

CORREG: Linear regression with highly correlated covariates

Clément THERY

April 26, 2014

To my sons,

Contents

1	Abstracts	4
2	Acknowledgments	5
3	The industrial context	6
4	State of the art	7
4.1	Ordinary least squares and associated problems	7
4.2	Penalized models	7
4.2.1	Ridge regression	7
4.2.2	LASSO: Least Absolute Shrinkage and Selection Operator	7
4.2.3	Adaptative LASSO and Random LASSO	7
4.2.4	Elasticnet	7
4.2.5	OSCAR: Octogonal Shrinkage and Clustering Algorithm for Regression	7
4.3	Modeling the parameters	7
4.3.1	CLERE: CLusterwise Effect REgression	7
4.3.2	Spike and Slab	8
4.4	Multiple Equations	8
4.4.1	SEM and Path Analysis	8
4.4.2	SUR: Seemingly Unrelated Regression	8
4.4.3	SPRING: Structured selection of Primordial Relationships IN the General linear model	8
4.4.4	Selvarclust: Linear regression within covariates for clustering	8
I	CorReg : the concept	9
5	Decorrelating covariates by a generative model	10
5.1	Generative model	10
5.2	Properties	10
5.2.1	general properties	10
5.2.2	Identifiability	10
5.3	About grouping effect	10
6	Estimation of the Structure of subregression by MCMC	11
6.1	How to compare structures ?	11
6.1.1	Bayesian criterion for quality	11
6.1.2	Some indicators for proximity	11
6.2	Neighbourhood	11
6.2.1	Classical	11
6.2.2	Active relaxation of the constraints	11
6.3	The walk	11
6.4	Numerical results	11

II	Further usage of the structure	12
7	Taking back the residuals	13
7.1	The model	13
7.2	Properties	13
7.3	Consistency	13
7.3.1	Consistency Issues	13
7.4	Numerical results	14
8	Missing values	15
8.1	How to manage missing values in the MCMC ?	15
8.1.1	Position of the missing value	15
8.1.2	Weighted penalty	15
8.1.3	Parameters estimation	16
8.2	Missing values in the main regression	16
8.2.1	explicative	16
8.2.2	predictive	16
9	CorReg: the package and its application in steel industry	17
9.1	CORREG package for R	17
9.2	Application in steel industry	17
9.2.1	The dataset	17
9.2.2	Found Structure	17
9.2.3	Results	17
10	Conclusion and perspectives	18
11	References	19
12	Appendices	22
12.1	Graphs and CorReg	22
12.1.1	Matricial notations	22
12.1.2	Properties	22
12.2	Mixture models	22
12.2.1	Linear combination	22
12.2.2	Industrial examples	22

Chapter 1

Abstracts

Chapter 2

Acknowledgments

Chapter 3

The industrial context

This work takes place in a steel industry context. The main objective is to be able to solve quality crisis when they occur. In such a case, a new type of unknown quality issue is observed and we have no idea of its origin. The defects, even generated at the beginning of the process, are often detected in its last part. The steel-making process includes several sub-process, each implying a whole manufactory. Thus we have many covariates and no a priori on the relevant ones. Moreover, the values of each covariates essentially depends on the characteristics of the final product, and many physical laws and tuning models are implied in the process. Therefore the covariates are highly correlated. We have several constraints :

- To be able to predict the defect and stop the process as early as possible to gain time (and money)
- To be able to understand the origin of the defect to try to optimize the process
- To be able to find parameters that can be changed because the objective is not only to understand but to correct the problematic part of the process.
- It also must be fast and automatic (without any a priori).

We will see in the state of the art that correlations are a real issue and that the number of variables increases the problem. The stakes are very high because of the high productivity of the steel plants but also because steel making is now well-known and optimized thus new defects only appears on innovative steels with high value. Any improvement on such crisis can have important impact on the market shares and when the customer is implied, each day won by the automation of the data mining process can lead to a gain of hundreds of thousands of euros, sometimes more. So we really need a kind of automatic method, able to manage the correlations without any a priori and giving an easily understandable and flexible model.

Chapter 4

State of the art

In the following we note classical norms: $\| \beta \|_2^2 = \sum_{i=1}^p (\beta_i)^2$, $\| \beta \|_1 = \sum_{i=1}^p |\beta_i|$ and $\| \beta \|_\infty = \max(|\beta_1|, \dots, |\beta_p|)$.

4.1 Ordinary least squares and associated problems

Linear regression is defined by this simple equation:

$$Y = X\beta + \varepsilon_Y \quad (4.1)$$

where $Y \in \mathbf{R}^n$ is the response variable vector observed on n individuals.

4.2 Penalized models

4.2.1 Ridge regression

[6] [8]

4.2.2 LASSO: Least Absolute Shrinkage and Selection Operator

[14] [13] [4] [19][18]

4.2.3 Adaptative LASSO and Random LASSO

[20][15]

4.2.4 Elasticnet

[21]

4.2.5 OSCAR: Octogonal Shrinkage and Clustering Algorithm for Regression

Like elasticnet, OSCAR [1] uses combination of two norms for its penalty. Here the objective is to group covariates with the same effect and give them exactly the same coefficient (reducing the dimension) with a simultaneous variable selection (group with null coefficient).

$$\hat{\beta} = \operatorname{argmin}_{\beta} \| Y - X\beta \|^2 \text{ subject to } \sum_{j=1}^p |\beta_j| + c \sum_{j < k} \max(|\beta_j|, |\beta_k|) \leq \lambda \quad (4.2)$$

4.3 Modeling the parameters

4.3.1 CLERE: CLusterwise Effect REgression

[16]

4.3.2 Spike and Slab

[7]

4.4 Multiple Equations

4.4.1 SEM and Path Analysis

4.4.2 SUR: Seemingly Unrelated Regression

[17]

4.4.3 SPRING: Structured selection of Primordial Relationships IN the General linear model

[2]

4.4.4 Selvarclust: Linear regression within covariates for clustering

[9] The idea is to allow covariates to have different roles : (S, R, U, W) . But:

- It is about clustering and not regression (not the same application field)
- No sub-regression allowed between relevant variables (in the True model)
- Using stepwise-like algorithm without protection against correlations [12] even it is known to be often unstable [11]

We provide an specific MCMC algorithm with the ability to have redundant covariates in the true model.

Part I

CorReg : the concept

Chapter 5

Decorrelating covariates by a generative model

5.1 Generative model

5.2 Properties

5.2.1 general properties

5.2.2 Identifiability

5.3 About grouping effect

Chapter 6

Estimation of the Structure of subregression by MCMC

6.1 How to compare structures ?

6.1.1 Bayesian criterion for quality

6.1.2 Some indicators for proximity

6.2 Neighbourhood

6.2.1 Classical

6.2.2 Active relaxation of the constraints

6.3 The walk

6.4 Numerical results

Part II

Further usage of the structure

Chapter 7

Taking back the residuals

7.1 The model

7.2 Properties

7.3 Consistency

7.3.1 Consistency Issues

Consistency issues of the LASSO are well known and Zhao [19] gives a very simple example to illustrate it. We have taken the same example to show how our method is more consistent. Here $p = 3$ and $n = 1000$. We define $\mathbf{X}_f, \mathbf{X}_r, \boldsymbol{\varepsilon}_Y, \boldsymbol{\varepsilon}_X i.i.d. \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_n)$ and then $X_3 = \frac{2}{3}X_1 + \frac{2}{3}X_2 + \frac{1}{3}\varepsilon_X$ and $Y = 2X_1 + 3X_2 + \varepsilon_Y$. We compare consistencies of complete, explicative and predictive model with LASSO (and LAR) for selection. It happens that the algorithm don't find the true structure but a permuted one so we also look at the results obtained with the true S (but \hat{B} is used) and with the structure found by the Markov chain after a few seconds.

True S is found 340 times on 1000 tries.

	Classical LASSO	CORREG Explicative	CORREG Predictive
True S	1.006479	1.005468	1.006093
\hat{Z}	1.006479	1.884175	1.006517

Table 7.1: MSE observer on a validation sample (1000 individuals)

We observe as we hoped that explicative model is better when using true S (coercing real zeros) and that explicative with \hat{S} is penalized (coercing wrong coefficients to be zeros). But the main point is that the predictive model stay better than the classical one whith the true S and corrects enough the explicative model to follow the classical LASSO closely when using \hat{S} . And when we look at the consistency :

	Classical LASSO	Explicative	Predictive
True S	0	1000	830
\hat{S}	0	340	621

Table 7.2: number of consistent model found (Y depending on X_1, X_2 and only them) on 1000 tries

299 times on 1000 tries, the predictive model using \hat{S} is better than classical LASSO in terms of MSE and consistent (classical LASSO is never consistent).

We also made the same experiment but with X_1, X_2 (and consequently X_3) following gaussian mixtures (to improve identifiability) randomly generated by our CORREG package for R. True S is now found 714 times on 1000 tries . So it confirms that non-gaussian models are easier to identify.

And when we look at the consistency :

	Classical LASSO	Explicative	Predictive
True S	1.571029	1.569559	1.570801
\hat{S}	1.005402	1.465768	1.005066

Table 7.3: MSE observed on a validation sample (1000 individuals)

	Classical LASSO	Explicative	Predictive
True S	0	1000	789
\hat{S}	0	714	608

Table 7.4: number of consistent model found (Y depending on X_1, X_2 and only them) on 1000 tries

299 times on 1000 tries, the predictive model using \hat{S} is better than classical LASSO in terms of MSE and consistent (classical LASSO is never consistent).

7.4 Numerical results

Chapter 8

Missing values

Missing values are a very recurrent issue in industry. We note M the binary matrix indicating whereas a value is missing (1) or not (0).

8.1 How to manage missing values in the MCMC ?

8.1.1 Position of the missing value

In the MCMC we need to compute the likelihood of the structure. When missing values occurs, we restrict the likelihood to the known values. So we look at each non-missing value separately. Each value is seen as different random variable noted $x_{i,j}$. But the structure itself makes things more complicated because known values are not all *iid* (if $j \in I_2$). For a given structure S , missing values can imply different consequences according to their position in the dataset. To compute the likelihood of a value $x_{i,j}$ in the dataset :

- if $M_{i,j} = 1$: $x_{i,j}$ is not considered because we restrict the likelihood to known values.
- else if $j \in I_1$: like in previous method, we use the density estimated (*e.g.* a Gaussian Mixture model estimated by MIXMOD) for X^j . Values in X^j are *iid*.
- else :

$$x_{i,j}|X_{i,I_1^j} \sim \sum_{\substack{1 \leq k \leq p \\ B_k^j \neq 0}} x_{i,k} B_k^j + \mathcal{N}(0; \sigma_j) \quad (8.1)$$

$$= \sum_{\substack{1 \leq k \leq p \\ B_k^j \neq 0 \\ M_{i,k} \neq 0}} x_{i,k} B_k^j + \mathcal{N}\left(\sum_{\substack{1 \leq k \leq p \\ B_k^j \neq 0 \\ M_{i,k} = 0}} x_{i,k} B_k^j ; \sigma_j\right) \quad (8.2)$$

$$(8.3)$$

8.1.2 Weighted penalty

Now we have defined the way to compute the likelihood, other questions remain : how to define the number of parameters in the structure ? How to take into account missingness (structures relying on highly missing covariates should be penalized) ? We have seen that for a same covariate X^j with $j \in I_2$, the number of parameters is not the same for each individual depending whether or not $M_{i,j} = 0$. But the penalty (for $\psi = BIC$) can't be added at the individual level (because $\log(1) = 0$ so it would be annihilated).

To penalize models that suppose dependencies based only on a few individuals, we propose to use the mean of the complexities obtained for a given covariate. Thus if a structure is only touched by one missing value the penalty will be smaller than another same shaped structure but with more missing values implied. Another way would be to use $\psi = RIC$ (see [5]) so the complexity is associated with

$\log(p)$ and can be added individually. Another idea would be to make a compromise and penalize by $\frac{k_i \log(p)}{\log(n)}$.

8.1.3 Parameters estimation

Estimating B with missing values is just estimating independent regressions with missing values. We have seen in equation (8.2) that we know the expression of this density for a given B . So it's just about maximizing the likelihood of this density on B . This can be done with an Expectation-Maximization (EM) [3] or one of its extensions [10]. But estimation of B is the most critical part of the MCMC in terms of computational time so it could be dangerous to put there another iterative algorithm. Alternatives does exist :

- Because sub-regression are supposed to be simple, we could imagine to use estimate each column of B with full submatrices of X . When relying on too much missing values, \hat{B} would be a bad candidates and then penalized directly by the likelihood (and it could be a good thing). Computational cost would be reduced significantly.
- To estimate B (and not for the global likelihood) we could use data imputation (by the mean) and then obtain a full matrix but still ignoring missing values when estimating the likelihood.

8.2 Missing values in the main regression

8.2.1 explicative

The reduced model (explicative one) is just a linear regression without structure so the method used for \hat{B} can also be used here.

8.2.2 predictive

Chapter 9

CorReg: the package and its application in steel industry

9.1 CorReg package for R

CORREG is already downloadable on the CRAN under CeCILL Licensing. This package permits to generate datasets according to our generative model, to estimate the structure (C++ code) of regression within a given dataset and to estimate both explicative and predictive model with many regression tools (OLS, stepwise, LASSO, elasticnet, clere, spike and slab, adaptative lasso and every models in the LARS package). So every simulation presented above can be done with CORREG. CORREG also provides tools to interpret found structures and visualize the dataset (missing values and correlations). More informations can be found on the website www.correg.org which is dedicated to CORREG.

9.2 Application in steel industry

9.2.1 The dataset

9.2.2 Found Structure

9.2.3 Results

Chapter 10

Conclusion and perspectives

Chapter 11

References

Bibliography

- [1] H.D. Bondell and B.J. Reich. Simultaneous regression shrinkage, variable selection, and supervised clustering of predictors with oscar. *Biometrics*, 64(1):115–123, 2008.
- [2] Mary-Huard T. Chiquet J. and Robin S. Multi-trait genomic selection via multivariate regression with structured regularization. *Proceedings of MLCB/NIPS'13 workshop*, 2013.
- [3] A.P. Dempster, N.M. Laird, D.B. Rubin, et al. Maximum likelihood from incomplete data via the em algorithm. *Journal of the Royal statistical Society*, 39(1):1–38, 1977.
- [4] B. Efron, T. Hastie, I. Johnstone, and R. Tibshirani. Least angle regression. *The Annals of statistics*, 32(2):407–499, 2004.
- [5] D.P. Foster and E.I. George. The risk inflation criterion for multiple regression. *The Annals of Statistics*, pages 1947–1975, 1994.
- [6] A.E. Hoerl and R.W. Kennard. Ridge regression: applications to nonorthogonal problems. *Technometrics*, pages 69–82, 1970.
- [7] H. Ishwaran and J.S. Rao. Spike and slab variable selection: frequentist and bayesian strategies. *Annals of Statistics*, pages 730–773, 2005.
- [8] D.W. Marquardt and R.D. Snee. Ridge regression in practice. *American Statistician*, pages 3–20, 1975.
- [9] Cathy Maugis, Gilles Celeux, and M-L Martin-Magniette. Variable selection in model-based clustering: A general variable role modeling. *Computational Statistics & Data Analysis*, 53(11):3872–3882, 2009.
- [10] G. McLachlan and T. Krishnan. *The EM algorithm and extensions*, volume 382. John Wiley & Sons, 2007.
- [11] Alan Miller. *Subset selection in regression*. CRC Press, 2002.
- [12] Adrian E Raftery and Nema Dean. Variable selection for model-based clustering. *Journal of the American Statistical Association*, 101(473):168–178, 2006.
- [13] R. Tibshirani. Regression shrinkage and selection via the lasso. *Journal of the Royal Statistical Society. Series B (Methodological)*, pages 267–288, 1996.
- [14] R. Tibshirani, G.N. Hoefling, P. Wang, and D. Witten. The lasso: some novel algorithms and applications.
- [15] S. Wang, B. Nan, S. Rosset, and J. Zhu. Random lasso. *The annals of applied statistics*, 5(1):468, 2011.
- [16] L. Yengo, J. Jacques, C. Biernacki, et al. Variable clustering in high dimensional linear regression models. 2012.
- [17] A. Zellner. An efficient method of estimating seemingly unrelated regressions and tests for aggregation bias. *Journal of the American statistical Association*, pages 348–368, 1962.

- [18] Yongli Zhang and Xiaotong Shen. Model selection procedure for high-dimensional data. *Statistical Analysis and Data Mining*, 3(5):350–358, 2010.
- [19] P. Zhao and B. Yu. On model selection consistency of lasso. *J. Mach. Learn. Res.*, 7:2541–2563, December 2006.
- [20] H. Zou. The adaptive lasso and its oracle properties. *Journal of the American statistical association*, 101(476):1418–1429, 2006.
- [21] H. Zou and T. Hastie. Regularization and variable selection via the elastic net. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 67(2):301–320, 2005.

Chapter 12

Appendices

12.1 Graphs and CorReg

12.1.1 Matricial notations

12.1.2 Properties

12.2 Mixture models

12.2.1 Linear combination

12.2.2 Industrial examples