Bayesian approaches for variable selection and shrinkage: An investigation of milk composition traits using infrared spectroscopy analysis

Yogasudha Veturi

&

Alessandro Ferragina

High dimensional data

- *p* > > *n; curse of dimensionality!*
- Microarray data, deep sequencing, biomedical imaging, high-frequency data in finance
- OLS performs poorly in both prediction and interpretation
- Variable selection and/or shrinkage estimation procedure needed

Variable selection and shrinkage procedures

- Penalized
  - LASSO, ridge regression, elastic net
- Bayesian
  - BayesA, BayesB, BayesC, Bayesian LASSO
- Semi-/nonparametric
  - Neural Networks, random forests, support vector regression, reproducing kernel Hilbert spaces

Variable selection and shrinkage procedures

- Penalized
  - LASSO, ridge regression, elastic net
- Bayesian
  - BayesA, BayesB, BayesC, Bayesian LASSO
- Semi-parametric approaches
  - Neural Networks, random forests, support vector regression, reproducing kernel Hilbert spaces

Bias-variance trade-off

- $MSE(\theta) = Var(\theta) + [Bias(\theta)]^2$
- Using OLS, for fixed *n*, as *p* increases, variance of estimates increases -> high MSE
- If estimates are shrunk towards zero, variance of estimator is reduced, although bias may increase
- E.g. Consider $\theta = \alpha(\theta) + (1-\alpha)0 \ \alpha \in [0,1]$
- $\mathrm{E}(\theta) = \alpha\theta$; $\mathrm{Var}(\theta) = \alpha^2 \, Var(\theta)$

de los Campos, Gustavo, et al. *Genetics* 193.2 (2013): 327-345.

Penalty/prior

- Different penalties / priors -> different solutions
- Choice of penalty/prior is based on:
  - Model comparison
    - model interpretation
    - model parsimony
    - Accuracy of predictions on future data
  - Parameter estimation
- Bayesian setting is more useful for parameter estimation

Penalized methods

$$(\mu,\beta)\downarrow argmin\{\sum i\uparrow\blacksquare(y\downarrow i-\mu-\sum j=1\uparrow p\blacksquare x\downarrow ij\ \beta\downarrow j\ )\uparrow 2+\lambda J(\beta)\}$$

- $J(\beta)$ = penalty function
- λ = regularization parameter (controls trade-offs between lack of fit and model complexity)
- Choice of penalty determines extent of shrinkage and/or variable selection

Penalized Estimators	$J(\beta)$
Bridge Regression	$\sum j=1 \uparrow p \blacksquare \lvert \beta \downarrow j \rvert \uparrow \gamma$
LASSO	$(\gamma=1)\ \sum j=1 \uparrow p \blacksquare \lvert \beta \downarrow j \rvert$
Ridge Regression	$(\gamma=2)\ \sum j=1 \uparrow p \blacksquare \beta \downarrow j \uparrow 2$
Subset selection	$(\gamma \rightarrow 0) \sum j=1 \uparrow p \blacksquare I(\beta \downarrow j \neq 0)$
Elastic Net	$\alpha \sum j=1 \uparrow p \blacksquare \lvert \beta \downarrow j \rvert + (1-\alpha) \sum j=1 \uparrow p \blacksquare \beta \downarrow j \uparrow 2$

LASSO

- Does both shrinkage and variable selection simultaneously

…however…

- Only selects *n* variables before it saturates
- Constraints on bound of the L1-norm
- Does not work well with correlated predictors - does not reveal grouping information
- Might result in low prediction power when $p > > n$

Ridge regression

- Better bias-variance trade-off than LASSO

…however…

- Keeps all variables in the model (no variable selection); model parsimony is not achieved

Subset selection

- Produces a sparse model
- Penalizes non-zero effects regardless of magnitude

…however…

- Only selects *n* variables before it saturates (like the LASSO)

Elastic Net

- Simultaneously does variable selection and shrinkage
- Can select groups of correlated variables; retains the "big fish"
- Algorithm "LARS-EN" can create the entire elastic net path with the computational efforts of a single OLS fit
- Also a good classifier; e.g. with microarray data, can do automatic gene selection (unlike other popular classifiers like LASSO, SVM, penalized logistic regression, nearest shrunken centroid)

…however…

Doesn't select related variables when the within-group correlations are non-extreme $(\rho \approx 0.85)$

Bayesian methods

$$p(\mu,\beta,\sigma^2 \mid y,\omega) \propto p(y \mid \mu,\beta,\sigma^2)\ p(\mu,\beta,\sigma^2 \mid \omega) \propto p(\sigma^2) \prod_{j=1}^{p} p(\beta_j \mid \omega)\ p(\sigma^2)$$

$$\prod_{i=1}^{n} N(y_i \mid \mu + \sum_{j=1}^{p} x_{ij}\beta_j,$$

Likelihood function

Prior distribution

Distribution of the unknowns given the data and hyper-parameters

Bayesian Estimators	$p\beta\downarrow j\ \omega$
Spike Slab models	$\pi N\beta\downarrow j\ 0,\ \sigma\downarrow\beta\downarrow 1\ \uparrow 2\ +(1-\pi)N\beta\downarrow j\ 0,\sigma\downarrow\beta\downarrow 2$
Bayes B	$\pi t\downarrow df,S+(1-\pi)I(\beta\downarrow j=0)$
Bayes A	$(\pi=1)\ t\downarrow df,S$
Bayes C	$(df\rightarrow\infty)\ \pi N\beta\downarrow j\ 0,\ \sigma\downarrow\beta\uparrow 2 +(1-\pi)I(\beta\downarrow j=0)$
Bayesian Ridge Regression	$(\pi=1,\ df\rightarrow\infty)\ N\beta\downarrow j\ 0,\sigma\downarrow\beta\uparrow 2$
Bayesian LASSO	Double-exponential

Gaussian prior (Bayesian Ridge Regression)

- Multivariate normal with posterior mean same as the RR with $\lambda=\sigma^2/\sigma^2\downarrow\beta$.
- Homogeneous shrinkage across markers
- May not be useful when correlation patterns vary across the dataset

Thick tailed priors (Bayes A and Bayesian LASSO)

- Higher mass at zero and thicker tails
  - Bayesian LASSO has posterior mean same as LASSO
- Induces less shrinkage of large effect estimates than BRR
- Commonly represented as infinite mixtures of scaled normal densities
- Scaled *t* (2 parameters) has more flexibility than DE to control the thickness of the tails

Spike slab priors

- Mixture of two densities; one with small variance (spike) and the other with large variance (slab)
- Combines variable selection and shrinkage
- Can mix Gaussian or non-Gaussian (e.g. scaled-*t* and double exponential) components

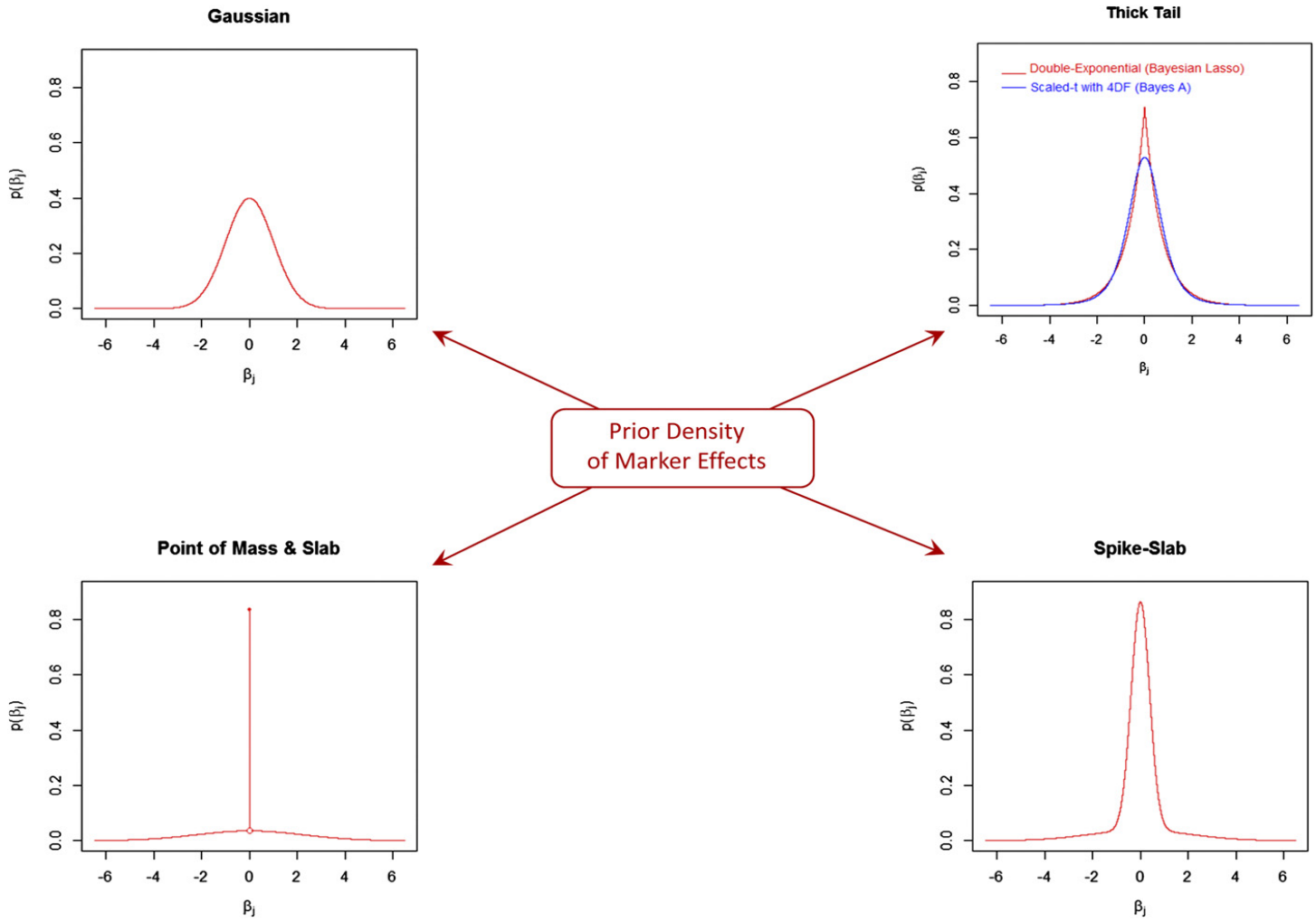
Point of mass and slab priors (Bayes B and Bayes C)

- Obtained from spike-slab models when

$(\sigma\downarrow\beta\downarrow 1\ \uparrow 2 \rightarrow 0)$

- Again, induce a combination of variable selection and shrinkage

Comparison of priors



de los Campos, Gustavo, et al. *Genetics* 193.2 (2013): 327-345.