Expressing model uncertainty in Bayesian variable selection using credible sets

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Introduction

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There are a number of classical approaches: subset selection, stepwise selection, penalized maximum likelihood (Lasso, elastic net, MCP, etc.).

Bayesian variable selection

Assume a parametric model $y \sim f(x^\gamma, \theta)$ where x^γ is a subset of included variables indexed by γ ($\gamma_i = 1$ if the i-th variable is included and 0 otherwise).

Put a prior on γ. For example, $\gamma_i \sim \text{Bernoulli}(\pi)$, $\pi \sim \text{Be}(a, b)$ then a and b can be chosen to encourage sparsity.

This leads to a posterior distribution $p(\gamma \mid \text{data})$, which expresses our uncertainty about γ.

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Recent work on high-dimensional problems

- MCMC methods – Importance Tempering (Zanella and Roberts, 2019), ASI (Griffin et al., 2021), PARNI (Liang et al., 2022)
- Stochastic search – SVEN (Li et al., 2023)

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To understand the relative importance of different variables, there are summaries

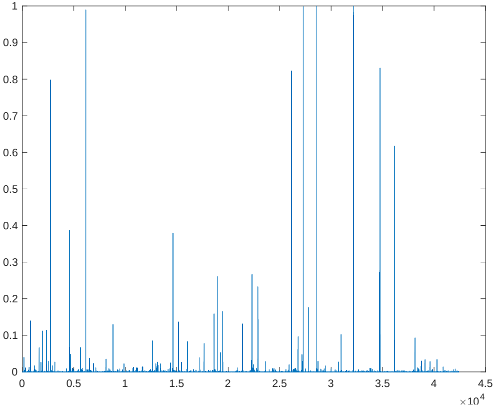
- Posterior inclusion probabilities (PIPs): $p(\gamma_i \mid \text{Data})$
- Maximum a posterior (MAP) model: the mode of $\gamma \mid \text{Data}$.
- Median model $\hat{\gamma}$ where $\hat{\gamma}_i = \mathrm{I}(p(\gamma_i \mid \text{Data}) > 0.5)$.

GWAS example: Systemic Lupus Erythematosus (case-control study)

chromosome 3
$n = 10,995$
Cases: 4,036
Controls: 6,959

$p = 42,430$

Median model has 13 variables



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Under an independent prior on γ, uncorrelated variables in linear models $\iff$ independence of γ_i's.

These relationships are due to multi-collinearity (*i.e.* correlation between variables). For example, due to linkage disequilibrium in GWAS.

Simulated example (George and McCulloch, 1997)

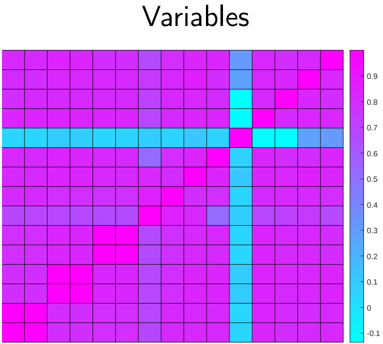
Linear regression example with $n = 180$ and $p = 15$.

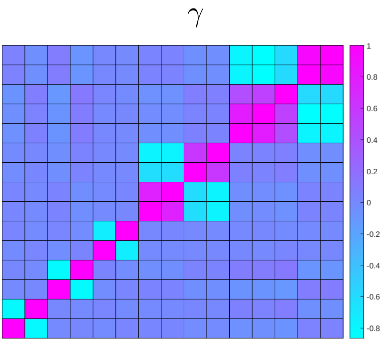
Non-zero regression coefficients are 1, 3, 5, 7, 8, 11, 12, 13.

Strong multicollinearity between variables:

- 1 and 2
- 3 and 4
- 5 and 6
- 7, 8, 9, 10
- 11, 12 13, 14, 15

Simulated example - Correlation





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There are summarisations methods for some problems (particularly clustering). How to represent uncertainty?

Credible sets

Let Γ be the set of all possible combination of variables then $A \subset \Gamma$ is a $100\alpha\%$ credible set (CS) if $p(A \mid \text{Data}) \geq \alpha$.

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The smallest $100\alpha\%$ CS can be found by

1. Rank the models by decreasing probability,

$$p(\gamma^{(1)} \mid \text{Data}) \geq p(\gamma^{(2)} \mid \text{Data}) \geq p(\gamma^{(3)} \mid \text{Data}) \geq \cdots \geq p(\gamma^{(2^p)} \mid \text{Data})$$

2. Find the smallest K such that $\sum_{k=1}^{K} p(\gamma^{(k)} \mid \text{Data}) \geq \alpha$ then $\left\{\gamma^{(1)}, \gamma^{(2)}, \ldots, \gamma^{(K)}\right\}$ is the smallest 100% CS.

Simulated example (smallest 50% credible set)

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	Prob
1	0	0	1	1	0	0	0	1	1	0	0	0	1	1	0.0849
1	0	1	0	1	0	0	0	1	1	0	0	0	1	1	0.0817
1	0	0	1	1	0	0	0	1	1	1	1	1	0	0	0.0424
1	0	0	1	1	0	0	0	1	1	0	0	1	1	1	0.0396
0	1	1	0	1	0	0	0	1	1	0	0	0	1	1	0.0345
0	1	0	1	1	0	0	0	1	1	0	0	0	1	1	0.0338
1	0	1	0	1	0	0	0	1	1	0	0	1	1	1	0.0279
0	1	0	1	1	0	0	0	1	1	1	1	1	0	0	0.0264
0	1	0	1	1	0	0	0	1	1	0	0	1	1	1	0.0248
1	0	1	0	1	0	0	0	1	1	1	1	1	0	0	0.0218
1	0	1	0	0	1	0	0	1	1	0	0	0	1	1	0.0218
1	0	0	1	0	1	0	0	1	1	0	0	0	1	1	0.0202
0	1	1	0	1	0	0	0	1	1	0	0	1	1	1	0.0183
1	0	1	1	1	0	0	0	1	1	0	0	0	1	1	0.0176
0	1	1	0	1	0	0	0	1	1	1	1	1	0	0	0.0142

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1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	Prob
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Strategy

Other 100α% CS may be easier to understand and calculable using MCMC output.

The strategy is

- Remove variables with low PIPs.
- Partition remaining variables into approximately uncorrelated blocks
- Approximate the distribution in each block.
- Construct the credible sets from the approximation.

Estimating the correlation structure

Calculate the correlation $\rho_{ij} = \text{Correlation}(\gamma_i, \gamma_j)$ under the posterior distribution.

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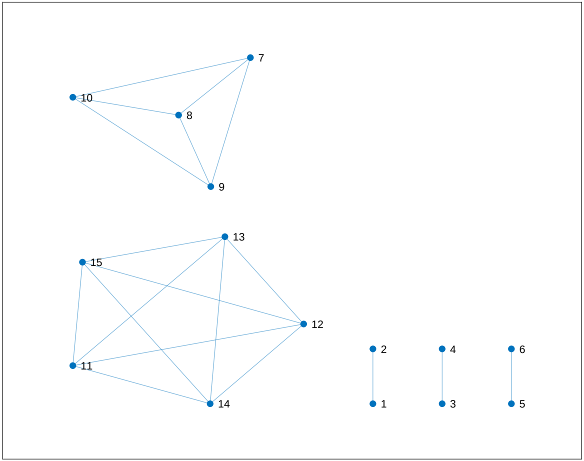
Define the matrix A by $A_{ij} = \mathrm{I}(|\rho_{ij}| > \tau)$ for some user-chosen threshold τ.

Find the components of the graph defined by the adjacency matrix A.

Simulated example



Choosing τ

Smaller τ leads to

- Larger components
- Smaller credible sets
- Harder to understand and compute the approximation

Multivariate Bernoulli distribution (Dai et al., 2013)

Let $\mathcal{D}$ be the set of non-empty subsets of $\{1, 2, \ldots, K\}$, *i.e.* $\mathcal{D} = \{\{1\}, \{2\}, \ldots, \{1, 2, \ldots, K\}\}$.

The K-dimensional multivariate Bernoulli distribution with parameters $\mathbf{f} = (f^{\epsilon} \in \mathbb{R} \mid \epsilon \in \mathcal{D})^T$ has the log probability mass function

$$\log p(y) = \sum_{r=1}^{K} \left(\sum_{1 \leq j_1 < j_2 < \cdots < j_r \leq K} f^{j_1 j_2 \cdots j_r} B^{j_1 j_2 \cdots j_r} \right) - b(\mathbf{f})$$

where $B^{j_1 j_2 \cdots j_r}(y) = y_{j_1} y_{j_2} \ldots y_{j_r}$ and $b(\mathbf{f})$ is the log normalizing constant.

Properties

- The multivariate Bernoulli distribution is a member of the exponential family and $\mathbf{f}$ are the natural parameters.
- These natural parameters can be linked to the general parameters using the relationship

$$\exp\{f^{j_1 j_2 \cdots j_r}\} = \frac{p\begin{pmatrix}\text{even \# zeros among } j_1, j_2, \ldots, j_r \text{ components} \\ \text{and other components are all zero}\end{pmatrix}}{p\begin{pmatrix}\text{odd \# zeros among } j_1, j_2, \ldots, j_r \text{ components} \\ \text{and other components are all zero}\end{pmatrix}}.$$

Properties

- For random vector $Y = (Y_1, \ldots, Y_K)$ following the multivariate Bernoulli distribution, suppose there are two blocks of nodes $Y' = (Y_1, Y_2, \ldots, Y_r)$ and $Y''. = (Y_{r+1}, Y_{r+2}, \ldots, Y_s)$, and denote index set $\tau_1 = \{1, 2, \ldots, r\}$ and $\tau_2 = \{r+1, r+2, \ldots, s\}$. Then Y' and Y'' are independent if and only if

$$f^{\tau} = 0, \forall \tau \cap \tau_1 = \emptyset \text{ and } \tau \cap \tau_2 = \emptyset.$$

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- Restricting the model to only first and second order terms, (*i.e.* $f^{j_1 j_2 \cdots j_r} = 0$ for all $j_1 j_2 \ldots j_r$ with $r > 2$) leads the quadratic exponential binary model (Cox and Weimurth, 1994).

Approximation

Suppose there are r blocks $\gamma_{m_1}, \ldots, \gamma_{m_r}$ and $q(\gamma|\mathbf{f})$ is the approximating multivariate Bernoulli distribution.

$$\begin{aligned}
\mathrm{KL} &= \sum p(\gamma \mid \text{Data}) \log p(\gamma) - \sum p(\gamma \mid \text{Data}) \log q(\gamma) \\
&= C - \sum p(\gamma \mid \text{Data}) \log q(\gamma \mid \mathbf{f}) \\
&= C - \sum_{j=1}^{q} p(\gamma_{m_j} | \text{Data}) \log q(\gamma_{m_j} \mid \mathbf{f})
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\end{aligned}$$

If there is a sample $\gamma^{(1)}, \gamma^{(2)}, \ldots, \gamma^{(N)} \sim p(\gamma \mid \mathrm{Data})$ then the a Monte Carlo approximation to the KL divergence is used

$$-\frac{1}{N} \sum_{j=1}^{q} \sum_{i=1}^{N} \log q\left(\gamma_{m_j}^{(i)} \middle| \mathbf{f}\right)$$

Finding the credible set

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The credible set $\mathcal{S}$ is a Cartesian product of $S_1, \ldots, S_r$ and then

$$p(\mathcal{S} \mid \text{Data}) = \prod_{i=1}^{r} p(Q_i \mid \text{Data}).$$

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$$p(\mathcal{S} \mid \text{Data}) = \prod_{i=1}^{r} p(Q_i \mid \text{Data}).$$

This allows the derivation of algorithms which control $p(\mathcal{S} \mid \text{Data})$ by changing the elements of $S_1, \ldots, S_r$.

Example (3 variables / 2 blocks)

$$\Gamma_1 = \{0, 1\}, \Gamma_2 = \{(0, 0), (0, 1), (1, 0), (1, 1)\}$$

	Block 1		Block 2			
	0	1	(0, 0)	(0, 1)	(1, 0)	(1, 1)
Prob	0.9	0.1	0	0.5	0.5	0

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Prob	0.9	0.1	0	0.5	0.5	0

$$S_1 = \{0, 1\} \Rightarrow p(S_1) = 1,$$
$$S_2 = \{(0,0), (0,1), (1,0), (1,1)\} \Rightarrow p(S_2) = 1,$$
$$\mathcal{S} = \{(0,0,0), (0,0,1), (0,1,0), (0,1,1), (1,0,0), (1,0,1), (1,1,0), (1,1,1)\} \Rightarrow p(\mathcal{S}) = 1.$$

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$$S_1 = \{0\} \Rightarrow p(S_1) = 0.9,\ S_2 = \{(0, 1), (1, 0)\} \Rightarrow p(S_2) = 1$$
$$\mathcal{S} = \{(0, 0, 1), (0, 1, 0)\} \Rightarrow p(\mathcal{S}) = 0.9.$$

Algorithms

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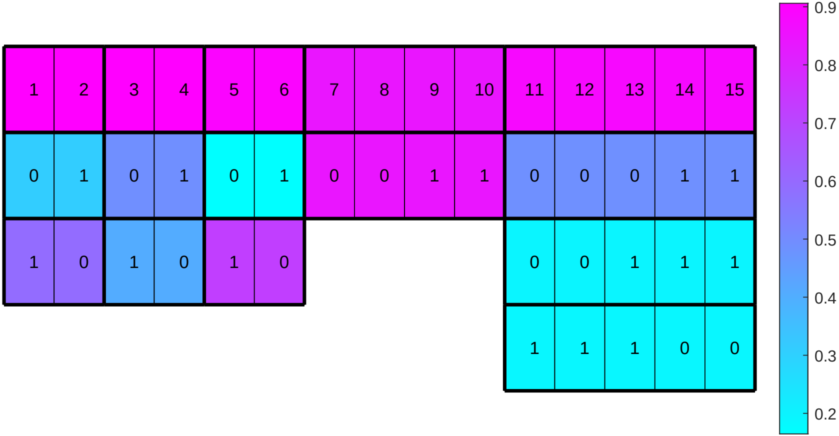
1. Calculate the probability of all possible credible sets (there are $2^{\#\Gamma_i}$). Find the smallest set with probability above the desired level.
2. Let Δ_i be the smallest change in $p(S_i)$ by removing an element from S_i. Choose $k = \arg\min(\Delta_1, \ldots, \Delta_r)$ and remove the corresponding element from S_k. Continue until removing any element leads to a probability below the desired level.

Simulated example (50 % credible set)



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1	0	0	1	1	0	0	0	1	1	0	0	1	1	1	0.0396
0	1	1	0	1	0	0	0	1	1	0	0	0	1	1	0.0345
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1	0	1	0	1	0	0	0	1	1	1	1	1	0	0	0.0218
1	0	1	0	0	1	0	0	1	1	0	0	0	1	1	0.0218
1	0	0	1	0	1	0	0	1	1	0	0	0	1	1	0.0202
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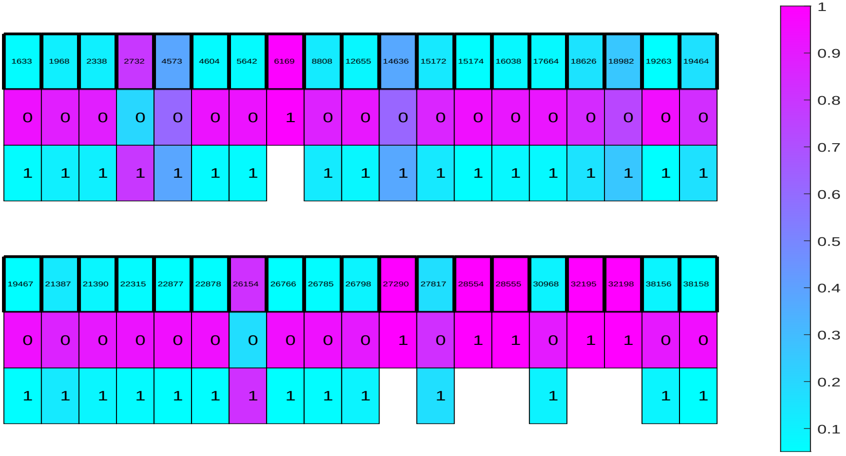
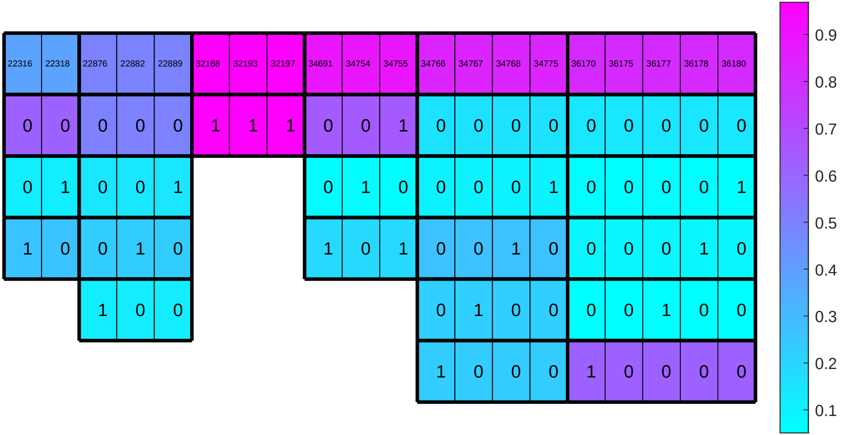
GWAS example



GWAS example



- One of 34766, 34767, 34768 and 34775 is included with probability 0.84 (individual PIPs are 0.10, 0.27, 0.22, 0.24)
- One of 22876, 22882, and 22889 is included with probability 0.50 (individual PIPs are 0.14, 0.23, 0.12)

Discussion

- Credible sets are useful way to explore uncertainty in the posterior distribution in Bayesian variable selection
- The method can identify blocks of highly correlated variables which can dilute marginal posterior inclusion probabilities
- The methods work with MCMC but could be easily extended to other inference frameworks (*e.g.* variational Bayes)
- These approaches could be extended to other discrete structures by finding a representation of the posterior with independence structure (*e.g.* factor models, etc.)

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