# On Variable Selection and Effective Estimations of Interactive and Quadratic Sensitivity Coefficients: A Collection of Regularized Regression Techniques

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# Background for variable selection and sensitivity estimation

- For parametric uncertainties the curse of dimensionality is still a problem
  - This is especially true for pairwise interactions and second-order sensitivity coefficients
- In some problems in engineered systems, high order sensitivity coefficients and variable significance are important
- Two potential ways: perturbation theory and random sampling based estimation
  - High order perturbation theory could be hard to implement in multiphysics codes
  - Random sampling based estimation equipped with regression is simple to implement, but for second-order and interaction coefficients, multi-collinearity leads to ill-conditioned problems.
- Our focus: regularized regressions
  - Add small constraints to the regression could bring in numerical stability and well-posedness
  - Different constraints result in different estimation process and results

- The general regression problem is written as

$$\mathbf{Y} = \mathbf{X}\beta + \varepsilon \tag{1}$$

- $\mathbf{Y}$: data (outcomes), $\mathbf{X}$: input matrix, $\beta$: regression coefficients, $\varepsilon$: errors
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$$\mathbf{Y} = \begin{pmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{pmatrix}, \quad \mathbf{X} = \begin{pmatrix} 1 & X_{11} & X_{12} & \cdots & X_{1p} \\ 1 & X_{21} & X_{22} & \cdots & X_{2p} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & X_{n1} & X_{n2} & \cdots & X_{np} \end{pmatrix}, \quad \beta = \begin{pmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{pmatrix} \quad \text{ar} \tag{2}$$

- $n$ is number of samples and $p$ is the number of independent variables
- Regression aim: estimate the coefficients, $\beta$, in Eq. (1).

# Conditioning Issues and Ordinary Least Squares

- The direct "solve" by ordinary least squares (OLS)

$$\beta \approx (\mathbf{X}^{\mathbf{T}}\mathbf{X})^{-1}\mathbf{X}^{\mathbf{T}}\mathbf{Y}.$$

- Several common situations can make OLS ill-conditioned or ill-posed:
  - $n < p$: Number of samples is smaller than number of parameters
  - $\mathbf{X}$ contains interdependencies, i.e., multi-collinearity, if high order terms are included
  - In either case, $\mathbf{X}^{\mathbf{T}}\mathbf{X}$ is rank deficient and not invertible
  - Alternative approaches like the pseudo-inverse can give unreasonable results as has been demonstrated in previous work.
- A possible cure is regularization: change the regression problem to make the system well-posed *and* give it better properties.

# Basic ideas

- Another way to think of OLS regression is as the minimizer of the $\ell_2$ norm of the error between the fit and the original data:

$$\beta = \underset{\beta}{\operatorname{argmin}} \|\mathbf{Y} - \mathbf{X}\beta\|_2^2 \tag{3}$$

  - Equivalent to a direct solve of the regression problem: $\beta_{\text{OLS}} = (X^T X)^{-1} X^T Y$
  - Ineffective and inaccurate for ill-conditioned problems
- Regularization: add additional information
  - Add a constraint term to the Lagrangian or cost function of the minimization problem
  - Different types of constraints have different effects
  - Certain regularizations can guarantee well-posedness.

# Non-Bayesian Regularization Regression Approaches

In these methods we explicitly change the minimization problem.

- Lasso regression (OLS plus an $\ell_1$ penalty based on size of $\beta$'s):

$$\beta = \underset{\beta}{\operatorname{argmin}}\{\|\mathbf{Y} - \mathbf{X}\beta\|_2^2 + \lambda_1\|\beta\|_1\} \tag{4}$$

- Ridge regression (OLS plus an $\ell_2$ penalty based on size of $\beta$'s):

$$\beta = \underset{\beta}{\operatorname{argmin}}\{\|\mathbf{Y} - \mathbf{X}\beta\|_2^2 + \lambda_2\|\beta\|_2^2\} \tag{5}$$

- Elastic net regression (Combination of Lasso and Ridge):

$$\beta = \underset{\beta}{\operatorname{argmin}}\left\{\|\mathbf{Y} - \mathbf{X}\beta\|_2^2 + \alpha\lambda_1\|\beta\|_1 + (1-\alpha)\lambda_2\|\beta\|_2^2\right\} \tag{6}$$

- Dantzig selector (Minimize $\ell_\infty$ error in fit with $\ell_1$ penalty on $\beta$'s):

$$\beta = \underset{\beta}{\operatorname{argmin}}\{\|\beta^T(\mathbf{Y} - \mathbf{X}\beta)\|_\infty + \lambda_1\|\beta\|_1\} \tag{7}$$

# Non-Bayesian Regularization Regression Approaches (cont'd)

- Non-Bayesian L-2 norm constraint put too much strength on limiting parameters with higher magnitudes: over-penalization

# Bayesian Regularization Regression Approaches

- The Bayesian version of regularized-regressions differs from non-Bayesian in the sense that hyperparameters, i.e. $\lambda$, are sampled in the Bayesian inference process.
- In other words, the Bayesian methods take similar forms to the non-Bayesian problems, but estimate the parameters through a Bayesian framework.
- Bayesian theory:

$$p(\beta|D) = \frac{p(D|\beta)p(\beta)}{\int d\beta \; p(D|\beta)p(\beta)} \tag{8}$$

- Bayesian inference short introduction:
  - Sample realizations of parameters from priors
  - Calculate posteriors
  - Modify the priors for the next iteration and repeat until reaching the maximum iteration
  - Do statistics with the results from the iterations

Bayesian lasso prior and posterior:

$$p(\beta|\sigma^2,\lambda_1) = \prod_{j=1}^{p} \frac{\lambda_1}{2\sqrt{\sigma^2}} \exp\left\{-\frac{\lambda_1|\beta_j|}{\sqrt{\sigma^2}}\right\} \tag{9a}$$

$$p(\beta|\sigma^2,\lambda_1,\mathbf{Y},\mathbf{X}) \propto \exp\left\{-\frac{1}{2\sigma^2}\|\mathbf{Y}-\mathbf{X}\beta\|_2^2 - \frac{\lambda_1\|\beta\|_1}{\sqrt{\sigma^2}}\right\} \tag{9b}$$

Bayesian ridge prior and posterior:

$$p(\beta|\sigma^2,\lambda_2) = \left(\frac{\lambda_2}{2\pi\sigma^2}\right)^{(n+1)/2} \exp\left\{-\frac{\lambda_2}{2\sigma^2}\|\beta\|_2^2\right\} \tag{10a}$$

$$p(\beta|\sigma^2,\lambda_2,\mathbf{Y},\mathbf{X}) \propto \exp\left\{-\frac{1}{2\sigma^2}\|\mathbf{Y}-\mathbf{X}\beta\|_2^2 - \frac{\lambda_2\|\beta\|_2^2}{\sigma^2}\right\} \tag{10b}$$

# Bayesian Regularization Regression Approaches

Automatic relevance determination (ARD) prior and posterior

$$p(\beta|\sigma^2, \lambda_2) \propto \exp\left\{-\sum_{j=1}^{p} \frac{\lambda_2}{2\sigma_j^2}|\beta_j|^2\right\}, \tag{11a}$$

$$p(\beta|\sigma^2, \lambda_2, \mathbf{Y}, \mathbf{X}) \propto \exp\left\{-\frac{1}{2\sigma^2}\|\mathbf{Y} - \mathbf{X}\beta\|_2^2 - \sum_{j=1}^{p} \frac{\lambda_2}{2\sigma_j^2}|\beta_j|^2\right\} \tag{11b}$$

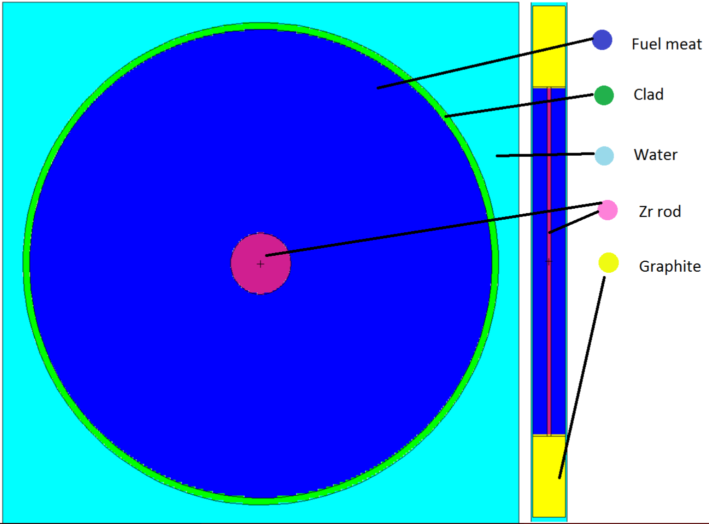
- ARD is very similar to Ridge regression except that it has a different $\sigma_j$, controlling the variance, for each variable.

# Section 2

# Problem settings

Lattice of TRIGA fuels pin modeled with MCNP

- QoI: $k_{\text{eff}}$



# Problem descriptions

There are 299 sensitivity coefficients taken into account in this problem:

- 23 input parameters:
  - 6 geometric parameters: e.g. r-fuel (fuel radius)
  - 17 material parameters: e.g. $\rho-\mathrm{Zr}$ (Zr rod mass density)
- 253 pairwise interactions (23 choose 2)
- 23 quadratic terms

The aim is to investigate the sensitivity of the criticality to the parameters, especially the second order terms. The model is:

$$\frac{\delta k}{k} \approx \sum_{i=1}^{23} c_i \left(\frac{\delta x_i}{x_i}\right) + \sum_{i=1}^{22} \sum_{j=i+1}^{23} c_{ij} \left(\frac{\delta x_i}{x_i}\right)\left(\frac{\delta x_j}{x_j}\right) + \sum_{i=1}^{23} c_{ii} \left(\frac{\delta x_i}{x_i}\right)^2 \quad (12)$$

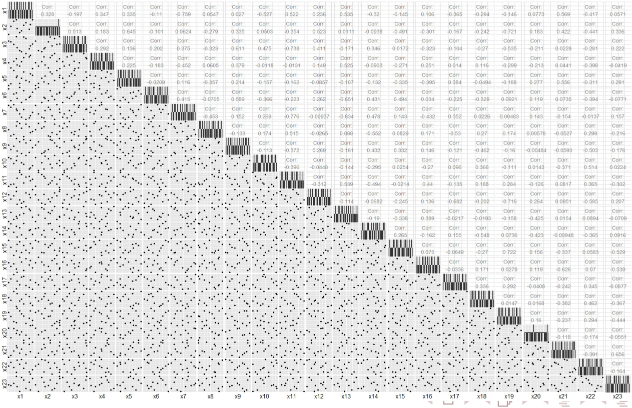
where $c_i$, $c_{ij}$ and $c_{ii}, i = 1, \cdots, 23, j \neq i$, are the first order, interactive and quadratic sensitivity coefficients, respectively.

# Reference data

- We are going to compare reference sensitivity coefficients to the coefficients computed by various regularized regression techniques using many few code runs (cases).
- The reference coefficients are computed using 1058 cases.
    - We need 46 total simulations for the linear and quadratic parameters
    - 1012 simulations are needed for the 253 interactions (4 simulations for each)
- The goal of this research is to see if regularized regression techniques can give coefficient estimates close to the references using many fewer simulation runs than the 1058 cases.

# Quasi-uniform multi-D sampling

- For the regression results we sample from the 23 parameters using by Latin Hypercube sampling.
- For any number of samples we fit the entire 299-sample sensitivity model for $k_{\text{eff}}$.
- A 12-sample example is shown below. 2D projections are uniform.



# Section 3

# Variable Selection

- One use of sensitivity analysis is to down-select from the large parametric uncertainty space to a smaller set of important parameters.
- After this variable selection process, a more detailed study can be performed on the important variables.
- In our case we would like to use a small number of samples (code-runs) to select the important variables.
- Below we'll discuss the selection of significant pairwise interaction and quadratic terms.

# Variable Selection: Interaction Terms

- Coefficients with a magnitude above 10% of the highest magnitude (from corresponding method) will be selected as significant.
- Reference result has 15 significant pairwise interactions

# Variable Selection: Interactions (cont'd)

| | True Positive | | | | | False Positive | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Sample size | OLS | Lasso | Ridge | DS | EN | OLS | Lasso | Ridge | DS | EN |
| 50 | 0 | 1 | 0 | 0 | 3 | 22 | 17 | 0 | 0 | 22 |
| 100 | 5 | 3 | 0 | 3 | 3 | 98 | 12 | 0 | 12 | 15 |
| 150 | 5 | 3 | 0 | 3 | 3 | 120 | 5 | 0 | 6 | 7 |
| 200 | 7 | 3 | 2 | 5 | 4 | 119 | 1 | 2 | 9 | 3 |
| 250 | 7 | 3 | 2 | 6 | 3 | 91 | 0 | 0 | 2 | 3 |
| 299 | 6 | 5 | 3 | 8 | 5 | 161 | 0 | 2 | 3 | 0 |

- Least square regression (OLS): gives hundreds of false positives
- Regularization helps remove false positives, though no method gets all 15 true parameters using the small number of samples considered.
- Lasso: 5 right with 0 wrong
- Dantzig selector (DS): more true positives with 3 wrong picks (borderline picks)
- Ridge: only 3 true positives but 2 false negatives: over-penalization

# Variable Selection: Interactions (cont'd)

| | True Positives | | | | | False Positives | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Sample size | OLS | Lasso | BRidge | BLasso | ARD | OLS | Lasso | BRidge | BLasso | ARD |
| 50 | 0 | 1 | 5 | 5 | 1 | 22 | 17 | 71 | 58 | 29 |
| 100 | 5 | 3 | 3 | 4 | 1 | 98 | 12 | 2 | 0 | 16 |
| 150 | 5 | 3 | 7 | 6 | 3 | 120 | 5 | 3 | 4 | 5 |
| 200 | 7 | 3 | 8 | 8 | 3 | 119 | 1 | 3 | 3 | 0 |
| 250 | 7 | 3 | 8 | 8 | 1 | 91 | 0 | 2 | 2 | 0 |
| 299 | 6 | 5 | 8 | 8 | 2 | 161 | 0 | 4 | 2 | 0 |

- Bayesian ridge and Bayesian lasso are comparable as both get 8 correct parameters at 200 samples.
- ARD seems makes most conservative picks: small false positives and small true positives.

# Variable Selection: Quadratic

- Same 10% threshold from interaction case.
- Reference result has 3 significant variables

| | True Positive | | | | | False Positive | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Sample size | OLS | Lasso | Ridge | DS | EN | OLS | Lasso | Ridge | DS | EN |
| 50 | 2 | 1 | 2 | 0 | 0 | 15 | 17 | 16 | 0 | 1 |
| 100 | 3 | 2 | 3 | 2 | 2 | 17 | 12 | 18 | 2 | 2 |
| 150 | 3 | 2 | 3 | 2 | 2 | 18 | 5 | 14 | 1 | 1 |
| 200 | 3 | 2 | 3 | 3 | 2 | 15 | 1 | 20 | 0 | 0 |
| 250 | 3 | 2 | 3 | 3 | 2 | 12 | 0 | 19 | 1 | 0 |
| 299 | 2 | 3 | 3 | 3 | 3 | 15 | 0 | 16 | 4 | 0 |

- OLS and Ridge not useful in this case.
- Lasso and elastic net converge to the correct answer.
- Dantzig selector does have a high number of false positives with 299 samples, but these could be borderline cases (near 10%)

# Variable Selection: Quadratic (cont'd)

| | True Positives | | | | | False Positives | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Sample size | OLS | Lasso | BRidge | BLasso | ARD | OLS | Lasso | BRidge | BLasso | ARD |
| 50 | 2 | 1 | 1 | 2 | 0 | 15 | 17 | 5 | 11 | 3 |
| 100 | 3 | 2 | 3 | 3 | 0 | 17 | 12 | 1 | 2 | 2 |
| 150 | 3 | 2 | 3 | 3 | 1 | 18 | 5 | 2 | 2 | 0 |
| 200 | 3 | 2 | 3 | 3 | 2 | 15 | 1 | 2 | 2 | 0 |
| 250 | 3 | 2 | 3 | 3 | 1 | 12 | 0 | 3 | 3 | 0 |
| 299 | 2 | 3 | 3 | 3 | 1 | 15 | 0 | 2 | 3 | 0 |

- BLasso, BRidge: similar with DS, borderline picks
- ARD: conservative

# Coefficient estimation

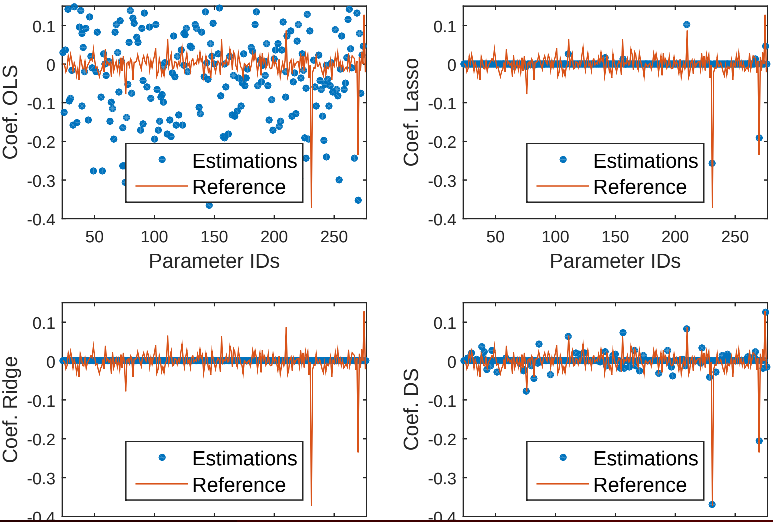
Now we ask a more difficult question of the methods: estimate the numeric value of the coefficients and compare with the reference result.

- Each parameter is assigned an ID
- IDs from 24 to 276: interactive coefficients
- IDs from 277 to 299: quadratic coefficients

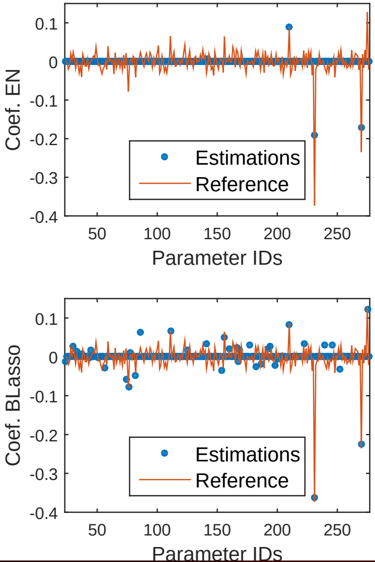
The results that follow all use 299 samples, about 28% of those used in the reference calculation.

# Coefficient Estimation: Interactions

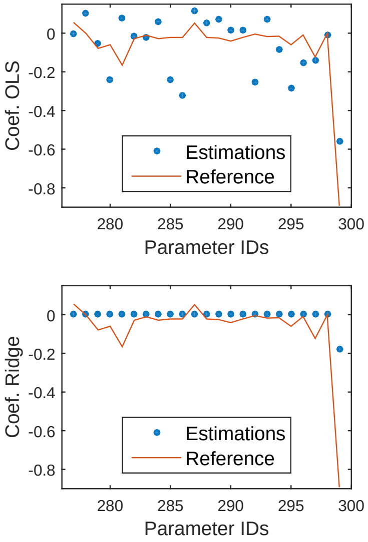
Blue dots are regression estimations, red lines are reference



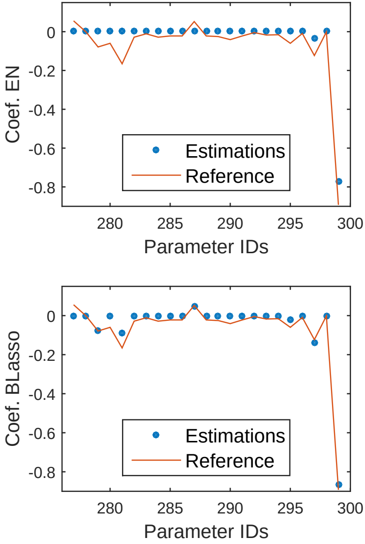
# Coefficient Estimation: Interactions (cont'd)



# Coefficient Estimation: Quadratic



# Coefficient estimation: quadratic (cont'd)



# Section 4

# Summaries

- Investigated seven types of regularization methods on second order variable selection and sensitivity coefficient estimations.
- On variable selection, we found Bayesian lasso, Bayesian ridge, Dantzig selector and elastic net are promising and comparable to lasso, a commonly used method in the statistics community.
- On coefficient estimation:
    - L-2 norm regularized methods: ARD and ridge are too conservative
        - Ridge has over-penalization
    - Lasso and EN present similar estimations that selects significant variables out but not with correct magnitudes
    - Dantzig selector, Bayesian lasso and Bayesian ridge present similar high accuracy on second order coefficient estimations
        - BRidge fixes the over-penalization

# Future work

- Other regularizations are worth investigation: e.g. $\ell_{0.5}$ "norm"
- Apply the methods with nuclear data sensitivity research
  - Include impact of covariances
  - Even higher dimensional problems common.

# Thank you!

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