Feature Selection under Multicollinearity & Causal Inference on Time Series

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Outline

High-dimensional Model

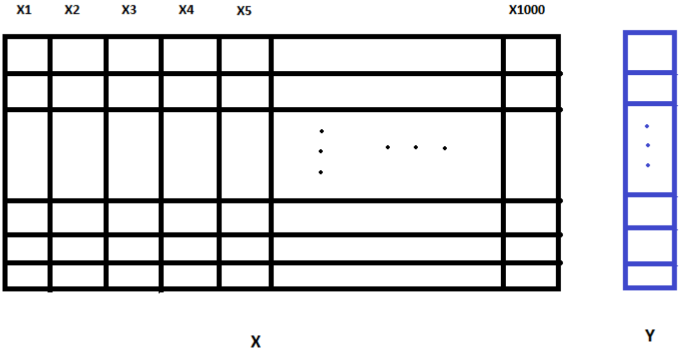

Figure: Model Estimation : $Y \approx f(X)$

Feature Selection ⇔ Sparse Estimation

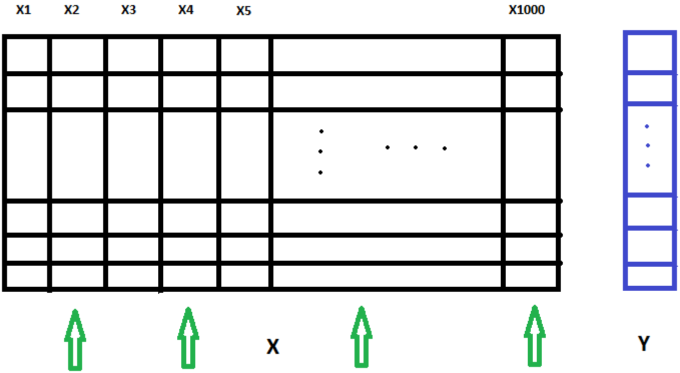

Figure: Sparse Estimation : $Y \approx f(\hat{X})$

Multicollinearity $\Leftrightarrow$ High Correlation

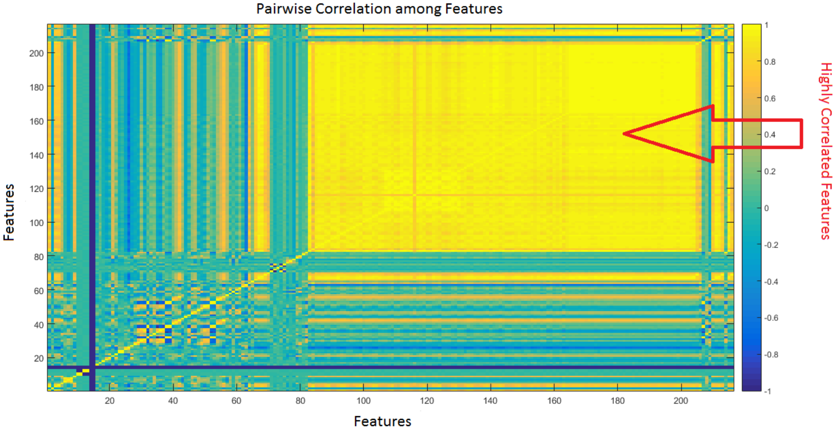

Figure: Shell Production Plant data heat map

Objective of Feature Selection

- Obtain a "sparse" and "significant" representation of output Y in terms of features from X
- Improve Prediction accuracy - balancing bias-variance trade-off
- Prevent model over-fitting issues
- Lower space and time usage
- Achieve significant savings in model training time
- Model interpretation - smaller subset shows the "big picture" - Occam's razor (Principle of Parsimony)

Challenges in Feature Selection

- Huge number of features (d) (e.g Text data)
- Lots of data points (n) too - Big data settings !
- X is a "fat matrix" ($d \gg n$)
- Strong Correlation among features - reality !
- Correlation affects consistent subset estimation
- Missing values for some data points
- Noisy observations also affects selection

Our Contribution

A new feature selection algorithm -
Bootstrap-enhanced **P**rojected **G**radient **D**escent, **BoPGD**

Our Contribution

A new feature selection algorithm -
Bootstrap-enhanced **P**rojected **G**radient **D**escent, **BoPGD**

- Offers scalability with dimensionality
- Consistent in true support recovery even when there is strong correlation among predictors
- Groups "strongly" correlated features together
- Uses re-sampling techniques to eliminate irrelevant, noisy features
- Provides a better interpretable model
- Orders of magnitude faster than existing algorithms ☺!

Outline

1. Feature Selection under Multicollinearity
   - Introduction
   - Problem Formulation
   - Existing algorithms for feature selection
   - Our algorithm - BoPGD
   - Experiments and Results
2. Causal Inference on Time Series
   - Introduction to Causality
   - Preliminaries and Model Assumptions
   - Existing approaches of Granger Causality
   - Our Concurrent Estimation Method
   - Experiments and Results

High-dimensional Sparse Estimation

- Given data points $X = [x_1, x_2, \ldots, x_n]^T$, each $x_i \in \mathcal{R}^d$
- A response vector $Y = [y_1, y_2, \ldots, y_n]^T$, each $y_i \in \mathcal{R}$
- Goal : Compute an s^*-sparse coefficient vector θ^* s.t,

$$\theta^* = \arg \min_{\theta : \|\theta\|_0 \leq s^*} f(\theta)$$

- $\|.\|_0$ is the L_0 norm function - Non-Convex in θ
- $f(\theta) = \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, \langle x_i, \theta \rangle)$ is the empirical risk function

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- Optimal estimation is infeasible due to NP-hardness ☹!

Our Model : Sparse Linear Regression

- Simple, yet useful high-dimensional linear model

$$Y = X\bar{\theta} + \zeta$$

- Loss function $f(\theta) = \frac{1}{n}\|Y - X\theta\|_2^2$
- ζ : an n-dimensional label noise vector where $\zeta_i \sim \mathcal{N}(0, \sigma^2)$

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- Goal : Jointly minimize the empirical risk and sparsity of estimation

Outline

Feature Selection methods

Broadly four main themes -

- Filter methods
- Classical methods a.k.a Wrapper methods
- Shrinkage methods a.k.a Embedded methods
- Iterative Hard-thresholding techniques a.k.a Project Gradient Descent methods [which can also be categorized as an embedded method]

Filter methods

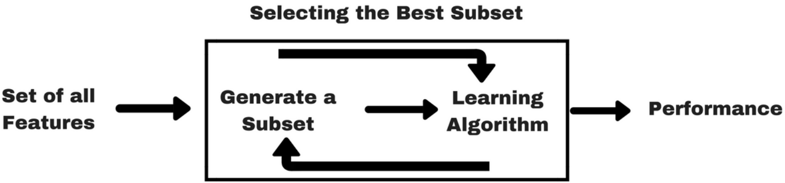
Set of all Features → **Selecting the Best Subset** → **Learning Algorithm** → **Performance**

- Feature selection done on the basis of scores in several statistical tests
- E.g.-
  - **Pearson's Correlation test** - quantifies linear dependence between two continuous-valued variables
  - **Chi-Square test** - evaluates the likelihood of correlation between two categorical variables
  - Others namely **LDA**, **ANOVA**, **Mutual Information** etc.

Drawbacks

- Determine the relevant feature subset without training a model on them
- Filter methods **do not** remove multicollinearity
- Selects all features correlated with the output
- Filter methods fail to find the best subset of features in many occasions

Classical methods

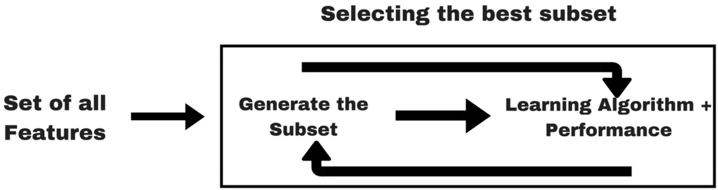


- **Best-Subset Selection** - Finds for each $k \in [d]$, the subset of size k having smallest residual sum of squares [FW00]
- **Forward or Backward Stepwise Selection** - Greedily adds (or removes) predictors one by one to the model
- **Forward Stage-wise Regression** - Iteratively identifies the variable most correlated with the current residual and adds it to the model

Drawbacks

- Infeasible when d is large ($d \approx 50$ usually works)
- "Slow-fitting" nature yields higher running time
- Sensitive to correlated variables
- Discrete process - variables either retained or discarded - often exhibits high variance
- Doesn't reduce the prediction error of the full model

Shrinkage methods



- Relax the non-convexity constraint of the L_0 norm by appropriate convex relaxations
- Promises to achieve global minima by optimizing over a larger constraint space which is convex
- Uses cross-validation to evaluate the performance of subset selection

Popular Shrinkage method based Algorithms

To name a few -

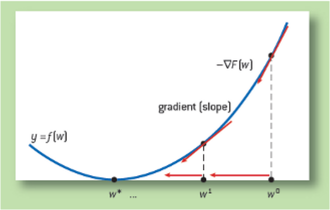
- Ridge [HK70] - L_2 norm relaxation of θ
- Lasso [Tib96] - L_1 norm relaxation of θ and its variants viz. Relaxed Lasso [Mei07], Adaptive Lasso [Zou06]
- Elastic Net [ZH05] - Combines L_1 and L_2 penalty
- OSCAR [BR08] - Combines L_1 and pairwise L_∞ norm penalization
- BoLasso [Bac08] - Bootstrap-enhanced Lasso support selection
- Cluster Representative Lasso (CRL) and Cluster Group Lasso [BRvdGZ13]

Drawbacks

- Not at all methods yield sparse solutions (e.g- ridge)
- Slower convergence rates - solves non-smooth optimization problems (e.g - Adaptive/Relaxed Lasso, OSCAR)
- Inconsistent estimation when X has high condition number - regular, sign, and pattern inconsistency (e.g - Lasso)
- Most of the methods do not take correlated structure of variables into account
- Even if some methods consider correlation (e.g CRL, CGL), they often overestimate $\hat{S}$ - lower precision and f1-score in true support recovery
- Higher running times when d is large

Off the Convex Path ...

Projected Gradient Descent (PGD) = Gradient Descent + Hard-thresholding



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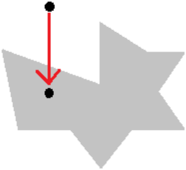

Figure: Empirical risk minimization with hard L_0 constraint

Iterative Hard-Thresholding techniques

- Iteratively do the following -
  - Gradient descent with gradient oracle
  - Hard threshold the gradient descent update onto the underlying non-convex set
- Projection can be performed efficiently for some interesting structures viz. sparsity, low rank
- Orders of magnitude faster than L_1 and greedy counterparts
- Achieves provable global guarantees when f is any arbitrary differentiable function satisfying RSC[1] and RSS[2] properties [JTK14]

[1] Restricted Strong Convexity
[2] Restricted Strong Smoothness

Outline

Our algorithm - BoPGD

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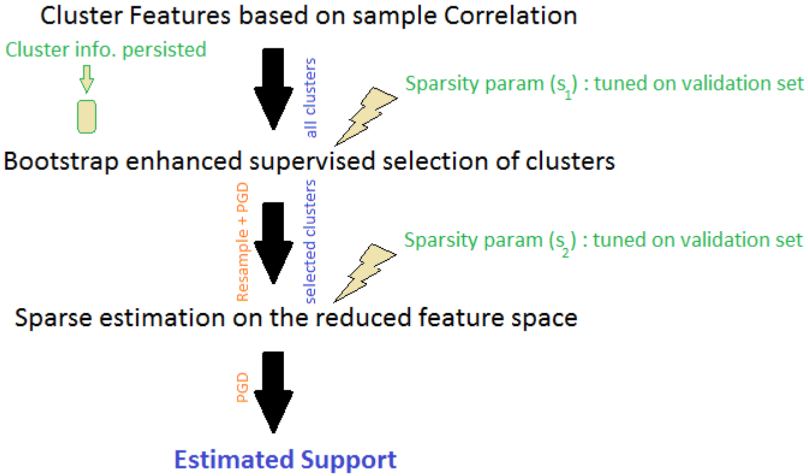
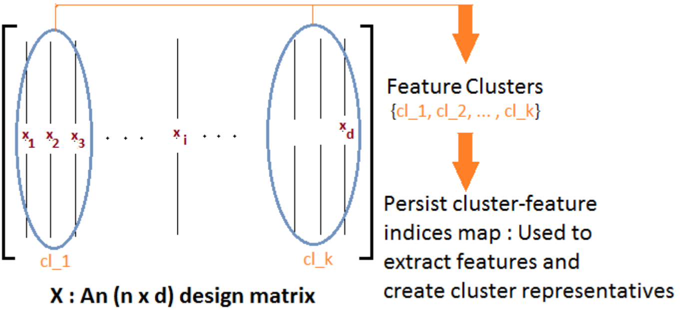
- Yields a "good" sparse model
- Scales well with the dimensionality of data

BoPGD - How it works



Clustering based on Inter-Feature Correlation

Objective : Take care of the strong correlation among the features - root cause of inconsistency in Lasso estimate !



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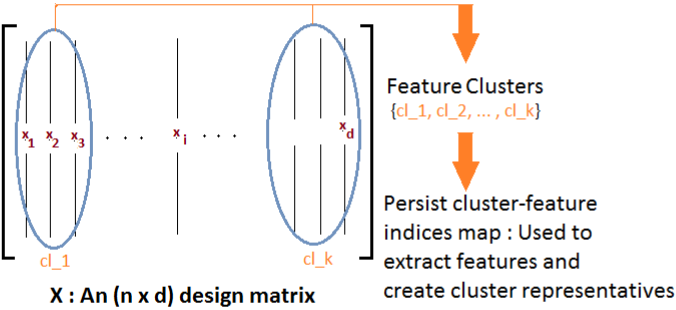
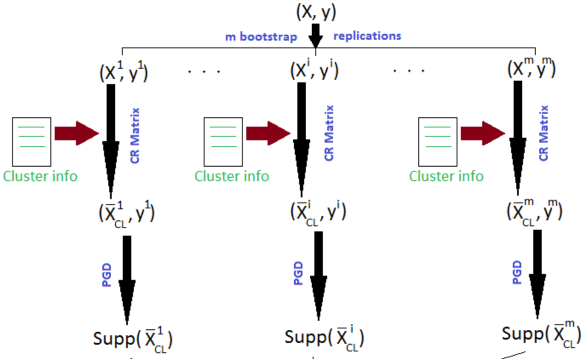


Note : $n \approx \Omega(\log d)$ to correctly cluster covariates [BRvdGZ13]

Bootstrapped Supervised Cluster Selection

Objective : Extract the significant set of feature-clusters and eliminate nuisance clusters using bootstrap based re-sampling



$$S_{CL} = \bigcap_{i=1}^{m} \mathrm{Supp}(\bar{X}^i_{CL})$$

Sparse estimation on down-sampled features

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- $\hat{\theta} = \textbf{PGD}(X_{\hat{S}^u}, s_2)$
- Sparsity parameter s_2 chosen via cross-validation - elbow point approach
- Report $\hat{S} = \{j : \hat{\theta}_j \neq 0\}$ as our "predicted" support

Outline

Evaluation Metrics

We used the following evaluation metrics :

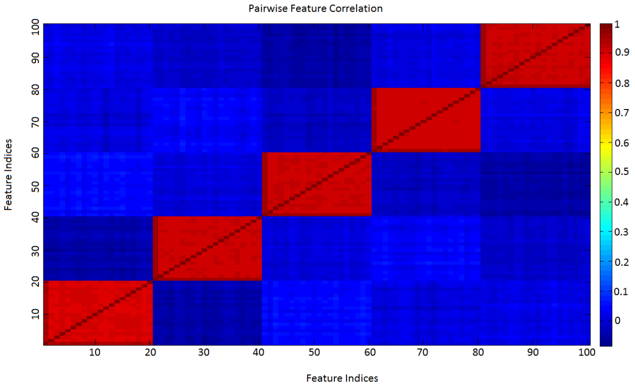
- Precision (P) $:= \frac{|\hat{S} \bigcap S^0|}{|\hat{S}|}$
- Recall (R) $:= \frac{|\hat{S} \bigcap S^0|}{|S^0|}$
- F-score $(F_1) := \frac{2PR}{P+R}$
- Mean Squared Error MSE $:= \frac{1}{n} \sum_{i=1}^{n} \mathbb{E}[(Y^i_{test} - \hat{Y}^i_{test})^2]$

where $\hat{S}$:= estimated support, S^0 := true support (if known)

Synthetic Experiments

Experiment 1. Single Block Model

- Data samples generated as $Z_i = (X_i, Y_i)$ where $X_i \sim \mathcal{N}(0, \Sigma)$ and $Y_i = \langle \theta, X_i \rangle + \zeta_i$ and $\zeta_i \sim \mathcal{N}(0, \sigma^2)$
- Σ block diagonal with high (≥ 0.85) intra-block and low (≤ 0.25) inter-block correlation



Comparison among different methods : Experiment 1

- The true support (S_0) is restricted to the first block
- $\mid S_0 \mid = 10$

Methods	**P**	**R**	**F$_1$**	**MSE**
Lasso	0.505	0.992	0.668	0.007
Elastic Net	0.464	0.996	0.631	0.006
BoLasso	0.756	0.996	0.859	0.005
CRL	0.500	1.000	0.667	0.005
PGD	0.913	0.988	0.947	0.006
BoPGD	**1.000**	0.996	**0.998**	0.006

Table: Results on Experiment 1 (averaged across 25 simulations)

Comparison among different methods : Experiment 2

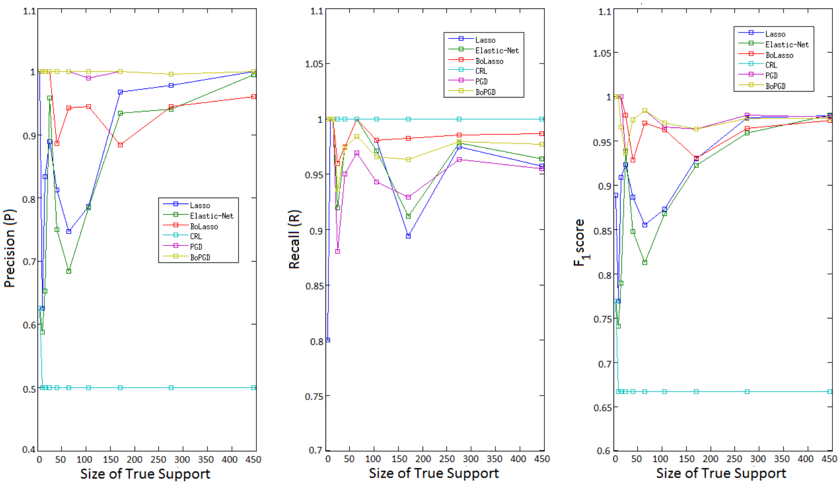
Experiment 2. Multi Block Model

- The true support is now spanned across all the five blocks
- From each block, half of the features are chosen randomly to be in support
- $\mid S_0 \mid = 50$

Methods	**P**	**R**	**F$_1$**	**MSE**
Lasso	0.710	0.941	0.809	0.013
Elastic Net	0.652	0.979	0.783	0.016
BoLasso	**0.934**	**0.921**	**0.927**	0.032
CRL	0.500	1.000	0.667	0.009
PGD	0.998	0.862	0.925	0.021
BoPGD	**0.978**	0.900	**0.938**	0.034

Table: Results on Experiment 2 (averaged across 25 simulations)

Performance of different algorithms as d varies



Experiments on Real data

Autompg data (UCI repository)

- The data concerns city-cycle fuel consumption in miles per gallon, to be predicted in terms of 3 multi-valued discrete and 5 continuous attributes
- There are 398 samples and 8 predictors viz. (2) cylinders, (3) displacement, (4) horsepower, (5) weight, (6) acceleration, (7) model year, (8) origin and (9) car name
- The target variable is (1) mpg (miles per gallon)
- Features $\{2, 3, 4, 5\}$ were strongly correlated ($\rho \geq 0.84$)
- Missing values (very less) were ignored

Results on Autompg data

Ftrs	Lasso	BoLasso	CRL	OSCAR	PGD	BoPGD
2	0	-0.716*	-0.648	-0.102	0	0
3	0	0.282*	1.890	-0.102	0.271	0.206
4	-0.002	0	-0.971	-0.102	0	0
5	-0.006	0.011	-5.285	-0.102*	-0.731	-0.661
6	0	0.082*	0	0	0	0
7	0.530	-0.007*	2.771	0.102*	0.353	0.349
8	0.387	0.160	1.174	0.061	0.163	0.166

- OSCAR does a “pretty decent” job of implicit clustering based on equality of coefficients

* marked coefficients are inconsistent (missed $\approx$ 5% of the cases)

Outline

Dependence vs Causation

"Stork deliver babies (p=0.008)" - [Mat00]

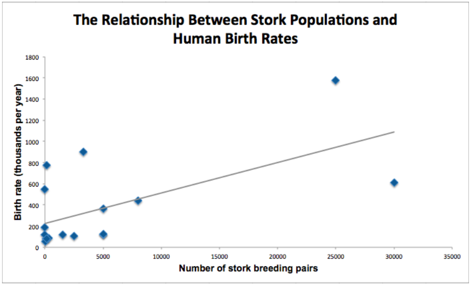


Figure: Human birth rate vs stork population across 17 European countries

Correlation $\not\Rightarrow$ Causation

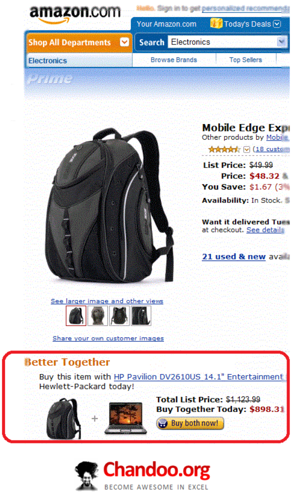


Figure: Snapshot from Amazon website (old)

Causal Inference on Time Series

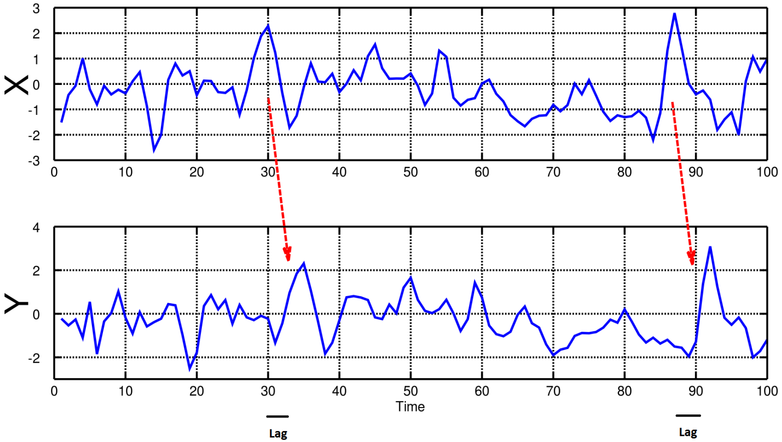


Figure: Time Series X influencing Y

From Data to Knowledge

Goal : Discover the underlying causal structure given as input large scale, high-dimensional time series data

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- Climate Change data - output the temporal causal graph of climate enforcing agents (viz. CO, CO_2, CH_4 etc.)
- Gene regulatory Network discovery given gene expression time series data
- Social influence Analysis etc.

From Data to Knowledge

Goal : Discover the underlying causal structure given as input large scale, high-dimensional time series data

- Climate Change data - output the temporal causal graph of climate enforcing agents (viz. CO, CO_2, CH_4 etc.)
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For the rest of the talk we focus only on **time series** data.

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- Effective number of features blows up with time-lagged variables
- Much more computationally intensive process
- Difficult when max lag L is unspecified or unknown

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- Both the algorithms scale well with dimensionality
- Data driven process - prior domain knowledge of the underlying physical data generating process not needed ☺!

Outline

Granger Causality [Gra69, Gra80]

- One of the most popular approaches to infer causal dependencies among time series variables
- Captures a statistical aspect of causality based on prediction
- X "granger causes" Y, denoted as $X \rightarrow Y$, if past values of X contain information that helps predict Y above and beyond that of contained in past values of Y alone
- Granger Causality principles -
  (a) The cause happens prior to the effect (Instantaneous causation is ignored !)
  (b) The cause makes unique changes in the effect

Linear Granger Causality tests - Bivariate data

- $X = \{x^t\}_{t=1}^T$, $Y = \{y^t\}_{t=1}^T$ time series variables (length T)
- $\mathbf{x}_t = [x^{(t-1)}, x^{(t-2)}, \dots, x^{(t-L)}]$, $\mathbf{y}_t = [y^{(t-1)}, y^{(t-2)}, \dots, y^{(t-L)}]$

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- Two different VAR models are fit to the Y as :

$$y^t \approx \langle \alpha, \mathbf{y}_t \rangle + \langle \beta, \mathbf{x}_t \rangle$$
$$y^t \approx \langle \gamma, \mathbf{y}_t \rangle$$

where $\alpha = [\alpha_1, \dots, \alpha_L]$, $\gamma = [\gamma_1, \dots, \gamma_L]$ and $\beta = [\beta_1, \dots, \beta_L]$

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  where $\alpha = [\alpha_1, \dots, \alpha_L]$, $\gamma = [\gamma_1, \dots, \gamma_L]$ and $\beta = [\beta_1, \dots, \beta_L]$
- Use any statistical significance tests (viz. F-statistic, χ^2 test) to ascertain whether the first model outperforms the second, and conclude X *"Granger causes"* Y

Linear Granger Causality tests - Multivariate data

- Given P time series $X_i = \{x_i^t\}_{t=1}^T, \forall i = \{1, 2, \ldots, P\}$

Linear Granger Causality tests - Multivariate data

- Given P time series $X_i = \{x_i^t\}_{t=1}^T$, $\forall i = \{1, 2, \ldots, P\}$
- A VAR model of order L is fit to X_i, $\forall t = L+1$ to T :

$$x_i^t = \sum_{j=1}^{P} \langle \beta_j^i, x_j^{(t,L)} \rangle + \epsilon_i^t$$

- $x_j^{(t,L)} = [x_j^{(t-1)}, \ldots, x_j^{(t-L)}]$ is the history of X_j up to time t
- $\beta_j^i = [\beta_j^i(1), \ldots, \beta_j^i(L)]$ is the coefficient vector
- ϵ_i^t is independent additive white noise
- No correlation among the residuals across time

Linear Granger Causality tests - Multivariate data

- Given P time series $X_i = \{x_i^t\}_{t=1}^T$, $\forall i = \{1, 2, \ldots, P\}$
- A VAR model of order L is fit to X_i, $\forall t = L+1$ to T :

$$x_i^t = \sum_{j=1}^{P} \langle \beta_j^i, x_j^{(t,L)} \rangle + \epsilon_i^t$$

- $x_j^{(t,L)} = [x_j^{(t-1)}, \ldots, x_j^{(t-L)}]$ is the history of X_j up to time t
- $\beta_j^i = [\beta_j^i(1), \ldots, \beta_j^i(L)]$ is the coefficient vector
- ϵ_i^t is independent additive white noise
- No correlation among the residuals across time
- X_j *"Granger causes"* X_i, if *at least one* value in β_j^i is *non-zero*

Outline

1. Feature Selection under Multicollinearity
   - Introduction
   - Problem Formulation
   - Existing algorithms for feature selection
   - Our algorithm - BoPGD
   - Experiments and Results
2. Causal Inference on Time Series
   - Introduction to Causality
   - Preliminaries and Model Assumptions
   - Existing approaches of Granger Causality
   - Our Concurrent Estimation Method
   - Experiments and Results

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- Lasso Granger [ALA07]
  - Lasso type formulation identifies sparse neighborhood structure
- Group Lasso Granger [LALR09]
  - Uses Group Lasso to leverage the group structure among the variables according to the time series they belong to

Lasso Granger Method [ALA07]

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$$\min_{\beta} \sum_{t=L+1}^{T} \left(x_i^t - \sum_{j=1}^{P} \langle \beta_j^i, x_j^{(t,L)} \rangle \right)^2 + \lambda \|\beta\|_1$$

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- Considers the natural *group structure* existing among the variables imposed by the respective time series they belong to
- Applies Group Lasso ([YL06]) type formulation
- Consider a partitioning of the set of predictors $\{x_1, \ldots, x_P\}$ into J groups
- Optimization problem of Group Lasso Granger :

$$\min_{\beta} \sum_{t=L+1}^{T} \left(x_i^t - \sum_{j=1}^{P} \langle \beta_j^i, x_j^{(t,L)} \rangle\right)^2 + \lambda \sum_{j=1}^{J} \sqrt{\rho_j}\, \left\|\beta_{\mathbb{G}_j}\right\|_2$$

- ρ_j accounts for the varying group size

Merits and Demerits

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Limitations :

- All the methods assume L is known beforehand
- Small values of L are considered in these models
- Pairwise tests instead of the full model yields spurious causality (e.g - exhaustive granger)
- Common Lag choice for all the features (e.g VAR granger) - unrealistic assumption !
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Advantages :

- Lasso and Group Lasso are consistent in sparse neighborhood selection [MB06]

Outline

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- We present two algorithms in this context :
  - **Lasso Granger++ :** Adapting Lasso Granger method to unknown lag
  - **Group Lasso Granger++ :** Extension of Group Lasso Granger method with unknown lag

Our method with initial lag L_0

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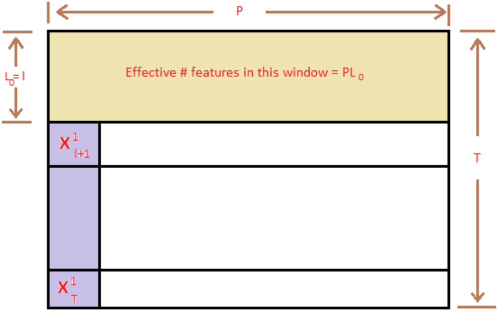

Figure: Lasso Granger++ with initial guess L_0

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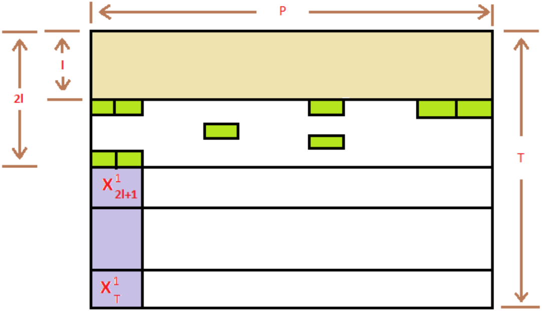


Figure: Lasso Granger++ with next guess L_1

Key points

- Choice of λ plays in key role in both the Lasso and Group Lasso routines - chosen via AIC(c)
- For each L_i we choose the "best" λ using AIC(c) [Aka98] score
- We select "best" maxlag $\hat{L}_i$ for X_i using minimum AIC(c) score

Space Complexity Analysis

Space complexity (κ) is :

$$\kappa = \mathcal{O}\Bigg(\sum_{j=1}^{\frac{T-2}{\ell}} (P\ell + s_{j-1})\Bigg), \quad where \quad 0 \le s_{j-1} \ll P(j-1)\ell$$

$$= \mathcal{O}\Bigg(T \max_j \big(P, \frac{s}{\ell}\big)\Bigg), \quad where \quad s = \max_j s_{j-1}$$

which is significantly smaller than $\frac{PT^2}{\ell}$ (brute force approach)

Time Complexity Analysis

Time complexity τ is :

$$\tau = \mathcal{O}\left(\sum_{j=1}^{\frac{T-2}{\ell}} (T - j\ell)(P\ell + s_{j-1})^2 \right), \quad where \quad 0 \leq s_{j-1} \ll P(j-1)\ell$$

$$= \mathcal{O}\left(T^2 \max_j \left(P^2\ell, \frac{s^2}{\ell}, Ps \right) \right), \quad where \quad s = \max_j s_{j-1}$$

which is significantly smaller than $\frac{P^2T^4}{\ell}$ (brute force approach)

Outline

Evaluation Criteria

- Let A denote the adjacency matrix of the source (original) feature causal graph
- Let $\hat{A}$ denote the same for the hypothesis (output) graph
- Precision (P) := $\frac{|\{(i,j) \in V \times V : \hat{A}(i,j) = A(i,j)\}|}{|\{(i,j) \in V \times V : \hat{A}(i,j) = 1\}|}$
- Recall (R) := $\frac{|\{(i,j) \in V \times V : \hat{A}(i,j) = A(i,j)\}|}{|\{(i,j) \in V \times V : A(i,j) = 1\}|}$
- F_1 score := $\frac{2PR}{P+R}$

Experiment 1

- We used one of the most cited benchmark datasets [Set10]
- 5 time series variables with small lags
- Ground truth is :

Variables	Causal Subset	Indiv. Lags	MaxLag
X_1	$\{X_1\}$	$\{1, 2\}$	2
X_2	$\{X_1\}$	$\{2\}$	2
X_3	$\{X_1\}$	$\{3\}$	3
X_4	$\{X_1, X_4, X_5\}$	$\{2, 1, 1\}$	2
X_5	$\{X_4, X_5\}$	$\{1, 1\}$	1

Results of Experiment 1

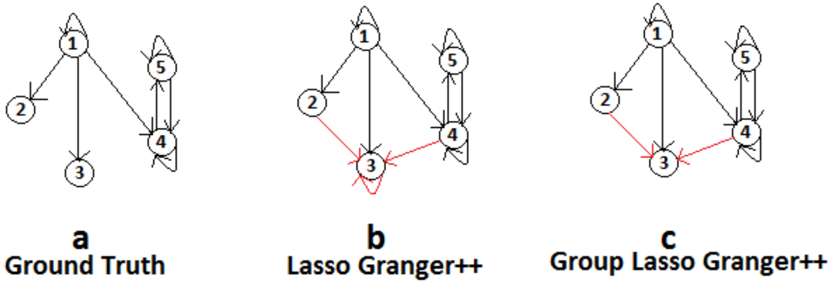


Figure: Ground Truth and the Hypothesis Causal Graphs inferred

Results of Experiment 1 - Contd ...

- Lasso Granger++ Lag prediction accuracy = 100%
- Group Lasso Granger++ Lag prediction accuracy = 100%

Methods	P	R	F_1
Lasso Granger++	0.727	1.000	0.842
Group Lasso Granger++	0.800	1.000	0.888
Standard Lasso Granger (L fixed)	0.701	1.000	0.821
Standard Group Lasso Granger (L fixed)	0.803	1.000	0.889

Table: Results on Experiment 1 (averaged across 10 simulations)

Experiment 2

- A star graph with 5 time series variables
- X_1 is the only target variable causally influenced by all other variables
- Variables $\{X_2, \ldots, X_5\}$ are independent noise processes
- Substantially different time lags along each edge from $X_j \to X_1$, $j \in \{2, \ldots, 5\}$
- Lag values chosen from $[1, 50]$ u.a.r (e.g. $L_2 = 46, L_3 = 7, L_4 = 46, L_5 = 32$)

Lasso Granger++ performance

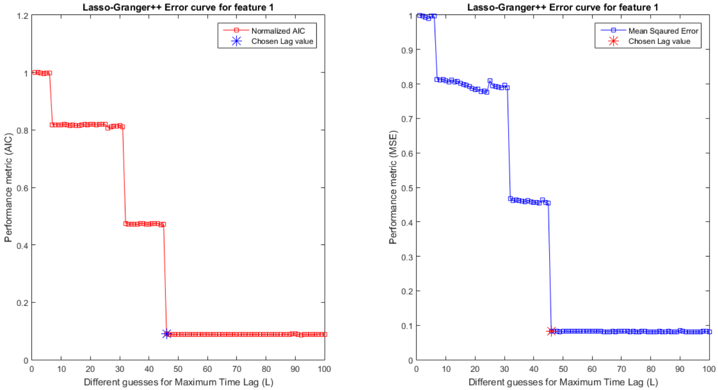
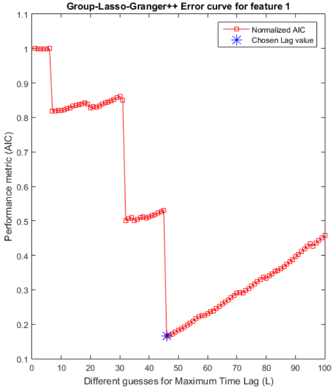


Figure: Lasso Granger++ step-wise error curve

Group Lasso Granger++ performance



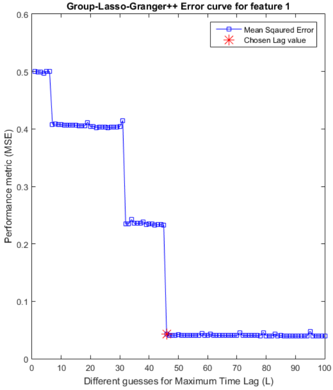
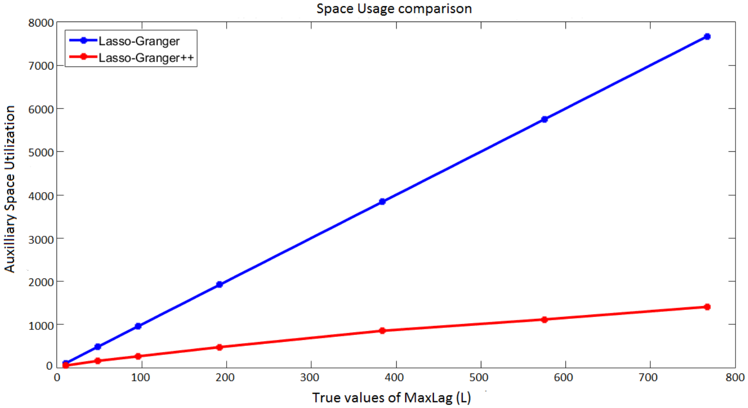


Figure: Group Lasso Granger++ step-wise error curve

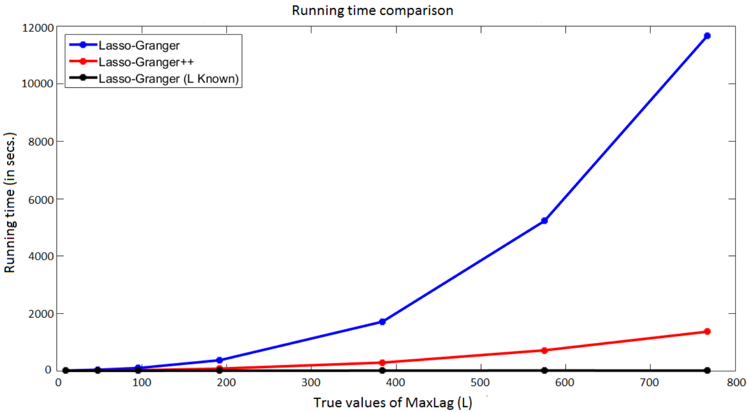
Performance tests of our Method I

1. Space Usage as a function of L



Performance tests of our Method II

2. Running time as a function of L



Publications based on the Thesis

Machine Learning and Statistical Analysis for Materials Science : Stability Analysis, Fingerprint Descriptors and Chemical Insights
- Published in The Journal of Chemistry of Materials, 2017
Authors : Praveen Pankajakshan, Suchismita Sanyal, Onno E. de Noord, Indranil Bhattacharya, Arnab Bhattacharyya, Umesh Waghmare.

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Thank You ☺!

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