Sparse High-Dimensional Regression: Exact Scalable Algorithms and Phase Transitions

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December 5, 2025

Reference

- Dimitris Bertsimas, Bart Van Parys, *Sparse High-Dimensional Regression: Exact Scalable Algorithms and Phase Transitions*, *The Annals of Statistics*, Vol. 48, No. 1, 2020.

Background

Problem (Best Subset Selection).
Given input data $X = (x_1, \ldots, x_n)^\top \in \mathbb{R}^{n \times p}$ and response $Y = (y_1, \ldots, y_n)^\top \in \mathbb{R}^n$, we seek a k-sparse linear predictor:

$$\min_{w \in \mathbb{R}^p} \frac{1}{2\gamma}\|w\|_2^2 + \frac{1}{2}\|Y - Xw\|_2^2 \quad \text{s.t.} \quad \|w\|_0 \leq k.$$

Why sparsity?

- In high dimensions ($p \gg n$), restricting to few variables improves interpretability and guards against overfitting. [3]
- Many scientific domains require explicit variable selection (e.g., genetics, networks, text), so the goal is not just prediction but identifying a small set of truly relevant features.

Challenges

Computational barrier.

- Best subset selection solves the *right* ℓ_0 problem, but is NP-hard and traditionally scales poorly. [4, 1]

Convex surrogates are scalable but imperfect.

- ℓ_1 relaxation (Lasso) is efficient, yet may yield biased estimates and unstable supports. [3, 5]

Gap. Can we obtain exact sparse regression *at scale*?
This paper: a new optimization view + scalable algorithm for high-dimensional best subset selection.

Main Idea & Contributions

Main idea.
Reformulate best subset selection into a convex integer optimization problem in binary variables, and solve it via a tailored cutting-plane / outer-approximation algorithm.

Contributions.

- New reformulation eliminates big-M constants and yields a pure binary convex program.
- Scalable algorithm with fast updates and warm starts, enabling problems with n, p up to 10^5.
- Empirical insights: reveals a statistical & computational phase transition where exact subset selection becomes easy beyond a sample-size threshold.

Talk roadmap.
Reformulation $\rightarrow$ Algorithm $\rightarrow$ Phase transition theory $\rightarrow$ Experiments.

Reformulation I: From ℓ_0 to Binary Selection

Start from the ℓ_0 problem.
We want at most k nonzero coefficients in w:

$$\min_{w \in \mathbb{R}^p} \frac{1}{2\gamma}\|w\|_2^2 + \frac{1}{2}\|Y - Xw\|_2^2 \quad \text{s.t.} \quad \|w\|_0 \le k. \tag{1}$$

Introduce binary selectors.
Let $s \in \{0,1\}^p$ indicate which variables are used:

$$S_k^p := \left\{ s \in \{0,1\}^p : \; \mathbf{1}^\top s \le k \right\}.$$

Then subset selection becomes: choose $s \in S_k^p$ and fit w only on active features.

Reformulation II-a: Kernel (Gram) from a Selected Subset

For each column $X_{:j} \in \mathbb{R}^n$, define a rank–1 Gram matrix

$$K_j := X_{:j} X_{:j}^\top \in \mathbb{R}^{n \times n}.$$

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Gram expansion $=$ sum of column outer products.

$$X_s X_s^\top = \sum_{t=1}^{k} X_{:j_t} X_{:j_t}^\top = \sum_{j=1}^{p} s_j \, X_{:j} X_{:j}^\top .$$

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Define

$$K_s := \sum_{j=1}^{p} s_j K_j \quad \Rightarrow \quad \boxed{K_s = X_s X_s^\top}.$$

Intuition: the subset Gram matrix is the sum of Gram contributions from each selected feature.

Reformulation II-b(1): Eliminating w

Inner ridge fit for a fixed subset.
For $s \in S_k^p$, solve ridge regression on X_s:

$$w_s^\star = \arg\min_{w_s} \ \frac{1}{2}\|Y - X_s w_s\|_2^2 + \frac{1}{2\gamma}\|w_s\|_2^2. \tag{7}$$

Closed-form ridge solution. First-order optimality gives

$$(X_s^\top X_s + \gamma^{-1} I) w_s = X_s^\top Y \quad \Rightarrow \quad w_s^\star = (X_s^\top X_s + \gamma^{-1} I)^{-1} X_s^\top Y.$$

Plug back to remove w_s.

$$c(s) = \frac{1}{2} Y^\top \Big(I_n - X_s (X_s^\top X_s + \gamma^{-1} I)^{-1} X_s^\top \Big) Y.$$

Reformulation II-b(2): Kernel view via Woodbury

Let $K_s = X_s X_s^\top$.

Matrix Inversion Lemma (Woodbury).

$$(A + UCV)^{-1} = A^{-1} - A^{-1}U(C^{-1} + VA^{-1}U)^{-1}VA^{-1}.$$

Set $A = I_n,\ U = X_s,\ C = \gamma I,\ V = X_s^\top$. Then

$$(I_n + \gamma X_s X_s^\top)^{-1} = I_n - X_s(X_s^\top X_s + \gamma^{-1} I)^{-1} X_s^\top.$$

Therefore the optimal value is

$$\boxed{c(s) = \frac{1}{2} Y^\top (I_n + \gamma K_s)^{-1} Y} \tag{10}$$

Resulting pure binary optimization.

$$\min_{s \in S_k^p} \ c(s) \quad \text{with } c(s) \text{ convex in } s. \tag{CIO}$$

So best subset selection becomes a convex integer optimization problem with no big-M constants.

Algorithm Intuition

We have a convex-integer problem.
After reformulation:

$$\min_{s \in S_k^p} c(s), \qquad s \in \{0,1\}^p,$$

where $c(s) = \frac{1}{2} Y^\top (I_n + \gamma K_s)^{-1} Y$ is convex and smooth in s.
Key idea.
Convexity implies a global linear lower bound at any point $s^{(t)}$:

$$c(s) \;\geq\; c(s^{(t)}) + \nabla c(s^{(t)})^\top (s - s^{(t)}).$$

Each bound is a cutting plane.
Outer approximation.
Collect many cuts to form a tight lower envelope, then search over binary s using a master MIO that gets tighter each iteration [2].

Takeaway: exploit convex geometry to guide combinatorial search.

Algorithm Overview

Algorithm: Cutting-Plane / Outer Approximation for Best Subset Selection

Input: Data (X, Y), sparsity level k, ridge parameter γ, tolerance ε.
Output: Globally optimal subset $s^\star$ (and coefficients $w^\star$).

1. **Initialize.** Obtain an initial subset $s^{(0)}$ (e.g., greedy warm start), set cut set $\mathcal{C} \leftarrow \emptyset$.
2. **Evaluate objective and gradient.** For current $s^{(t)}$, compute

$$c(s^{(t)}) = \tfrac{1}{2} Y^\top (I_n + \gamma K_{s^{(t)}})^{-1} Y, \qquad \nabla c(s^{(t)}).$$

3. **Add a cutting plane.** Introduce η as a *lower bound on the optimal value.* Each tangent cut is a *global lower bound* on $c(s)$::

$$\eta \;\geq\; c(s^{(t)}) + \nabla c(s^{(t)})^\top (s - s^{(t)}).$$

4. **Solve the master MIO.** *Minimize the best lower bound implied by all cuts.*

$$\min_{s \in S_k^p,\ \eta} \quad \eta \quad \text{s.t. all cuts in } \mathcal{C}.$$

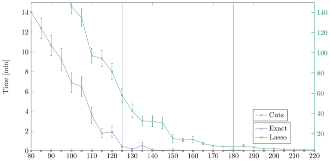
   Let the solution be $(s^{(t+1)}, \eta^{(t+1)})$.

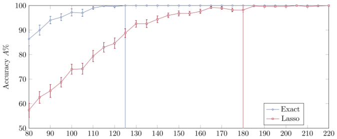
5. **Check convergence.** If $\eta^{(t+1)} \geq c(s^{(t+1)}) - \varepsilon$, stop and output $s^\star = s^{(t+1)}$.

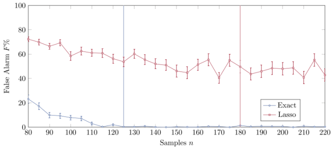
Empirical Teaser: Phase Transition

What happens as sample size n increases?

Exact best subset selection exhibits a sharp phase transition: from poor recovery to near-perfect recovery, and (surprisingly) from hard to easy computation.







Theory Setup for Phase Transition

Data model.
Assume a sparse linear model with true support $S^\star$:

$$Y = Xw^\star + \varepsilon, \qquad |S^\star| = k, \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 I_n).$$

Two regimes.

- Undersampled regime $(n < n_t)$: many subsets fit similarly well $\Rightarrow$ hard recovery and heavy computation.
- Oversampled regime $(n > n_t)$: true subset separates clearly $\Rightarrow$ accurate recovery and easy computation.

Goal of theory.
Characterize the threshold n_t and show exact subset selection succeeds *earlier* than ℓ_1 surrogates.

Main Theoretical Results

Theorem. Statistical phase transition

Assume the design is uncorrelated ($\rho = 0$), set the ridge parameter $\gamma = 1/n$, and suppose $p - k > k$. Then there exist numerical constants $c_8, c_9 > 0$ (independent of n, k, p, σ^2) such that for all $\theta \geq 1$,

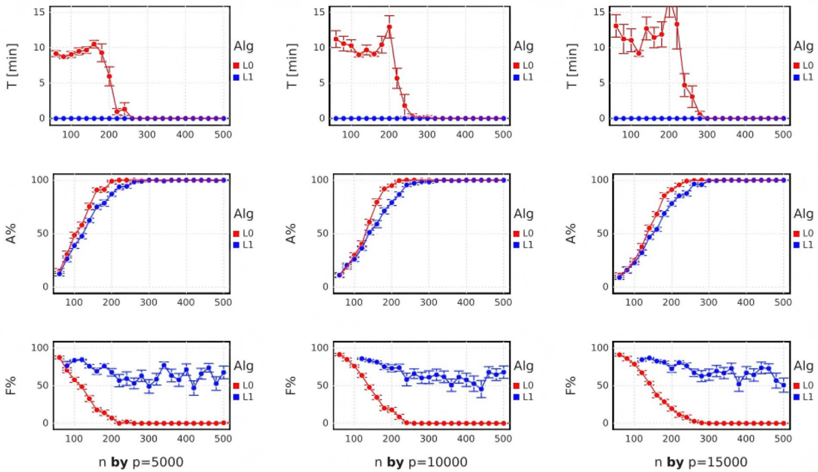
$$n \;\geq\; \theta\, n_1 \quad \Longrightarrow \quad \mathbb{P}\big[s^\star = s_1^\star = s^{\text{true}}\big] \;\geq\; 1 - c_9 \exp(-\theta\, c_8).$$

Corollary. Earlier success than Lasso

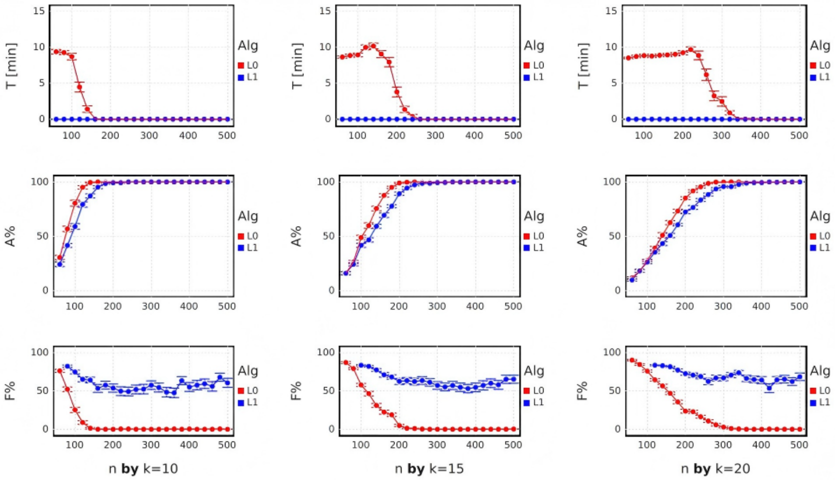
Exact ℓ_0 subset selection achieves full support recovery once n exceeds its threshold (around n_0 / n_t), and this occurs *strictly earlier* than the Lasso accuracy threshold n_1:

$$n_t^{(\ell_0)} < n_1^{(\ell_1)}.$$

Phase Transition vs. Dimension p



Phase Transition vs. Sparsity k



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