Solar: a least-angle regression for accurate and stable variable selection in high-dimensional data

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Overview

1. Motivation
   - Dimensions, computataion load and complicated structure
   - Motivating examples
2. Solar algorithm
   - Pseudo code
   - Computation flow
3. Simulation results
   - p/n approaching 0
   - p/n approaching 1
   - p/n does not change
   - irrepresentable condition simulation

subsample ordering

subsample ordering : a new regularization method developed originally for Gaussian process regression and neural network for Google Cloud. The prototype Python packages can be found on my Github https://github.com/isaac2math

- DeepFrame: a fast and accurate GPU-based library for neural network training (with Dr. Chunnan Sheng, Tesla/Xiaopeng Motors.ai; submitted to Journal of Machine Learning Research)
- Solar: a least-angle regression for accurate and stable variable selection in high-dimensional data (submitted to Journal of Computational and Graphical Statistics)
- Data-driven detection of endogeneity and instrument variable via Probabilistic Graph Modelling (working on, with Prof. Tim Fisher and Dr. Jian Hong, School of Econ)
- Subsample ordering: a fast and accurate solver for high-dimensional Gaussian Process regression (working on, with Dr. Peter Exterkate, School of Econ)

The curse of dimensionality

- Dimensionality : p (number of variables) for natural language processing can easily go beyond 10 million;
- Greater dimensions requires
  1. improvements of the variable selection algorithm (e.g., better sparsity and accruracy);
  2. restraining the growth of computation load for variable selection
- More complicated dependence structures in datasets (more severe multicollinearity if the structure is linear);

These challenges compel variable-selection algorithms to enhance the accuracy, stability and robustness of variable-selection in high dimensional spaces.

Bayesian Network (Koller and Friedman, 2009)

Directed acyclic graphs (DAG) are used to describe dependence structure of the data.

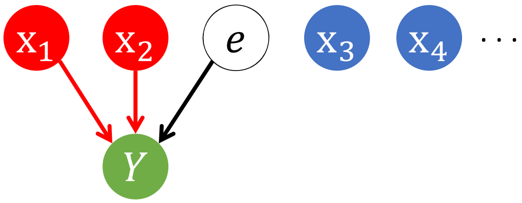


Figure: the DAG (referred to as the *standard structure*) typically assumed in the regression analysis, where $\{\mathbf{x}_1, \mathbf{x}_2\}$ are the 'parents' of Y; Y is the 'child' of $\{\mathbf{x}_1, \mathbf{x}_2\}$ and $\mathbf{x}_1$ is a 'spouse' of $\mathbf{x}_2$.

Example 1 (Lim and Yu, 2016)

Assuming the standard strcture, consider the lars-lasso algorithm, which uses the L_1-norm fraction $t \in [0, 1]$ as a tuning parameter. In each CV training-validation split, for all β on the solution path,

$$t = \frac{\|\beta\|_1}{\|\beta_{\max}\|_1}, \tag{1}$$

where $\|\beta_{\max}\|_1$ is defined as the L_1 norm of the non-shrinked solution on the solution path.

Example 1 (Lim and Yu, 2016)

The solution path of lars-lasso is unstable in high dimensions (also applies to coordinate descend of lasso).

- When $p > n$, $\beta_{\max}$ is the traditional forward regression solution with n selected variables.
- $\beta_{\max}$ uses up all n degrees of freedom (a saturated fit)
- Hence, due to the resampling randomness in CV, $\|\beta_{\max}\|_1$ may vary substantially across validation sets.
- As a result, the same value of t may correspond to different amounts of shrinkage (or λ) on the solution paths of different CV training-validation splits.

Example 1 (Lim and Yu, 2016)

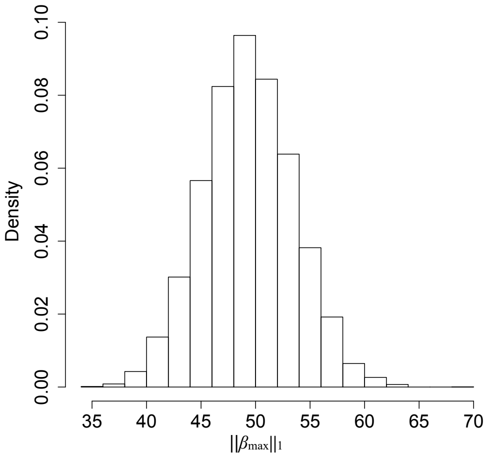


Figure: Histogram of $\|\beta_{\max}\|_1$ from 10,000 bootstrap lasso estimates from a Gaussian simulation, where the variance of each variable is 1, pairwise correlations are 0.5, $n = 100$ and $p = 150$ (Lim and Yu, 2016, Section 3.1.1.).

Example 2. (Zhao and Yu, 2006)

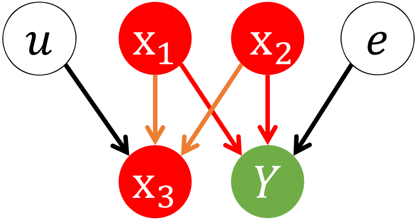


Figure: Example 2 dependence structure.

$$\begin{cases} \mathbf{x}_3 = \omega_1 \mathbf{x}_1 + \omega_2 \mathbf{x}_2 + \sqrt{1 - 2\omega^2} \cdot u \\ Y = \beta_1 \mathbf{x}_1 + \beta_2 \mathbf{x}_2 + \delta e \end{cases} \tag{2}$$

irrepresentable condition: for variable selection consistency of any lasso-type estimator, $\sum_i |\omega_i| < 1$

Example 2. (Zhao and Yu, 2006)

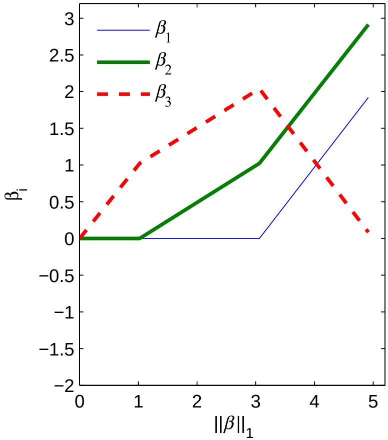


Figure: $\sum_i |\omega_i| > 1$: the irrepresentable condition fails and lasso selects redundant variables

Solar algorithm

Algorithm 1: average L_0 solution path estimation

input : (Y, X).

generate K subsamples $\left\{\left(Y^k, X^k\right)\right\}_{k=1}^{K}$;

set $\widetilde{p} = \min\left\{n_{\mathrm{sub}}, p\right\}$;

for *$k := 1$ to K, stepsize $= 1$* **do**

  run an unrestricted lars (Algorithm 3.2 in Friedman et al. (2001)) on $\left(Y^k, X^k\right)$ and record the order of variable inclusion at each stage;

  define $\widehat{q}^k = \mathbf{0} \in \mathbb{R}^p$;

  for all i and l, if $\mathbf{x}_i$ is included at stage l, set $\widehat{q}_i^k = (\widetilde{p} + 1 - l)/\widetilde{p}$, where $\widehat{q}_i^k$ is the i^{th} entry of $\widehat{q}^k$;

end

$\widehat{q} := \frac{1}{K}\sum_{k=1}^{K} \widehat{q}^k$;

return $\widehat{q}$

Solar algorithm

Algorithm 2: Subsample-ordered least-angle regression (solar)

input : (Y, X)

Randomly select 20% of the points in (Y, X) to be the validation set (Y_v, X_v); denote the remaining points (Y_r, X_r);
estimate $\widehat{q}$ using Algorithm 1 on (Y_r, X_r);
for $c := 1$ *to* 0, *stepsize* $= -0.02$ **do**
    set $Q(c) = \{\mathbf{x}_j \mid \widehat{q}_j \geqslant c, \forall j\}$ and add all variables in $Q(c)$ into an OLS model;
    if *sample size of* (Y_r, X_r) *is not less than* $|Q(c)|$ **then**
        train the OLS model on (Y_r, X_r) and compute its validation error on (Y_v, X_v);
    else
        break the if-else statement and for loop
    end
end
find c^*, the value of c associated with the minimal validation error on (Y_v, X_v); find $Q(c^*)$;
return $\widehat{q}$, $\beta\left(Q\left(c^*\right), Y\right)$

Solar algorithm demo

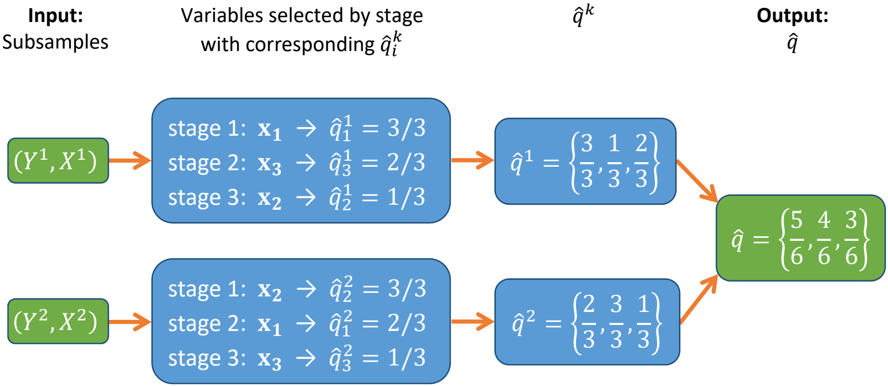


Figure: Computation of $\widehat{q}$ on 2 subsamples, where $\{\mathbf{x}_1, \mathbf{x}_2\}$ are informative and $\mathbf{x}_3$ is redundant.

Solar algorithm demo

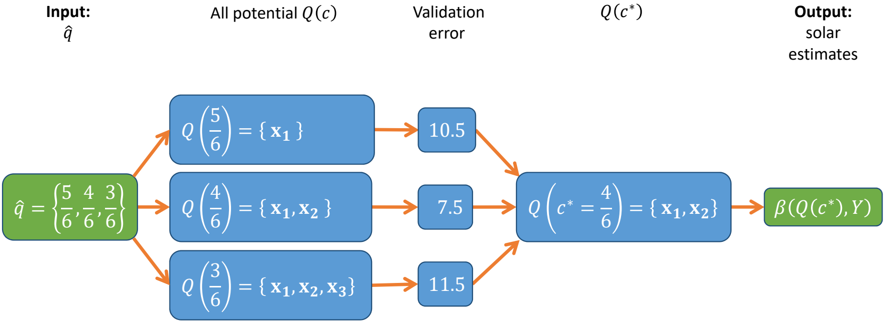


Figure: Computation flow for Algorithm 2 (continued from Figure 5).

Solar algorithm demo

- Same computation load as CV-lars-lasso: one least-angle regression on each subsample to compute $\hat{q}$; Another one for selecting variable.
- less computational expensive than coordinate descend
- My goal: outperform lasso-type estimators withouting increasing the computation load

Comparison simulation

vs CV-lars-lasso and cross-validated, cyclic pathwise coordinate descent with warm start (CV-cd, for short)

- when p/n approaches 0 ;
- when p/n approaches 1 ;
- when n and p both increase rapidly in high-dimensional space;
- when the dependence structure gets complicated and voilates the irrepresentable condition;

Simulation settings

$$Y = X\beta + e = 2\mathbf{x}_0 + 3\mathbf{x}_1 + 4\mathbf{x}_2 + 5\mathbf{x}_3 + 6\mathbf{x}_4 + e \tag{3}$$

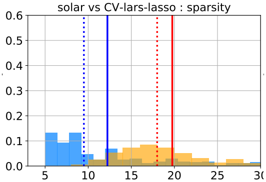
- $X \in \mathbb{R}^{n \times p}$ is generated from a zero-mean, multivariate Gaussian distribution with covariance matrix with 1 on the main diagonal and 0.5 for the off-diagonal elements.
- All data points are identically and independently distributed. Each $\mathbf{x}_j$ is independent from the noise term e, which is standard Gaussian.
- n is the sample size and p is the dimension.
- we generate 200 samples, on each of which we run lasso solvers and solar. We average the performance of each algorithm on 200 samples.

Simulation result : p/n approaching 0

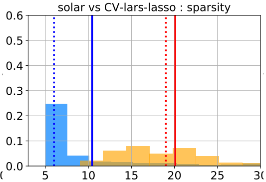
Table: Number of variables selected

		p/n		
		100/50	100/100	100/200
mean	solar	12.33	10.43	7.58
	CV-lars-lasso	19.75	20.09	19.19
	CV-cd	20.77	20.46	20.00
median	solar	9.5	6	5
	CV-lars-lasso	18	19	18
	CV-cd	18	19	18
Pr(only select $\{\mathbf{x}_0, \mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4\}$)	solar	0.025	0.305	0.560
	CV-lars-lasso	0	0	0
	CV-cd	0	0	0

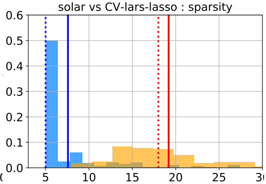
Histogram of the number of variables selected by solar



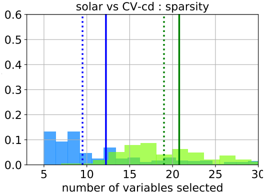
(a) $p/n = 100/50$, vs CV-lars-lasso



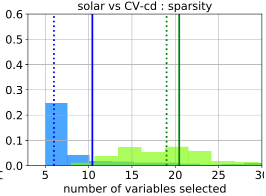
(b) $p/n = 100/100$, vs CV-lars-lasso



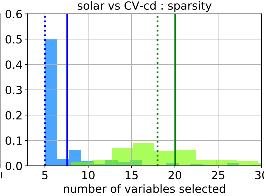
(c) $p/n = 100/200$, vs CV-lars-lasso



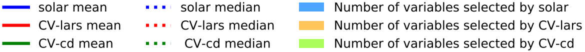
(d) $p/n = 100/50$, vs CV-cd



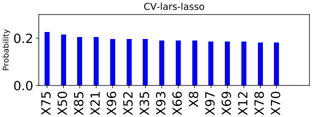
(e) $p/n = 100/100$, vs CV-cd



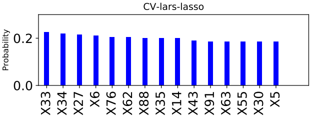
(f) $p/n = 100/200$, vs CV-cd



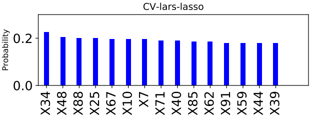
Probability of selecting redundant variables (top 15).



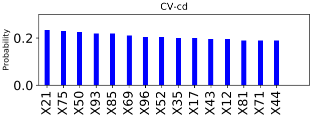
(a) $p/n = 100/50$, CV-lars-lasso



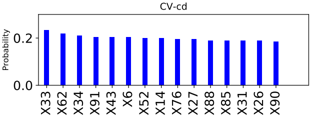
(b) $p/n = 100/100$, CV-lars-lasso



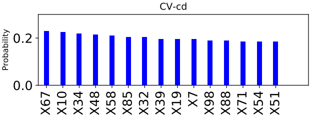
(c) $p/n = 100/200$, CV-lars-lasso



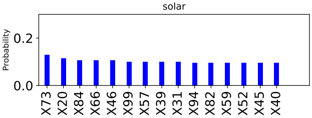
(d) $p/n = 100/50$, CV-cd



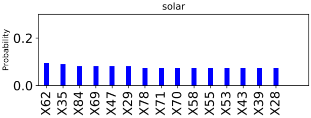
(e) $p/n = 100/100$, CV-cd



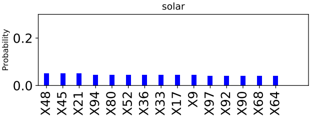
(f) $p/n = 100/200$, CV-cd



(g) $p/n = 100/50$, solar

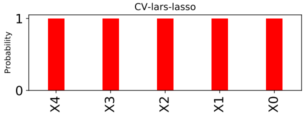


(h) $p/n = 100/100$, solar

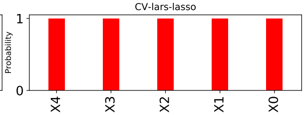


(i) $p/n = 100/200$, solar

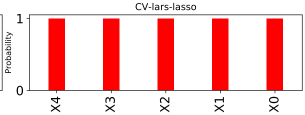
Probability of selecting informative variables.



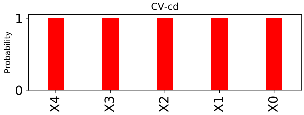
(a) $p/n = 100/50$, CV-lars-lasso



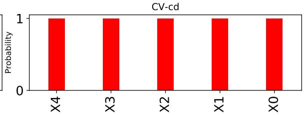
(b) $p/n = 100/100$, CV-lars-lasso



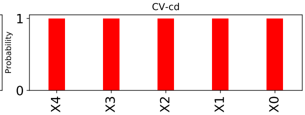
(c) $p/n = 100/200$, CV-lars-lasso



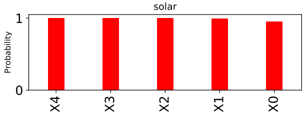
(d) $p/n = 100/50$, CV-cd



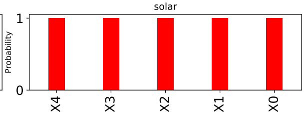
(e) $p/n = 100/100$, CV-cd



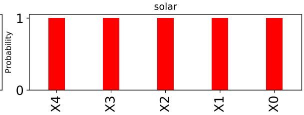
(f) $p/n = 100/200$, CV-cd



(g) $p/n = 100/50$, solar (95% for x_0 and 99.5% for x_1)

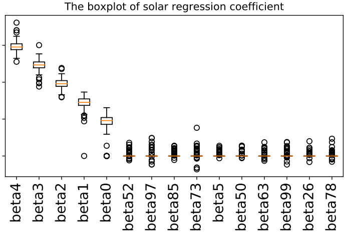


(h) $p/n = 100/100$, solar

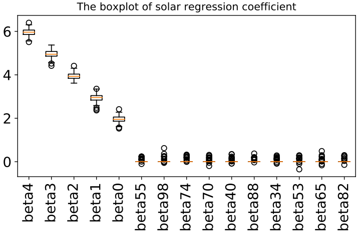


(i) $p/n = 100/200$, solar

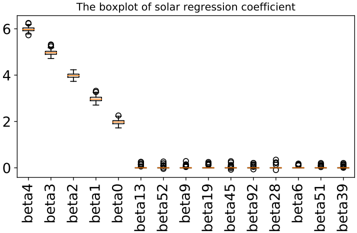
Solar regression coefficient boxplots (top 15 by mean)



(a) $p/n = 100/50$



(b) $p/n = 100/100$



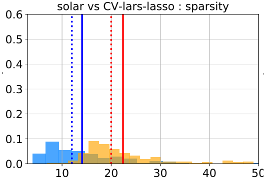
(c) $p/n = 100/200$

Simulation result: p/n approaching 1

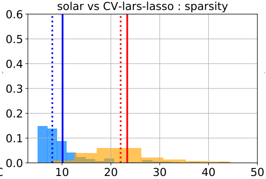
Table: Number of variables selected

		p/n		
		150/50	200/100	250/150
mean	solar	14.07	10.10	9.7
	CV-lars-lasso	22.41	23.34	25.37
	CV-cd	24.37	24.92	26.96
median	solar	12	8	6
	CV-lars-lasso	20	22	23
	CV-cd	20	22	23
Pr(only select $\{\mathbf{x}_0, \mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4\}$)	solar	0.015	0.115	0.445
	CV-lars-lasso	0	0	0
	CV-cd	0	0	0

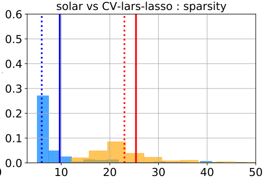
Histogram of the number of variables selected by solar



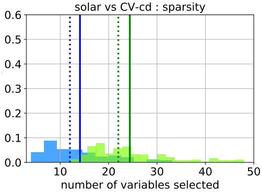
(a) $p/n = 150/50$, vs CV-lars-lasso



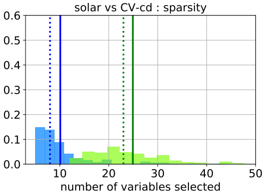
(b) $p/n = 200/100$, vs CV-lars-lasso



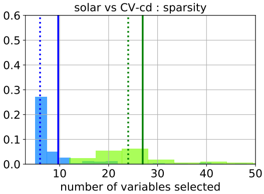
(c) $p/n = 250/150$, vs CV-lars-lasso



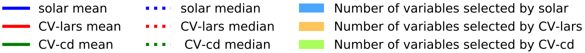
(d) $p/n = 150/50$, vs CV-cd



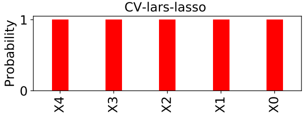
(e) $p/n = 200/100$, vs CV-cd



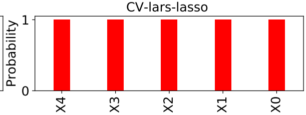
(f) $p/n = 250/150$, vs CV-cd



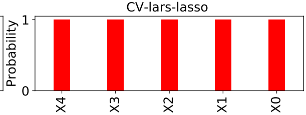
Probability of selecting informative variables



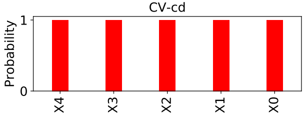
(a) $p/n = 150/50$, CV-lars-lasso



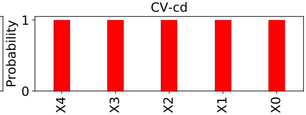
(b) $p/n = 200/100$, CV-lars-lasso



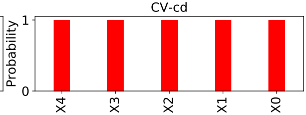
(c) $p/n = 250/150$, CV-lars-lasso



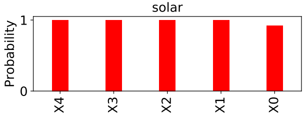
(d) $p/n = 150/50$, CV-cd



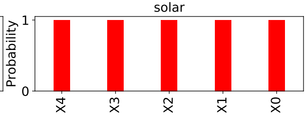
(e) $p/n = 200/100$, CV-cd



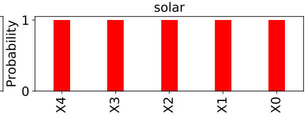
(f) $p/n = 250/150$, CV-cd



(g) $p/n = 150/50$, solar (92.01% for x_0 and 99.5% for x_1)

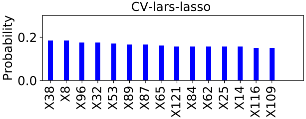


(h) $p/n = 200/100$, solar

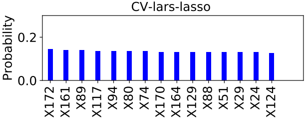


(i) $p/n = 250/150$, solar

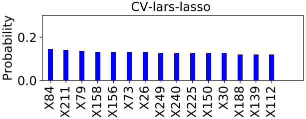
Probability of selecting redundant variables (top 15)



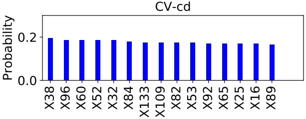
(a) $p/n = 150/50$, CV-lars-lasso



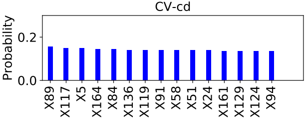
(b) $p/n = 200/100$, CV-lars-lasso



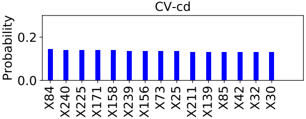
(c) $p/n = 250/150$, CV-lars-lasso



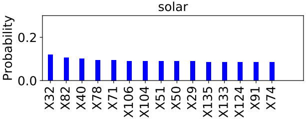
(d) $p/n = 150/50$, CV-cd



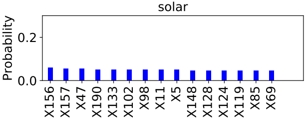
(e) $p/n = 200/100$, CV-cd



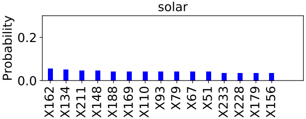
(f) $p/n = 250/150$, CV-cd



(g) $p/n = 150/50$, solar

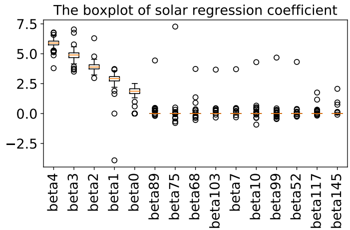


(h) $p/n = 200/100$, solar

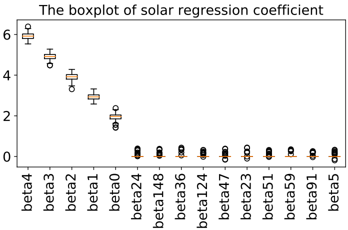


(i) $p/n = 250/150$, solar

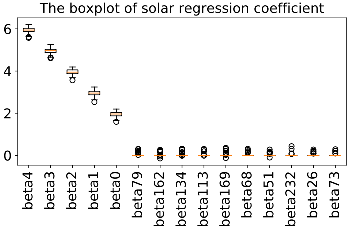
Solar regression coefficient boxplots (top 15 by mean)



(a) $p/n = 150/50$



(b) $p/n = 200/100$



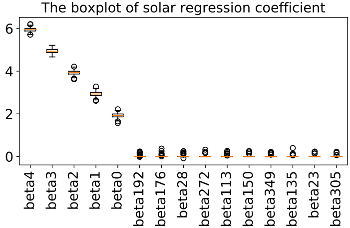
(c) $p/n = 250/150$

Simulation result: p/n does not change

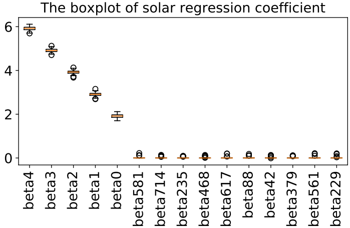
Table: Number of variables selected.

		p/n		
		400/200	800/400	1200/600
mean	solar	10.88	13.80	14.85
	CV-lars-lasso	28.17	33.13	36.90
	CV-cd	29.58	35.07	38.76
median	solar	7	11	13
	CV-lars-lasso	26	31	33
	CV-cd	26	31	33
Pr(active set $= \{\mathbf{x}_0, \mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4\}$)	solar	0.150	0.010	0
	CV-lars-lasso	0	0	0
	CV-cd	0	0	0

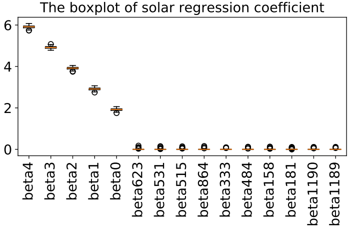
Solar regression coefficient boxplots (top 15 by mean)



(a) $p/n = 400/200$

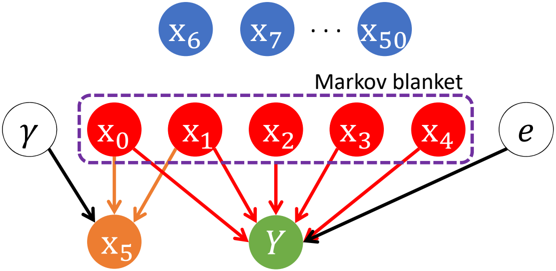


(b) $p/n = 800/400$



(c) $p/n = 1200/600$

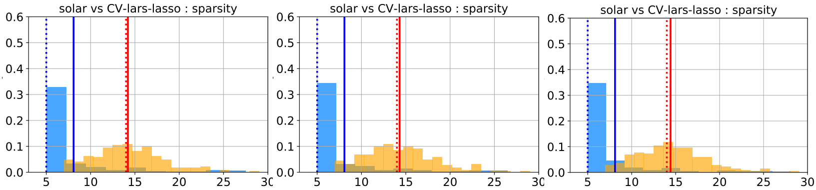
simulation setting about irrepresentable condition



$$\begin{cases} \mathbf{x}_5 = \omega_1 \mathbf{x}_0 + \omega_2 \mathbf{x}_1 + \gamma \cdot \sqrt{1 - 2\omega^2} \\ Y = 2\mathbf{x}_0 + 3\mathbf{x}_1 + 4\mathbf{x}_2 + 5\mathbf{x}_3 + 6\mathbf{x}_4 + e \end{cases} \tag{4}$$

where $n = 150$, $p = 50$, $\omega_i \in \mathbb{R}$ and γ, e are both standard Gaussian noise terms, independent from each other and all the other variables in the simulation. By setting ω_i to either $1/4$, $1/3$ or $1/2$, the population value of $\sum_i |\omega_i|$ changes, respectively, to either $1/2$, $2/3$ or 1.

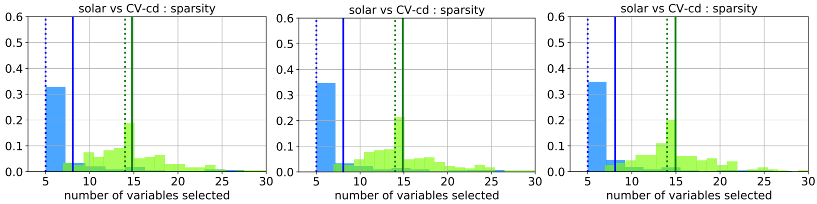
Histogram of the number of variables selected by solar



(a) $\omega = 1/4$, vs CV-lars-lasso

(b) $\omega = 1/3$, vs CV-lars-lasso

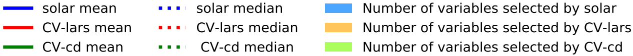
(c) $\omega = 1/2$, vs CV-lars-lasso



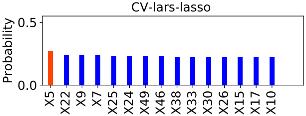
(d) $\omega = 1/4$, vs CV-cd

(e) $\omega = 1/3$, vs CV-cd

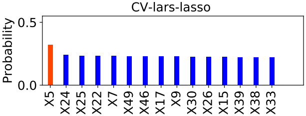
(f) $\omega = 1/2$, vs CV-cd



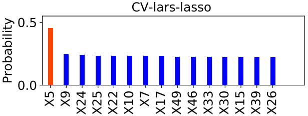
Probability of selecting redundant variables ($\mathbf{x}_5$ in orange, top 15 by probability)



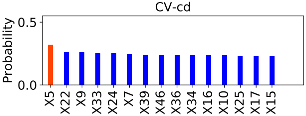
(a) $\omega = 1/4$, CV-lars-lasso



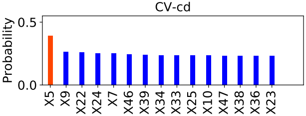
(b) $\omega = 1/3$, CV-lars-lasso



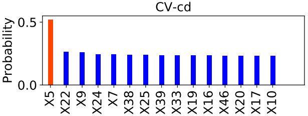
(c) $\omega = 1/2$, CV-lars-lasso



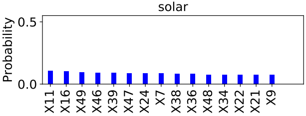
(d) $\omega = 1/4$, CV-cd



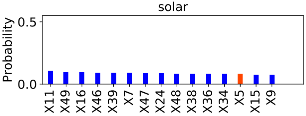
(e) $\omega = 1/3$, CV-cd



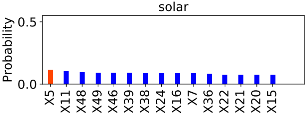
(f) $\omega = 1/2$, CV-cd



(g) $\omega = 1/4$, solar

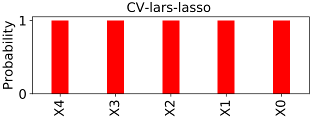


(h) $\omega = 1/3$, solar

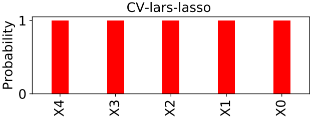


(i) $\omega = 1/2$, solar

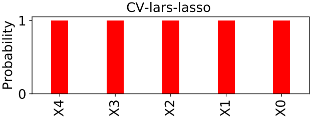
Probability of selecting informative variables



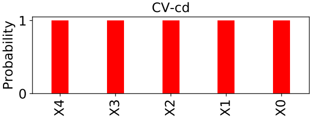
(a) $\omega = 1/4$, CV-lars-lasso



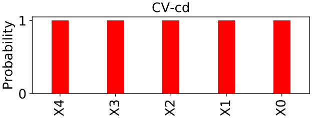
(b) $\omega = 1/3$, CV-lars-lasso



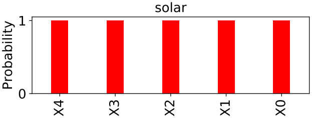
(c) $\omega = 1/2$, CV-lars-lasso



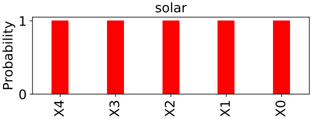
(d) $\omega = 1/4$, CV-cd



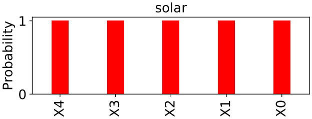
(e) $\omega = 1/3$, CV-cd



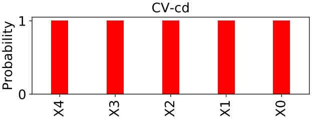
(f) $\omega = 1/2$, CV-cd



(g) $\omega = 1/4$, solar



(h) $\omega = 1/3$, solar



(i) $\omega = 1/2$, solar

Reference

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Koller, D., Friedman, N., 2009. Probabilistic graphical models: principles and techniques. MIT press.

Lim, C., Yu, B., 2016. Estimation stability with cross-validation (ESCV). Journal of Computational and Graphical Statistics 25 (2), 464–492.

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