Exact Support Recovery via (Refined) Least Squares

Stefan Steinerberger
(joint with Ofir Lindenbaum)
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known \uparrow

\[ \uparrow \]

unknown
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Gaussian Noise

lots of 0s

unknown
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We have \( y = A\theta + \omega \). We know \( y \) and \( A \), \( \omega \) is an (unknown) random Gaussian vector. Goal: recover \( \theta \in \{-1, 0, 1\}^D \).
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Clearly impossible: the system is underdetermined and we have noise. What if \( \theta \) is sparse?

Formally: \( A \in \mathbb{R}^{N \times D} \) and \( \theta \) vanishes on all but \( k \) coordinates.

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A first idea

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Suppose that \( \theta \) only has one nonzero entry in the \( i \)-th position.

Somebody gives you \( y = v_i + \omega \). How do you have the best chance of getting \( v_i \)?
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Suppose that \( \theta \) only has one nonzero entry in the \( i \)-th position. Then

\[ y = \pm A_{.,i} + \omega \]

and \( A_{.,i} \) is the \( i \)-th column of the matrix (but we do not know which one).
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Suppose that $\theta$ only has one nonzero entry in the $i$–th position. Then

$$y = \pm A_{.,i} + \omega$$

and $A_{.,i}$ is the $i$–th column of the matrix (but we do not know which one). A good idea is to take the inner product

$$\langle y, A_{.,j} \rangle = \langle \pm A_{.,i}, A_{.,j} \rangle + \langle \omega, A_{.,j} \rangle$$
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The first term is only big when \( i = j \), the second is always equally random. Pick the \( j \) for which the inner product is the largest.
Example!

We take the following matrix $A \in \mathbb{R}^{20 \times 30}$.

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where $\theta = (1, 1, 0, 0, \ldots)$ and $\omega_i \sim \mathcal{N}(0, 1)$. How to get $\theta$ from $y$?
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Clearly the first two coordinates stick out.
\[ y = \theta + \omega \]

Such methods are known as **Matching Pursuit** (Mallat & Zhang, Gilbert & Tropp). There are many variations on it, for example RandOMP (Elad & Yavneh), regularized OMP (Needell & Vershynin), . . .
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The Lasso (Tibshirani 1996)

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\|y - Ax\|_2^2 \rightarrow \min
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\|x\|_1 \leq R
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Many variations, such as

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\|y - Ax\|_2^2 + \lambda \cdot \|x\|_2 \rightarrow \min
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One version we will also consider is the 'Trimmed Lasso' where

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T_k(x) = \min \|\phi\|_0 \leq k \|x - \phi\|_1.
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T_k(x) = \min_{\|\phi\|_0 \leq k} \|x - \phi\|_1.
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Other approaches

Because of time constraints, I am not going to explain

- Iterative Support Detection (ISD), Wang & Yin 2010
- Iterated Reweighted $\ell^1$—minimization (IRL1), Candes, Wakin & Boyd (2008)
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There are also many other methods.
How do these methods compare?

64 unknown variables (say, genes) and \( \theta \in \{-1, 0, 1\}^{64} \) has 30 nonzero entries (not that sparse) and \( \mathcal{N}(0, 1) \) Gaussian noise.
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64 unknown variables and $\mathcal{N}(0, 1)$ Gaussian noise. Success as a function of sparsity.
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*I will mainly emphasize the underlying new idea. It seems very likely that the underlying idea can be used to boost many other methods (example later).*
Refined Least Squares (RLS)

We take the same example as above. $A \in \mathbb{R}^{20 \times 30}$ as above

\[
y = \begin{bmatrix} 1 \\ 10 \\ 20 \\ 30 \\ 1 \\ 5 \\ 10 \\ 15 \\ 20 \end{bmatrix}
\]

$\theta + \omega$ where $\theta = (1, 1, 0, 0, ...) \text{ and } \omega_i \sim N(0, 1)$. How to get $\theta$ from $y$?

Simplest possible idea. Let's just do least squares

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\[ \| y - Ax \|_2 \to \text{min} . \]
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$$\|y - Ax\|_2 \rightarrow \text{min}.$$ 

This is very bad. Certainly the first two coefficients are not small but many others are bigger.
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Least Squares does not work – but it works *on average*. Let’s take the same example, \( \theta = (1, 1, 0, 0 \ldots, 0) \) and average the behavior of Least Squares over 100 random choices of \( A, \omega \).
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That works! But it’s clearly cheating: 100 random matrices is like having 100 times the number of equations...
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How to get more equations *without cheating*:

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Just pick some random subset of rows: this gives you a ‘new’ problem. It’s easy to create many ‘new’ problems like this.
Refined Least Squares (RLS)

Let's do an example.

$y = \theta + \omega$
Refined Least Squares (RLS)

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$$y = \theta + \omega$$
The diagram illustrates the relationship between the variable index and the coefficient, highlighting the strongest coefficients with a green dotted line. The variable index ranges from 0 to 60, and the coefficient ranges from $-1.5$ to $1.5$. The strongest coefficients are marked as $m=9$. The data points are scattered across the graph, indicating variability in the coefficient values.
The diagram shows a plot of coefficients against the variable index, with a threshold at $S = 10$. The $x$-axis represents the variable index, ranging from 0 to 60, and the $y$-axis represents the coefficient, ranging from -1.5 to 1.5. The green dots indicate the strongest coefficients, with $m = 13$. The pattern suggests a decrease in coefficients as the variable index increases, with a notable drop at the threshold $S = 10$. The coefficients fluctuate around zero, with some values approaching 1.5.
m=15

Coefficient

Variable index

Strongest Coeff.
The diagram shows a scatter plot with the variable index on the x-axis and the coefficient on the y-axis. The plot is labeled with "$m=19$". The variable index ranges from 0 to 60, and the coefficient ranges from -1.5 to 1.5. The plot includes a vertical dashed line at the index 10, and two sets of data points: green dots representing the strongest coefficients, and red dots indicating another set of data points.
Refined Least Squares (RLS)

Outline of the algorithm.

1. Pick a random subset of the equations and solve the problem with least squares.
2. Average the results.
3. Pick the largest entry in the average as a guess for a coordinate with a nonzero entry. Use the sign as a guess for the sign.
4. Remove the corresponding coordinate to get a new problem with the same number of equations and one less unknown.
5. Go back up to 1.
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How do you have the best chance of getting $v_i$? At this stage, we switch back to Inner Products (the OMP selection rule).
Refined Least Squares (RLS)

Underlying idea: by looking at subsets of the equations, we get a harder problem.
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Underlying idea: by looking at subsets of the equations, we get a harder problem. However, we get many harder problems and the gain from being able to average exceeds the increase of difficulty.
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(\langle\langle\text{reduced RHS}, \text{reduced column}_i\rangle\rangle)_{i=1}^{\text{#columns}}.
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Experiments suggests that this boosts OMP to a **very competitive** method (it seems slightly worse than RLS but only slightly).
Some Theory

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Proposition (Lindenbaum, S, 21)
If we fix the ratio \( N/D < 1 \) and let the dimensions of the matrix go to infinity, then

\[
\mathbb{E}_{X,\omega} \| X^\dagger y - X^\dagger X\theta^* \| = (1 + o(1)) \sqrt{\frac{N}{D - N}}.
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Some Theory

Figure 3. Numerical evaluation of the relation predicted by Theorem 1 for $D = 300$ and $10 \leq N \leq 290$. As the number of equations $N$ tends to $D$ (the number of variables), the expected $\ell^2$ norm of $X^\dagger y - X^\dagger X \theta^*$ (black dots) grows like $N^{1/2}(D - N)^{-1/2}$ (red line).
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Proof.

A fun computation: relevant are the inverse singular values of $X$. Use the Marchenko-Pastur distribution. One integral

$$
\int \frac{\sqrt{(\lambda_+ - x)(x - \lambda_-)}}{x^2} \, dx =
\begin{align*}
&= \frac{1}{x} \sqrt{-\lambda^2 - (x - 1)^2 + 2\lambda(1 + x)} \\
&\quad + \arctan \left( \frac{1 + \lambda - x}{\sqrt{-\lambda^2 - (x - 1)^2 + 2\lambda(1 + x)}} \right) \\
&\quad - \frac{1 + \lambda}{1 - \lambda} \arctan \left( \frac{x + \lambda(2 + x) - \lambda^2 - 1}{(\lambda - 1)\sqrt{\lambda^2 + 2\lambda(1 + x) - (1 + x)^2}} \right).
\end{align*}
$$
Another theoretical perspective: we are given

$$y = X \theta^* + \omega,$$

where $X \in \mathbb{R}^{N \times D}$. 

**Theorem (Lindenbaum, S, 2020)**

Averaging over random subsets $A$ of the equations of size $n < D$, we have

$$\mathbb{E} \left\| X \theta^* - \hat{\theta}^*_A \right\| \lesssim n \sqrt{N} \sqrt{\frac{D}{n}} + n D.$$
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**Theorem (Lindenbaum, S, 2020)**

Averaging over random subsets \( A \) of the equations of size \( n < 0.9D \), we have

\[ \mathbb{E}_{X,\omega} \left\| \mathbb{E}_A \left( \pi_A \theta^* - \hat{\theta}_A \right) \right\| \lesssim \frac{n}{\sqrt{N\sqrt{D}}} + \frac{n}{D}. \]
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This leads to a dichotomy:

1. If $n$ is small, then the error is small but the projection $\pi_A \theta^*$ has little to do with the ground truth.
2. If $n$ is large, then the error increases but the projection is more accurate.
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Main Question

1. Which methods are best suited for this type of averaging?
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2. Better way of selecting equations than just randomly?
3. Any chance of proving bounds with good constants?
\[ y = \theta + \omega \]

Thank you!