

import numpy as np
from sklearn.linear_model import OrthogonalMatchingPursuit as omp

Remarks about ℓ_2 -normalized columns of the measurement matrix A:

• It is not strictly required. However, if we work with a general matrix A, we need to adjust the steps in the iterations accordingly.

• For
$$A = [\mathbf{a}_1 \, \mathbf{a}_2 \, \dots \mathbf{a}_n] \in \mathbb{C}^{m \times n}$$
 and $\mathbf{w} = [w_1, w_2, \dots, w_n]^T \in \mathbb{C}^n$, we have

$$A\mathbf{w} = \sum_{k=1}^{n} w_k \mathbf{a}_k = \sum_{k=1}^{n} \left(w_k \|\mathbf{a}_k\|_2 \right) \frac{\mathbf{a}_k}{\|\mathbf{a}_k\|_2} = \hat{A}\hat{\mathbf{w}},$$

where $\hat{A} = \begin{bmatrix} \frac{\mathbf{a}_1}{\|\mathbf{a}_1\|_2} & \frac{\mathbf{a}_2}{\|\mathbf{a}_2\|_2} & \cdots & \frac{\mathbf{a}_n}{\|\mathbf{a}_n\|_2} \end{bmatrix}$ and $\hat{w}_k = w_k \|\mathbf{a}_k\|_2.$

Using OMP to solve:

Find
$$\hat{\mathbf{w}}$$
 sparse s.t. $\mathbf{y} = \hat{A}\hat{\mathbf{w}}$,

and get back to the original solution w.

Orthogonal Matching Pursuit: Some Remarks

1. Recall:
$$j_{k+1} := \arg \max_{j \in [n]} \{ | (A^*(y - Aw^k))_j | \}, \quad A^*_{S^k}y = A^*_{S^k}A_{S^k}w^k_{S^k}.$$

- 2. How to speed up?
 - Use QR decomposition of the matrix A_{Sk}
 - Fast algorithm to update QR decomposition of $A_{S^{k+1}}$ from A_{S^k} .
 - Use fast matrix-vector multiplication for A (Fourier transform)
- 3. Stopping criterions:
 - 3.1 If we know the sparsity level s, stop after Cs iterations.
 - 3.2 To account for measurement and computational errors, stop when

$$\|y - Aw^k\|_2 \le \varepsilon$$
, or $\|A^*(y - Aw^k)\|_\infty \le \varepsilon$,

where ε is a chosen tolerance.

- 1. OMP never selects the same index twice because the residual is orthogonal to *Az* of related chosen indices.
- 2. OMP works well if *s* is small. If *s* is not small compared to *n*, the OMP may require more time. In that case, suitable basis pursuit algorithms can be significantly faster than OMP.
- Cons: Once an incorrect index has been selected in a target support S^k, it remains in al the subsequent target supports.

• Consider an $n \times n$ matrix with ℓ_2 -normalized columns defined by

$$A = \begin{bmatrix} Id_{n \times n} & | & \frac{\eta}{n-1} \mathbf{1}_n \\ 0 & | & \sqrt{1-\frac{\eta^2}{n}} \end{bmatrix}$$

The *n*-sparse vector **x** = [1,...,1,0]^T is not recovered from **y** = A**x** after *n* iterations since the wrong index *n* + 1 is picked at the first iteration. (See page 157 in the textbook)

Here are some important results to least squares problems.

Proposition (Prop. A.20.) Let $A \in \mathbb{C}^{m \times n}$ and $\mathbf{y} \in \mathbb{C}^m$. Define

 $\mathcal{M} := \{ \mathbf{x} \in \mathbb{C}^n \quad s.t. \ \mathbf{x} \text{ is a minimizer of } \min \|A\mathbf{z} - \mathbf{y}\|_2 \}.$

Then the optimization problem

$$\min_{\mathbf{x}\in\mathcal{M}}\|x\|_2$$

has the unique solution $\mathbf{x}^{\#} = A^{\dagger} \mathbf{y}$.

Corollary

Let $A \in \mathbb{C}^{m \times n}$ s.t. rank $(A) = \min\{m, n\}$ (full rank) and let $\mathbf{y} \in \mathbb{C}^m$. Then

1. If $m \ge n$, then the least squares problem

$$\min_{\mathbf{x}\in\mathbb{C}^n}\|A\mathbf{x}-\mathbf{y}\|_2$$

has the unique solution $\mathbf{x}^{\#} = A^{\dagger} \mathbf{y}$.

2. If $n \ge m$, then the least squares problem

$$\min_{\mathbf{x}\in\mathbb{C}^n}\|x\|_2 \quad s.t. \quad A\mathbf{x}=\mathbf{y}$$

has the unique solution $\mathbf{x}^{\#} = A^{\dagger} \mathbf{y}$.

Orthogonal Matching Pursuit (OMP)

Iterative Hard Thresholding (IHT)

Hard Thresholding Pursuit (HTP)

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Problem: Given $A \in \mathbb{C}^{m \times n}$ and $\mathbf{y} \in \mathbb{C}^m$. Find

$$\mathbf{w} \in \mathbb{C}^n$$
 such that $\mathbf{y} = A\mathbf{w}$ and $\|\mathbf{w}\|_0 \leq s$.

Motivation: Solve $A\mathbf{w} = \mathbf{y}$ by iteration methods. Indeed, from $\mathbf{y} = A\mathbf{w}$, we have:

$$\begin{split} 0 &= A^*(\mathbf{y} - A\mathbf{w}) \\ \mathbf{w} &= \mathbf{w} + \gamma A^*(\mathbf{y} - A\mathbf{w}), \quad \text{where} \quad \gamma \in \mathbb{R} \\ \mathbf{w}^{k+1} &= \mathbf{w}^k + \gamma A^*(\mathbf{y} - A\mathbf{w}^k) \quad (\text{fixed-point iterate}) \end{split}$$

Then we apply a projection method to ensure the iterates \mathbf{w}^k have at most *s* nonzero entries.

Theorem

Given $p \in [1, \infty]$. Assume that:

- (i) *M* is a closed, nonempty set in the Banach space \mathbb{C}^n or \mathbb{R}^n .
- (ii) The operator $\mathcal{A} : M \to M$ is L-contractive for some fixed $L \in [0, 1)$:

$$\|\mathcal{A}\mathbf{u} - \mathcal{A}\mathbf{v}\|_p \leq L \|\mathbf{u} - \mathbf{v}\|_p$$
 for all $\mathbf{u}, \mathbf{v} \in M$.

Then the following statements hold true:

- 1. The equation $\mathbf{u} = A\mathbf{u}, \mathbf{u} \in M$, has exactly one solution $\mathbf{u}_* \in M$.
- 2. For each given $\mathbf{u}^0 \in M$, the sequence $\{\mathbf{u}^k\}$ constructed by the iteration method, $\mathbf{u}^{k+1} = \mathcal{A}\mathbf{u}^k$, converges to the unique solution \mathbf{u}_* of $\mathbf{u} = \mathcal{A}\mathbf{u}$ and

$$\|\mathbf{u}^{k}-\mathbf{u}_{*}\|_{p}\leq rac{L^{k}}{1-L}\|\mathbf{u}^{1}-\mathbf{u}^{0}\|_{p},$$

Denote

$$\begin{split} \mathcal{L}_s(\mathbf{z}) &:= \text{Index set of } s \text{ largest absolute entries of } \mathbf{z} \in \mathbb{C}^n, \\ \mathcal{H}_s(\mathbf{z}) &:= \mathbf{z} \mathcal{L}_s(\mathbf{z}). \end{split}$$

Iterative Hard Thresholding (IHT)

Input: Measurement matrix A, measurement vector \mathbf{y} , sparsity level s, hyperparameter γ .

Initialization: *s*-sparse vector \mathbf{w}^0 , typically $\mathbf{w}^0 = 0$.

Iteration: Repeat until a stopping criterion is met.

$$\mathbf{w}^{k+1} = H_s(\mathbf{w}^k + \gamma A^*(\mathbf{y} - A\mathbf{w}^k)).$$

Output: The *s*-sparse vector **w**[#].

Remark: The IHT does not require the computation of any orthogonal projection.

Orthogonal Matching Pursuit (OMP)

Iterative Hard Thresholding (IHT)

Hard Thresholding Pursuit (HTP)

Motivation: Basic Thresholding + Orthogonal Projection

Hard Thresholding Pursuit

Input: Measurement matrix A, measurement vector \mathbf{y} , sparsity level s, hyperparameter γ .

Initialization: *s*-sparse vector \mathbf{w}^0 , typically $\mathbf{w}^0 = 0$.

Iteration: Repeat until a stopping criterion is met.

$$S^{k+1} = L_s(\mathbf{w}^k + \gamma A^*(\mathbf{y} - A\mathbf{w}^k)),$$

$$\mathbf{w}^{k+1} = \underset{\mathbf{z} \in \mathbb{C}^n}{\operatorname{argmin}} \{ \|\mathbf{y} - A\mathbf{z}\|_2, \quad \operatorname{supp}(\mathbf{z}) \subseteq S^{k+1} \}$$

Output: The *s*-sparse vector **w**[#].

Remarks:

 If we don't know the sparsity s, we can base on the absolute values of entries in each iteration and decide how many entries we would like to keep. For example, in the input of IHT, instead of using the sparsity level s, we can choose a hyperparameter ε and H_s is replaced by H_ε, where

$$\mathcal{H}_arepsilon(z) = egin{cases} z & ext{if } |z| > arepsilon, \ 0 & ext{otherwise} \end{cases}$$

• The error estimations rely on the property of the matrix A (for e.g, RIP-like condition).

- First criterion the minimal number of measurements for a sparsity level *s* and a signal length *N* may vary with each algorithm (Study later)
- 2nd criterion Speed of the algorithm. In general, when s is small, OMP is extremely fast because the speed depends on the number of iterations (which is s when the algorithm succeeds). The runtime of IHT is almost not influenced by the sparsity s.

Exercises

- 1. (Prob. 3.11) Implement OMP, IHT, HTP. Choose $A \in \mathbb{R}^{m \times N}$ with independent random entries equal to $1/\sqrt{m}$ or $-1/\sqrt{m}$, each with probability 1/2. Test the algorithms on randomly generated *s*-sparse signals, where first support is chosen at random and then the nonzero coefficients. By varying N, m, s, evaluate the empirical success probability of recovery.
- 2. (Prob. 3.7) Given $A \in \mathbb{C}^{m \times N}$ and $\tau > 0$, show that the solution of

$$\min \|\mathbf{A}\mathbf{z} - \mathbf{y}\|_2^2 + \tau \|\mathbf{z}\|_2^2$$

is given by

$$\mathbf{z}^{\#} = (A^*A + \tau Id)^{-1}A^*\mathbf{y}.$$

(Prob. 3.3.) Let A ∈ ℝ^{m×N} and y ∈ ℝ^m. Assuming the uniqueness of the minimizer x[#] of

$$\min_{\mathbf{z}\in\mathbb{R}^N} \|\boldsymbol{z}\|_1 \quad \text{s.t.} \quad \|\boldsymbol{A}\mathbf{z}-\mathbf{y}\| \le \eta,$$

where $\eta \geq 0$ and $\|\cdot\|$ is an arbitrary norm on $\mathbb{R}^m,$ prove that $\mathbf{x}^\#$ is necessarily m-sparse.

4. QR property of a matrix after adding one column vector.

Appendix: Some Proofs

Proof Sketch of Lemma 3.3.

Let $\mathbf{v} \in \mathbb{C}^n$ s.t. supp $(\mathbf{v}) \subseteq S$.

• For any $t \in \mathbb{C}$, $\operatorname{supp}(\mathbf{v} + t\mathbf{e}_j) \subseteq S \cup \{j\}$, show that

$$\|\mathbf{y} - A(\mathbf{v} + t\mathbf{e}_j)\|_2^2 \ge \|\mathbf{y} - A\mathbf{v}\|_2^2 - |(A^*(\mathbf{y} - A\mathbf{v}))_j|^2,$$

and the quality holds when $|t| = |(A^*(\mathbf{y} - A\mathbf{v}))_j|$.

• Therefore,

$$\begin{aligned} \|\mathbf{y} - A\mathbf{w}\|_2^2 &= \min\{\|\mathbf{y} - A\mathbf{z}\|_2^2: \ \operatorname{supp}(\mathbf{z}) \subseteq S \cup \{j\}\} \\ &\leq \min_{t \in \mathbb{C}} \|\mathbf{y} - A(\mathbf{v} + t\mathbf{e}_j)\|_2^2 \\ &\leq \|\mathbf{y} - A\mathbf{v}\|_2^2 - |(A^*(\mathbf{y} - A\mathbf{v}))_j|^2. \end{aligned}$$

Proof. We have

$$\begin{aligned} \|y - A(v + te_j)\|_2^2 &= \|y - Av - tAe_j\|_2^2 \\ &= \|y - Av\|_2^2 + |t|^2 \|Ae_j\|_2^2 - 2\operatorname{Re}\langle y - Av, tAe_j\rangle \\ &= \|y - Av\|_2^2 + |t|^2 - 2\operatorname{Re}\left(\overline{t}e_j^T A^*(y - Av)\right) \\ &\geq \|y - Av\|_2^2 + |t|^2 - 2|t||(A^*(y - Av))_j| \\ &\geq \|y - Av\|_2^2 - |(A^*(y - Av))_j|^2. \end{aligned}$$

The equality holds when $|t| = |(A^*(y - Av))_j|$ and

$$\operatorname{Re}\left(\overline{t}e_{j}^{T}A^{*}(y-Av)\right)=|t||\overline{t}e_{j}^{T}A^{*}(y-Av)|.$$

Therefore,

$$\min_{t\in\mathbb{C}} \|y - A(v + te_j)\|_2^2 = \|y - Av\|_2^2 - |(A^*(y - Av))_j|^2,$$

and

$$\begin{aligned} \|y - Aw\|_2^2 &= \min_{supp(z) \subseteq S \cup \{j\}} \{ \|y - Az\|_2^2 \} \le \min_{t \in \mathbb{C}} \|y - A(v + te_j)\|_2^2 \\ &\le \|y - Av\|_2^2 - |(A^*(y - Av))_j|^2. \end{aligned}$$

Proof of Lemma 3.4. We rewrite the constraint optimization problem

$$\mathbf{v} := \operatorname*{argmin}_{\mathbf{z} \in \mathbb{C}^n} \{ \|\mathbf{y} - A\mathbf{z}\|_2, \operatorname{supp}(\mathbf{z}) \subseteq S \}$$

to an unconstraint optimization problem:

$$\nu = \underset{\mathbf{z} \in \mathbb{C}^n}{\operatorname{argmin}} \{ \|\mathbf{y} - A_{\mathcal{S}} \mathbf{z}_{\mathcal{S}}\|_2 \} = \underset{\mathbf{u} \in \mathbb{C}^{|\mathcal{S}|}}{\operatorname{argmin}} \{ \|\mathbf{y} - A_{\mathcal{S}} \mathbf{u}\|_2 \}$$

By the orthogonality condition, we have

$$A_S^*\mathbf{y}=A_S^*A_S\mathbf{v}_S.$$