Bayesian approaches for variable selection and shrinkage

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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

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Bias-variance trade-off

- $MSE(\hat{\theta}) = Var(\hat{\theta}) + [Bias(\hat{\theta})]^2$
- 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 $\tilde{\theta} = \alpha(\hat{\theta}) + (1 - \alpha)0 \ \alpha \in [0,1]$
- $\mathrm{E}(\tilde{\theta})$ = $\alpha\theta$; $\mathrm{Var}(\tilde{\theta})$ = $\alpha^2 Var(\hat{\theta})$

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

$$(\hat{\mu}, \hat{\beta})_{argmin} \left\{ \sum_{i} (y_i - \mu - \sum_{j=1}^{p} x_{ij}\beta_j)^2 + \lambda J(\beta) \right\}$$

- $J(\beta)$ = 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	$\sum_{j=1}^{p} \lvert\beta_j\rvert^\gamma$
LASSO	$(\gamma = 1) \sum_{j=1}^{p} \lvert\beta_j\rvert$
Ridge Regression	$(\gamma = 2) \sum_{j=1}^{p} {\beta_j}^2$
Subset selection	$(\gamma \to 0) \sum_{j=1}^{p} I(\beta_j \neq 0)$
Elastic Net	$\alpha \sum_{j=1}^{p} \lvert\beta_j\rvert + (1-\alpha) \sum_{j=1}^{p} {\beta_j}^2$

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 a<u>utomatic gene selection </u>(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

$$p(\mu, \beta, \sigma^2 | y, \omega) \propto p(y | \mu, \beta, \sigma^2) p(\mu, \beta, \sigma^2 | \omega)$$

$$\propto \prod_{i=1}^{n} N(y_i | \mu + \sum_{j=1}^{p} x_{ij}\beta_j, \sigma^2) \prod_{j=1}^{p} p(\beta_j | \omega) \, p(\sigma^2)$$

Likelihood function

Prior distribution

Distribution of the unknowns given the data and hyper-parameters

Bayesian Estimators	$p(\beta_j \vert \omega)$
Spike Slab models	$\pi N(\beta_j \vert 0, \sigma^2_{\beta_1}) + (1-\pi) N(\beta_j \vert 0, \sigma^2_{\beta_2})$
Bayes B	$\pi t_{df,S} + (1-\pi) I(\beta_j = 0)$
Bayes A	$(\pi = 1)\ t_{df,S}$
Bayes C	$(df \rightarrow \infty)\ \pi N(\beta_j \vert 0, \sigma^2_\beta) + (1-\pi) I(\beta_j = 0)$
Bayesian Ridge Regression	$(\pi = 1, df \rightarrow \infty)\ N(\beta_j \vert 0, \sigma^2_\beta)$
Bayesian LASSO	Double-exponential

Gaussian prior (Bayesian Ridge Regression)

- Multivariate normal with posterior mean same as the RR with $\lambda = \frac{\sigma^2}{{\sigma^2}_{\beta}}$.
- 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

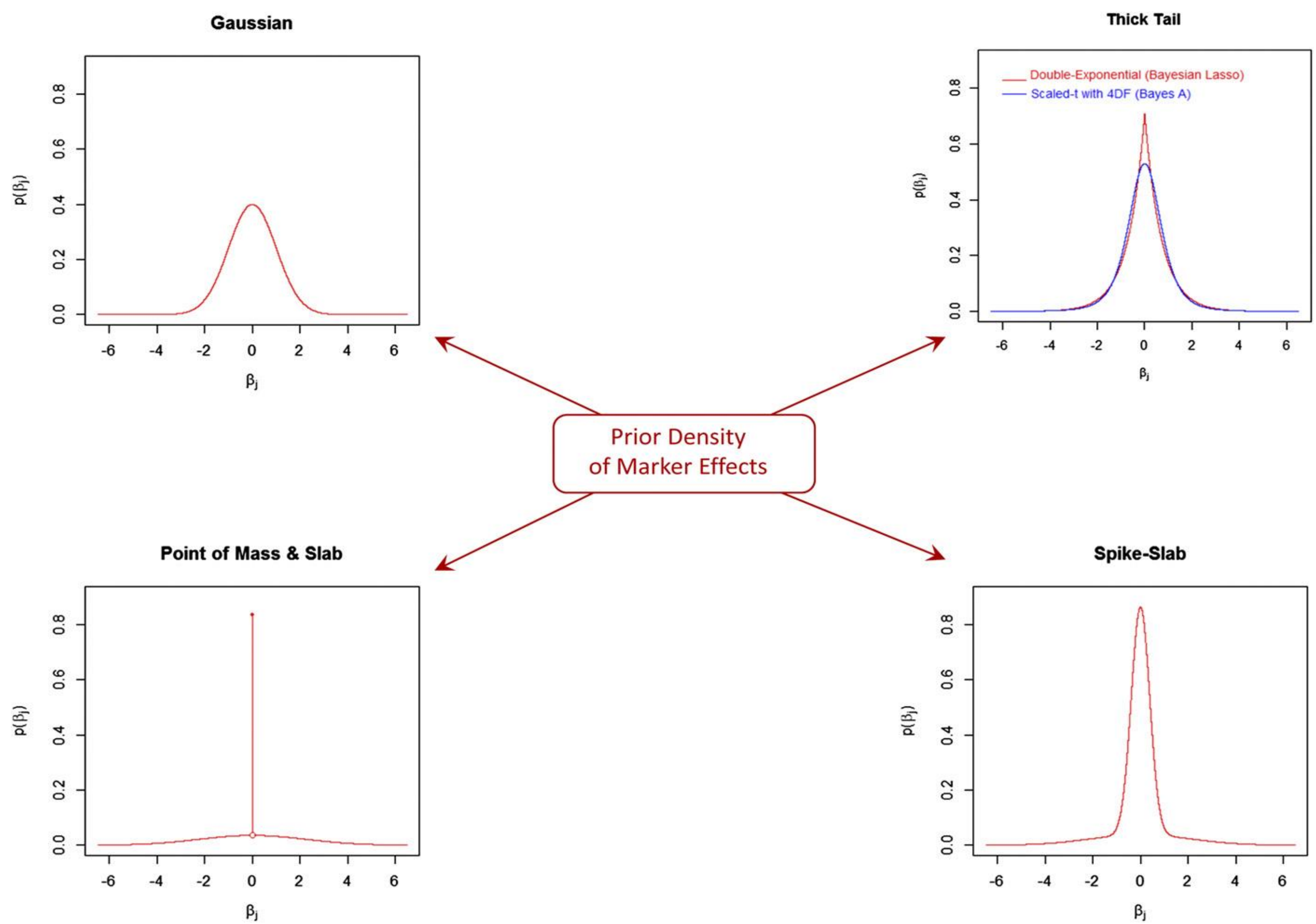
Spike slab priors

- 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
$$(\sigma^2_{\beta_1} \to 0)$$
- Again, induce a combination of variable selection and shrinkage

Comparison of priors



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