Sequentially-Allocated Latent Structure Optimization

David B. Dahl — Brigham Young University Peter Müller — University of Texas at Austin

Bayes Comp 2020 University of Florida January 8, 2020

Motivation

- In a typical Bayesian analysis, considerable effort is placed on "fitting the model" (e.g., sampling from the posterior) but this is only half of the inference problem.
- Meaningful inference also requires summarizing the posterior distribution of the parameters of interest for, e.g., subsequent analysis or communicating results.
- If the parameters of interest live in \mathbb{R}^n , common posterior summaries are **means** and **medians**.
- Summarizing posterior distributions of parameters with complicated structure is more challenging, e.g., the "average" clustering, feature allocation, or network is not easily defined.
- In this paper, we consider summarizing partition/clustering distributions.

Setting the Stage

MCMC Samples from the Posterior Clustering Distribution

	[,1]	[,2]	[,3]	$\lfloor,4\rfloor$	[,5]
[1,]	1	2	1	2	2
[2,]	1	1	1	2	3
[3,]	1	1	2	1	1
[4,]	1	2	2	2	2
[5,]	1	1	2	1	1
[6,]	1	1	2	2	1
[7,]	1	1	1	1	1
[8,]	1	2	2	2	1
[9,]	1	2	1	1	1
[10,]	1	2	2	3	4
[11,]	1	2	2	2	1
[12,]	1	1	1	1	1
[13,]	1	1	1	1	2
[14,]	1	1	1	1	1

Example: First Clustering in MCMC Output

Clustering in *cluster label* notation:

$$c^{(1)} = (1, 2, 1, 2, 2)$$

Clustering in **set partition** notation:

$$\pi^{(1)} = \{\{1,3\},\{2,4,5\}\}\$$

Clustering in *adjacency matrix* notation;

$$A(c^{(1)}) = \begin{bmatrix} 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 & 1 \end{bmatrix}$$

Example: First Clustering in MCMC Output

Clustering in *cluster label* notation:

$$c^{(1)} = (\clubsuit, \heartsuit, \clubsuit, \heartsuit, \heartsuit)$$

Clustering in **set partition** notation:

$$\pi^{(1)} = \{\{1,3\},\{2,4,5\}\}\$$

Clustering in *adjacency matrix* notation;

$$A(c^{(1)}) = \begin{bmatrix} 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 & 1 \end{bmatrix}$$

Example: Second Clustering in MCMC Output

Clustering in *cluster label* notation:

$$c^{(2)} = (1, 1, 1, 2, 3)$$

Clustering in **set partition** notation:

$$\pi^{(2)} = \{\{1, 2, 3\}, \{4\}, \{5\}\}\$$

Clustering in *adjacency matrix* notation:

$$A(c^{(2)}) = \begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

Example: Third Clustering in MCMC Output

Clustering in *cluster label* notation:

$$c^{(3)} = (1, 1, 2, 1, 2)$$

Clustering in **set partition** notation:

$$\pi^{(3)} = \{\{1, 2, 4\}, \{3, 5\}\}\$$

Clustering in *adjacency matrix* notation:

$$A(c^{(3)}) = \begin{bmatrix} 1 & 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ 1 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \end{bmatrix}$$

Example: Averaging the MCMC Clustering Output

Averaging the vector of cluster labels **does not make sense**.

Averaging the set partitions is **not defined**.

Averaging adjacency matrices does make sense:

$$\bar{A} = \frac{1}{B} \sum_{b=1}^{B} A(c^{(b)}) = \begin{bmatrix} 1 & 2/3 & 2/3 & 1/3 & 0 \\ 2/3 & 1 & 1/3 & 2/3 & 1/3 \\ 2/3 & 1/3 & 1 & 0 & 1/3 \\ 1/3 & 2/3 & 0 & 1 & 1/3 \\ 0 & 1/3 & 1/3 & 1/3 & 1 \end{bmatrix}$$

 \bar{A} is the **pairwise similarity matrix (PSM)**. Denote $\hat{\mu}_{ij}$ as it's (i,j) element, which estimates $\mu_{ij} = \Pr(c_i = c_j \mid \text{data})$.

Overview

- We present the sequentially-allocated latent structure optimization (SALSO) method to minimize an objective criterion to obtain a point estimate based on a collection of randomly-sampled clusterings/partitions.
- SALSO is a stochastic search method involving a series of micro optimizations.
- Currently implementation handles two loss functions:
 - "binder": Loss function of Binder (1978) loss
 - "VI.Ib": Lower bound of the variation of information loss of Wade & Ghahramani (2018).

Loss Functions and Bayes Estimators

- A Bayes estimator minimizes the posterior expected value of a loss function.
- The 0-1 loss function:

$$L(c, \hat{c}) = I\{c = \hat{c}\},\$$

yielding the maximum a posteriori (MAP) clustering:

$$\mathrm{argmax}_{\hat{c}}\ p(\hat{c}\mid \mathsf{data})$$

- Equal loss for clusterings that differs by one label and clusterings that differs by many labels!?
- Mode may not represent well the "center" of a distribution.

Loss Functions and Bayes Estimators

Dahl (2006) suggested the clustering that minimizes:

$$f_{\text{Isclust}}(\hat{c}) = \sum_{i=1}^{n} \sum_{j=1}^{n} (A(\hat{c})_{ij} - \hat{\mu}_{ij})^2,$$

where $\hat{\mu}_{ij}$ is a Monte Carlo estimate of $\mu_{ij} = Pr(c_i = c_j)$.

 Lau & Green (2007) studied the Binder (1978) loss function in a Bayesian nonparametric context:

$$L(c, \hat{c}) = \sum_{i < j} I\{c_i = c_j\} I\{\hat{c}_i \neq \hat{c}_j\} + I\{c_i \neq c_j\} I\{\hat{c}_i = \hat{c}_j\},$$

yielding a clustering minimizing the Monte Carlo estimate of the expectation of the Binder loss:

$$f_{\text{binder}}(\hat{c}) = \sum_{i=1}^{n} \sum_{j=1}^{n} I\{\hat{c}_i = \hat{c}_j\}(0.5 - \hat{\mu}_{ij})$$

■ Dahl & Newton (2007) noted that minimizing $f_{lsclust}$ is equivalent to minimizing f_{binder} .

Loss Functions and Bayes Estimators

 Wade & Ghahramani (2018) suggested the variation of information of Meilă (2007) as a loss function:

$$L(c, \hat{c}) = \sum_{i=1}^{n} \left(\log \left(\sum_{j=1}^{n} I\{\hat{c}_j = \hat{c}_i\} \right) - 2E \left(\log \left(\sum_{j=1}^{n} I\{\hat{c}_j = \hat{c}_i, c_j = c_i\} \right) \middle| \mathsf{data} \right) \right)$$

which is computationally expensive. Instead, minimize the Monte Carlo estimate of the **lower bound** of the posterior expectation of the variation of information loss (VI.Ib):

$$f_{\text{VI.lb}}(\hat{c}) = \sum_{i=1}^{n} \left(\log \left(\sum_{j=1}^{n} I\{\hat{c}_j = \hat{c}_i\} \right) - 2 \log \left(\sum_{j=1}^{n} I\{\hat{c}_j = \hat{c}_i\} \hat{\mu}_{ij} \right) \right)$$

 Paulon, Trippa, Müller (2018) propose a scientifically-tailored loss function.

12

Monte Carlo Estimate the Posterior Expected Loss

- For a given \hat{c} , both the Binder and the lower bound of the VI objective functions are based on the $\hat{\mu}_{ij}$'s.
- But having a way to estimate the posterior expected loss for a given \hat{c} does *not* give a search algorithm for its minimization.

Methods for Optimization Given a Loss Function

- 1. Exhaustive search. Feasible for small n only, e.g., B(15)=1,382,958,545.
- 2. Round the elements of the pairwise similarity matrix. May not lead to a clustering, e.g.:

$$\bar{A} = \begin{bmatrix} 1 & 2/3 & 2/3 & 1/3 & 0 \\ 2/3 & 1 & 1/3 & 2/3 & 1/3 \\ 2/3 & 1/3 & 1 & 0 & 1/3 \\ 1/3 & 2/3 & 0 & 1 & 1/3 \\ 0 & 1/3 & 1/3 & 1/3 & 1 \end{bmatrix} \Rightarrow \begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

- 3. Medvedovic and Sivaganesan (2002) selected a clustering using hierarchical clustering using $1-\bar{A}$ as the distance matrix.
- 4. Dahl (2006) selected the clustering in the MCMC output that minimizes the objective function.

Methods for Optimization Given a Loss Function

- 5. Lau & Green (2007) proposed a heuristic item-swapping algorithm based on binary integer programming to minimize the posterior expectation of Binder loss.
- Wade & Ghahramani (2018) proposed a greedy search algorithm based on neighborhoods defined by the Hasse diagram, which can be used for Binder or VI.lb loss.
- 7. We propose the **sequentially-allocated latent structure optimization (SALSO)** method to perform a *series of micro optimizations* to stochastically search for the minimizer of the posterior expectation of Binder or VI.lb loss.

cls.draw2

Example 4: Output of a Dirichlet process mixture model with normal components fitted to the dataset Ysim2 from the mcclust package.

Size: 400 observations

Method	Binder	Time	VI.lb	Time
SALSO (10)	3402	0.1	0.5900	0.2
SALSO (100)	3402	0.5	0.5896	1.6
SALSO (1000)	3402	4.7	0.5896	16.3
W & G	3409	5:23:01.3	0.5913	9:49:51.7
L & G	3402	1:11:36.3	_	_
M & S (avg)	3481	0.0	0.5933	0.0
M & S (comp)	3562	0.0	0.6129	0.0
Draws	3917	0.5	0.7239	0.4

Sequentially-Allocated Latent

Structure Optimization

Sequentially-Allocated Latent Structure Optimization

- The steps of the SALSO algorithm are:
 - 1. Randomly sample a permutation $\sigma = (\sigma_1, \dots, \sigma_n)$ of $\{1, \dots, n\}$, giving the sequence in which the n items are allocated.
 - Starting for an empty structure, build up a full structure by sequentially allocating items to minimize the objective function (but rarely make a sub-optimal allocation).
 - Improve the full structure by a series of one-at-a-time reallocations to minimize the objective function (but, again, rarely make a sub-optimal allocation).
 - Do the above steps many times for randomly-selected permutations and choose the structure that minimizes the objective function.

Illustration of SALSO Method

- To illustrate the SALSO method, consider clustering 5 items.
- For simplicity, suppose $\sigma = (\sigma_1, \dots, \sigma_5) = (1, 2, 3, 4, 5)$.
- Recall the steps to SALSO are:
 - 1. Sample a permutation.
 - 2. Build up a full structure from an empty structure.
 - 3. Improve the full structure.
 - 4. Do it for many random permutations (not just $\sigma=(1,2,3,4,5)$).

Step 1: Sample a permutation

Permutation: 1 2 3 4 5 Item 1 is allocated first,

Item 2 is allocated second,

etc.

Clustering: ~ ~ ~ ~ ~

Clustering: ? ~ ~ ~ Candidates for ? are: 1

Clustering: 1 ~ ~ ~ ~

Clustering: 1 ? ~ ~ ~ Candidates for ? are: 1, 2

$$f(\hat{c}) = f((1,1)) = 0.27$$

 $f(\hat{c}) = f((1,2)) = 0.73$

Clustering: 1 1 ~ ~ ~

Clustering: 1 1 ? ~ ~ Candidates for ? are: 1, 2

$$f(\hat{c}) = f((1,1,1)) = 0.79$$

 $f(\hat{c}) = f((1,1,2)) = 0.49$

Clustering: 1 1 2 ~ ~

Clustering: 1 1 2 ? ~ Candidates for ? are: 1, 2, 3

$$f(\hat{c}) = f((1,1,2,1)) = 1.01$$

 $f(\hat{c}) = f((1,1,2,2)) = 0.79$
 $f(\hat{c}) = f((1,1,2,3)) = 0.71$

Clustering: 1 1 2 2 ~

Here, we took the second best.

We allow this for each allocation with very small probability.

Clustering: 1 1 2 2 ? Candidates for ? are: 1, 2, 3

$$f(\hat{c}) = f((1,1,2,2,1)) = 1.31$$

 $f(\hat{c}) = f((1,1,2,2,2)) = 0.89$
 $f(\hat{c}) = f((1,1,2,2,3)) = 1.05$

Clustering: 1 1 2 2 2

Clustering: 1 1 2 2 2

Clustering: ? 1 2 2 2 $\,$ Candidates for ? are: 1, 2, 3

$$f(\hat{c}) = f((1,1,2,2,2)) = 0.89$$

 $f(\hat{c}) = f((2,1,2,2,2)) = 1.26$
 $f(\hat{c}) = f((3,1,2,2,2)) = 1.07$

Clustering: 1 1 2 2 2

Clustering: 1 ? 2 2 2 Candidates for ? are: 1, 2, 3

$$f(\hat{c}) = f((1,1,2,2,2)) = 0.89$$

 $f(\hat{c}) = f((1,2,2,2,2)) = 1.27$
 $f(\hat{c}) = f((1,3,2,2,2)) = 1.07$

Clustering: 1 1 2 2 2

Clustering: 1 1 ? 2 2 Candidates for ? are: 1, 2, 3

$$f(\hat{c}) = f((1,1,1,2,2)) = 1.04$$

 $f(\hat{c}) = f((1,1,2,2,2)) = 0.89$
 $f(\hat{c}) = f((1,1,3,2,2)) = 0.86$

Clustering: 1 1 3 2 2

Clustering: 1 1 3 ? 2 Candidates for ? are: 1, 2, 3, 4

$$f(\hat{c}) = f((1,1,3,1,2)) = 1.22$$

 $f(\hat{c}) = f((1,1,3,2,2)) = 0.86$
 $f(\hat{c}) = f((1,1,3,3,2)) = 1.05$
 $f(\hat{c}) = f((1,1,3,4,2)) = 0.98$

Clustering: 1 1 3 2 2

Clustering: 1 1 3 2 ? Candidates for ? are: 1, 2, 3, 4

$$f(\hat{c}) = f((1,1,3,2,1)) = 1.25$$

 $f(\hat{c}) = f((1,1,3,2,2)) = 0.86$
 $f(\hat{c}) = f((1,1,3,2,3)) = 1.04$
 $f(\hat{c}) = f((1,1,3,2,4)) = 0.98$

Clustering: 1 1 3 2 2

Clustering: 1 1 3 2 2 Scan completed

Clustering: 1 1 3 2 2 Put in canonical form

Clustering: 1 1 2 3 3

Clustering: 1 1 2 3 3 Any change from start of scan?

Clustering: 1 1 2 3 3 Yes, so perform another scan

Clustering: ? 1 2 3 3 Candidates for ? are: 1, 2, 3, 4

$$f(\hat{c}) = f((1,1,2,3,3)) = 0.86$$

$$f(\hat{c}) = f((2,1,2,3,3)) = 1.19$$

$$f(\hat{c}) = f((3,1,2,3,3)) = 1.29$$

$$f(\hat{c}) = f((4,1,2,3,3)) = 1.04$$

Clustering: 1 ? 2 3 3 Candidates for ? are: 1, 2, 3, 4

$$f(\hat{c}) = f((1,1,2,3,3)) = 0.86$$

$$f(\hat{c}) = f((1,2,2,3,3)) = 1.20$$

$$f(\hat{c}) = f((1,3,2,3,3)) = 1.29$$

$$f(\hat{c}) = f((1,4,2,3,3)) = 1.04$$

Clustering: 1 1 ? 3 3 Candidates for ? are: 1, 2, 3

$$f(\hat{c}) = f((1,1,1,3,3)) = 1.04$$

 $f(\hat{c}) = f((1,1,2,3,3)) = 0.86$
 $f(\hat{c}) = f((1,1,3,3,3)) = 0.89$

$$f(\hat{c}) = f((1,1,2,1,3)) = 1.22$$

$$f(\hat{c}) = f((1,1,2,2,3)) = 1.05$$

$$f(\hat{c}) = f((1,1,2,3,3)) = 0.86$$

$$f(\hat{c}) = f((1,1,2,4,3)) = 0.98$$

Clustering: 1 1 2 3 ? Candidates for ? are: 1, 2, 3, 4

$$f(\hat{c}) = f((1,1,2,3,1)) = 1.25$$

 $f(\hat{c}) = f((1,1,2,3,2)) = 1.04$
 $f(\hat{c}) = f((1,1,2,3,3)) = 0.86$
 $f(\hat{c}) = f((1,1,2,3,4)) = 0.98$

Clustering: 1 1 2 3 3 Put in canonical form

Clustering: 1 1 2 3 3 Any change from start of scan?

Clustering: 1 1 2 3 3 $\,$ No, so move on to Step 4

Step 4: Do It For Many Permutations

- The permutation many lead to a local minimizer.
- Improve the chances of finding the global minimizer by repeating Steps 1-3 for many random permutations.
 - This is embarrassingly parallel.
- Select the structure the minimizes the posterior expected loss among all those good structures obtained by using many random permutations.

Review of the Steps of the SALSO Method

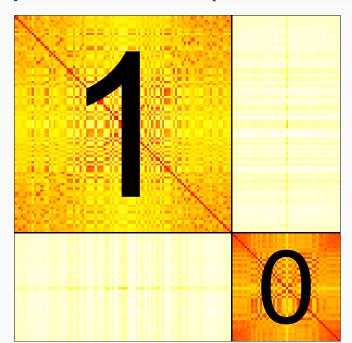
- 1. Sample a random permutation.
- 2. Build up a full structure from an empty structure.
- 3. Improve the full structure.
- 4. Do it for many random permutations.

Software and Empirical Comparison

Software Implementation

SALSO is implemented in the R package "salso" available on CRAN. library(salso) dim(iris.clusterings) ## [1] 1000 150 probs <- psm(iris.clusterings)</pre> estimate <- salso(probs)\$estimate table(estimate) ## estimate ## 0 ## 50 100

plot(confidence(estimate, probs))



Comparison Methodology

- Various optimization methods:
 - Hierarchical clustering of Medvedovic and Sivaganesan (2002) using average or complete linkage [base R]
 - Draws method of Dahl (2006) [salso, mcclust]
 - Linear programming method of Lau & Green (2007) [mcclust]
 - Greedy search by Wade & Ghahramani (2018) [mcclust.ext]
 - SALSO method [salso]
- Loss functions
 - Binder loss (Binder 1978)
 - Lower bound of the variation of information loss (Wade & Ghahramani 2018)

DPbetabinom

Example 1: Posterior density sample for a semiparametric beta-binomial model using a Dirichlet process prior, from the DPbetabinom example code in the DPpackage library.

Size: 106 observations

Method	Binder	Time	VI.lb	Time
SALSO (10)	1914	0.0	1.44	0.0
SALSO (100)	1914	0.1	1.44	0.7
SALSO (1000)	1914	1.3	1.44	1.9
W & G	2015	30.3	1.44	1:39.7
L & G	1914	30.4	_	_
M & S (avg)	2123	0.0	1.55	0.0
M & S (comp)	2104	0.0	1.59	0.0
Draws	2067	0.7	1.67	1.4

DPbinary

Example 2: Posterior density sample for a semiparametric binary regression model, from the DPbinary example code in the DPpackage library.

Size: 150 observations

Method	Binder	Time	VI.lb	Time
SALSO (10)	906.6	0.4	3.69	0.1
SALSO (100)	906.6	0.4	3.69	0.7
SALSO (1000)	906.6	1.5	3.68	5.5
W & G	906.8	19.2	3.70	35.0
L & G	906.6	59.0	_	-
M & S (avg)	5303.3	0.0	3.71	0.0
M & S (comp)	5303.3	0.0	3.71	0.0
Draws	1115.2	1.3	4.27	2.0

ex2.draw

Example 3: Clusterings from a Dirichlet process scale-location mixture model with normal components fitted to a simulated dataset as found in ex2.draw from the mcclust.ext package.

Size: 200 observations

Method	Binder	Time	VI.lb	Time
SALSO (10)	1761	0.0	0.6683	0.1
SALSO (100)	1761	0.2	0.6683	0.7
SALSO (1000)	1761	1.2	0.6683	4.1
W & G	4449	10:00.6	0.6684	21:00.0
L & G	1761	5:31.1	_	_
M & S (avg)	1878	0.0	0.6725	0.0
M & S (comp)	2006	0.0	0.8555	0.0
Draws	1875	1.5	0.7225	2.4

cls.draw2

Example 4: Output of a Dirichlet process mixture model with normal components fitted to the dataset Ysim2 from the mcclust package.

Size: 400 observations

Method	Binder	Time	VI.lb	Time
SALSO (10)	3402	0.1	0.5900	0.2
SALSO (100)	3402	0.5	0.5896	1.6
SALSO (1000)	3402	4.7	0.5896	16.3
W & G	3409	5:23:01.3	0.5913	9:49:51.7
L & G	3402	1:11:36.3	_	_
M & S (avg)	3481	0.0	0.5933	0.0
M & S (comp)	3562	0.0	0.6129	0.0
Draws	3917	0.5	0.7239	0.4

Comparing the Quality of Estimates — Subset of Size 15

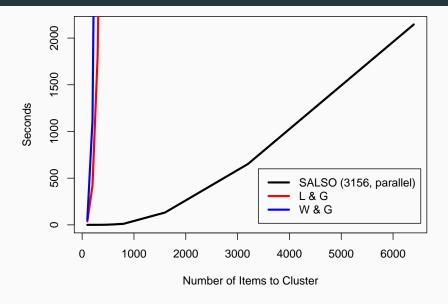
- Random subsets of size 15 were taken from cls.draw2 so the global minimum can be found via enumeration.
- Record the number of random subsets until the first difference between i. SALSO and ii. W & G or L & G.
- In each difference, SALSO produced the global minimum.

# of Subsets	W & G (Binder)	W & G (VI.lb)	L & G (Binder)
Mean	11	11	523
Median	6	11	391
Std. Dev.	11	7	510

Comparing the Quality of Estimates — Subset of Sizes 100 & 200

- Randomly sample datasets of 100 or 200 items from the 400 items in the cls.draw2 dataset.
- L & G and SALSO estimates differ in about:
 - 0.7% of the $\binom{400}{100}$ datasets of size 100
 - 3% of the $\binom{400}{200}$ datasets of size 200
- Among 200 such cases, every time SALSO provided a smaller posterior expected loss.

How Well Does Computation Scale?



Constrained Optimization

- We may want to constrain the optimization.
 - e.g.: For the sake of interpretation, it may be helpful to limit the number of clusters or features.
- Solution: Tweak the loss function to give infinite loss for violated constraints.
 - e.g.: Infinite loss for clusterings with more clusters than desired.
- Implementation: During micro optimization, never create a structure that violates the constraint.
 - e.g.: Don't consider allocations that create clusters beyond the desired maxSize.

Suppose we want at most three clusters.

Clustering: ? 1 2 3 3 Candidates for ? are: 1, 2, 3 but not: 4

Conclusion

- We presented the sequentially-allocated latent structure optimization (SALSO) method to minimize an objective criterion to obtain a point estimate based on a collection of randomly-sampled clusterings.
- SALSO is a stochastic search method involving a series of micro optimizations.
- Status:
 - Well-developed for clusterings
 - Implemented in the "salso" "sdols" package on CRAN.
 - Want to apply to other structures, e.g., feature allocations, networks, variable selection.
- Summaries other than point estimates?