

Summarizing Distributions of Latent Structures

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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.
- Posterior summaries are important for subsequent analyses or in communicating the results to a diverse audience.
- 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” network in the network distribution is not easily defined.
- We consider summarizing distributions of latent structures, e.g., clusterings, feature allocations, and networks.

- 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*.
- Several objective criterion can be used, including squared error loss, absolute error loss, Binder (1978) loss, or the lower bound of the variation of information loss (Wade & Ghahramani 2018), respectively.

Setting the Stage

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 as ***pairwise allocation matrix*** (i.e., adjacency matrix):

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

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 as *pairwise allocation matrix* (i.e., adjacency matrix):

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

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 as *pairwise allocation matrix* (i.e., adjacency matrix):

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

Example: Averaging the MCMC Clustering Output

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

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

Averaging pairwise allocation 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 estimated **expected pairwise allocation matrix (EPAM)** because it's (i, j) element estimates $\mu_{ij} = \Pr(c_i = c_j \mid \text{data})$.

More Realistic Example

Suppose MCMC output contains 1,000 posterior samples for the partition of 150 observations (encoded with cluster labels), e.g.:

```
iris.clusterings[1,]
```

```
##      [1] 1 1 1 1 2 2 1 2 1 1 1 1 1 1 2 2 1 1 1 2 1 2
##     [23] 2 1 1 1 1 1 1 1 1 1 2 2 1 1 1 2 1 1 2 3 1 1
##     [45] 1 1 2 1 2 1 4 4 4 4 4 4 4 3 4 4 3 4 3 4 4 4
##     [67] 5 3 3 3 4 4 3 4 4 4 6 4 4 3 7 3 3 4 4 4 4 3
##     [89] 4 4 3 4 3 3 3 4 4 4 3 4 4 4 3 4 3 4 4 4 3 4
##    [111] 4 3 3 3 3 4 4 4 4 3 4 4 4 4 4 4 4 4 3 4 4 4
##    [133] 3 4 3 4 4 4 4 4 4 4 4 4 4 3 3 3 4 4
```

What is the Bayes estimate of the partition from these 1,000 samples?

Loss Functions and Bayes Estimators

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

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

yielding the maximum *a posteriori* (MAP) clustering:

$$\operatorname{argmax}_{\hat{c}} p(\hat{c} \mid \text{data})$$

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

Loss Functions and Bayes Estimators

- Dahl (2006) suggested a least-squares criterion:

$$\operatorname{argmin}_{\hat{c}} \sum_{i=1}^n \sum_{j=1}^n (A(\hat{c})_{ij} - \mu_{ij})^2$$

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

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

yielding the clustering:

$$\operatorname{argmin}_{\hat{c}} \sum_{i=1}^n \sum_{j=1}^n \mathbf{I}\{\hat{c}_i = \hat{c}_j\} (0.5 - \mu_{ij})$$

- Dahl & Newton (2007) noted that minimizing the posterior expected loss of Binder (1978) is equivalent to the least-squares criterion in Dahl (2006).

Loss Functions and Bayes Estimators

- Wade & Ghahramani (2018) used the variation of information (VI) of Meilă (2007) as a loss function, yielding the clustering:

$$\operatorname{argmin}_{\hat{c}} \sum_{i=1}^n \left(\log \left(\sum_{j=1}^n \mathbf{I}\{\hat{c}_j = \hat{c}_i\} \right) - 2\mathbb{E} \left(\log \left(\sum_{j=1}^n \mathbf{I}\{\hat{c}_j = \hat{c}_i, c_j = c_i\} \right) \middle| \text{data} \right) \right)$$

which is computationally expensive. Instead, they suggest the clustering that minimizes the **lower bound** of the posterior expected value of the variation of information loss (VI.lb):

$$\operatorname{argmin}_{\hat{c}} \sum_{i=1}^n \left(\log \left(\sum_{j=1}^n \mathbf{I}\{\hat{c}_j = \hat{c}_i\} \right) - 2 \log \left(\sum_{j=1}^n \mathbf{I}\{\hat{c}_j = \hat{c}_i\} \mu_{ij} \right) \right)$$

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

Monte Carlo Estimate the Posterior Expected Loss

- For a given \hat{c} , both the Binder and the lower bound of the VI loss are based on the μ_{ij} 's.
- The (i, j) elements of \bar{A} are Monte Carlo estimates of the μ_{ij} 's, leading to a Monte Carlo estimate of the posterior expected loss.
- 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

- Exhaustive search. Infeasible for even moderate n , e.g., $B(15) = 1,382,958,545$.
- Round the estimated expected pairwise allocation matrix (EPAM). May not lead to a clustering, e.g.:

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

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

Methods for Optimization Given a Loss Function

- More sophisticated search algorithms:
 - Lau & Green (2007) proposed a heuristic item-swapping algorithm based on binary integer programming to minimize the posterior expected 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.
- 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 expected value of Binder or VI.lb loss.

Sequentially-Allocated Latent Structure Optimization

Sequentially-Allocated Latent Structure Optimization

- The SALSO method is applicable for many types of latent structure, including clusterings, feature allocations, & networks.
- The steps to SALSO are:
 1. Starting for an empty structure, build up a full structure by sequentially optimizing the allocation of items.
 2. Improve the full structure by a series of one-at-a-time optimizations.
 3. Do the above steps many times for randomly-selected permutations and choose the structure that minimizes the posterior expected loss.
- The random order in which items are allocated is not necessarily their order in the dataset; the permutation $\sigma = (\sigma_1, \dots, \sigma_n)$ of $\{1, \dots, n\}$ gives the sequence in which the n items are allocated.

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. Build up a full structure from an empty structure
 2. Improve the full structure
 3. Do it for many random permutations (not just $\sigma = (1, 2, 3, 4, 5)$)

Step 1: Build Up a Full Structure

Clustering: ~ ~ ~ ~ ~

Step 1: Build Up a Full Structure

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

Step 1: Build Up a Full Structure

Clustering: 1 ~ ~ ~ ~

Step 1: Build Up a Full Structure

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

Step 1: Build Up a Full Structure

Clustering: 1 1 ~ ~ ~

Step 1: Build Up a Full Structure

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

Step 1: Build Up a Full Structure

Clustering: 1 1 2 ~ ~

Step 1: Build Up a Full Structure

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

Step 1: Build Up a Full Structure

Clustering: 1 1 2 3 ~

Step 1: Build Up a Full Structure

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

Step 1: Build Up a Full Structure

Clustering: 1 1 2 3 3

Step 2: Improving the Full Structure

Clustering: 1 1 2 3 3

Step 2: Improving the Full Structure

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

Step 2: Improving the Full Structure

Clustering: 2 1 2 3 3

Step 2: Improving the Full Structure

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

Step 2: Improving the Full Structure

Clustering: 2 2 2 3 3

Step 2: Improving the Full Structure

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

Step 2: Improving the Full Structure

Clustering: 2 2 2 3 3

Step 2: Improving the Full Structure

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

Step 2: Improving the Full Structure

Clustering: 2 2 2 1 3

Step 2: Improving the Full Structure

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

Step 2: Improving the Full Structure

Clustering: 2 2 2 1 3

Step 2: Improving the Full Structure

Clustering: 2 2 2 1 3 Scan completed

Step 2: Improving the Full Structure

Clustering: 2 2 2 1 3 Put in canonical form

Step 2: Improving the Full Structure

Clustering: 1 1 1 2 3

Step 2: Improving the Full Structure

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

Step 2: Improving the Full Structure

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

Step 3: Do It For Many Permutations

- The permutation many lead to a local minimizer.
- Improve the chances of finding the global minimizer by repeating Step 1 and 2 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. Build up a full structure from an empty structure
2. Improve the full structure
3. Do it for many random permutations

Software and Empirical Comparison

Software Implementation

SALSO is implemented in the R package “sdols” available on CRAN.

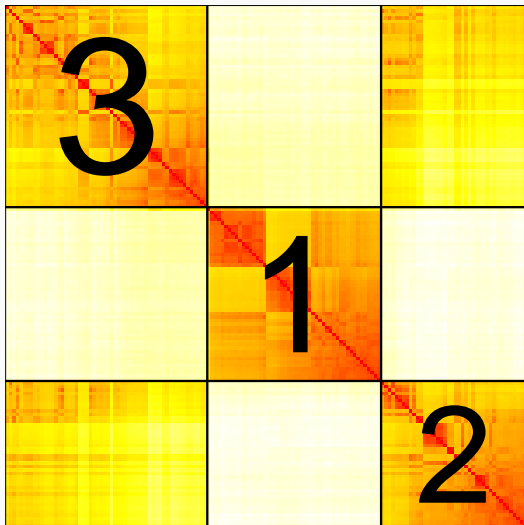
```
library(sdols)
dim(iris.clusterings)

## [1] 1000 150

epam <- expectedPairwiseAllocationMatrix(iris.clusterings)
estimate <- salso(epam, nCandidates=100,
                  budgetInSeconds=20, maxSize=3)
table(estimate)

## estimate
## 1 2 3
## 50 42 58
```

```
plot(confidence(estimate, epam))
```



Comparison Methodology

- Various optimization methods:
 - Hierarchical clustering of Medvedovic and Sivaganesan (2002) using average or complete linkage [mcclust]
 - Draws method of Dahl (2006) [sdols, mcclust]
 - Linear programming method of Lau & Green (2007) [mcclust]
 - Greedy search by Wade & Ghahramani (2018) [mcclust.ext]
 - SALSO method [sdols]
- Loss functions
 - Binder loss (Binder 1978)
 - Lower bound of the variation of information loss (Wade & Ghahramani 2018)
- Datasets: Three sets of MCMC output from a variety of models with 1,000 samples each.

Example 1: Ewens Pitman attraction distribution (Dahl, Day, Tsai 2017) applied to iris data.

Size: 150 observations

Method	Binder	Time
SALSO (12)	3493.16	0.039 seconds
SALSO (100)	3493.16	0.218 seconds
M & S (avg)	3497.01	0.055 seconds
W & G	3500.12	3.8 minutes
M & S (comp)	3512.90	0.055 seconds
L & G	3560.01	2.7 minutes
Draws	3607.48	0.085 seconds

Example 1: Ewens Pitman attraction distribution (Dahl, Day, Tsai 2017) applied to iris data.

Size: 150 observations

Method	VI.lb	Time
M & S (comp)	1.3246	0.026 seconds
M & S (avg)	1.3246	0.026 seconds
SALSO (12)	1.3246	0.033 seconds
SALSO (100)	1.3246	0.197 seconds
W & G	1.3246	7.9 minutes
Draws	1.3320	0.102 seconds
L & G	—	—

Example 2: Gaussian likelihood with a spatial PPM (Page & Quintana 2016) prior.

Size: 600 observations

Method	Binder	Time
SALSO (12)	7509.7	0.843 seconds
SALSO (100)	7509.7	7.033 seconds
L & G	7509.7	8.2 hours
M & W (comp)	8060.7	1.615 seconds
W & G	8365.6	18.8 hours
M & S (avg)	9409.1	1.604 seconds
Draws	10464.5	0.765 seconds

Example 2: Gaussian likelihood with a spatial PPM (Page & Quintana 2016) prior.

Size: 600 observations

Method	VI.lb	Time
M & S (avg)	2.7543	0.700 seconds
SALSO (12)	2.8241	3.94 seconds
M & W (comp)	2.8526	0.715 seconds
SALSO (100)	2.8633	26.61 seconds
Draws	3.7788	1.176 seconds
W & G	4.6411	36.3 hours
L & G	—	—

Example 3: Bivariate Gaussian likelihood with a spatial PPM (Page & Quintana 2016) prior.

Size: 600 observations

Method	Binder	Time
SALSO (12)	46270.74	0.937 seconds
SALSO (100)	46270.74	7.709 seconds
L & G	46271.21	9.8 hours
M & S (avg)	46724.64	1.609 seconds
M & S (comp)	47844.03	1.641 seconds
Draws	53182.66	1.005 seconds
W & G	57761.10	24.1 hours

Example 3: Bivariate Gaussian likelihood with a spatial PPM (Page & Quintana 2016) prior.

Size: 600 observations

Method	VI.lb	Time
SALSO (100)	1.5620	14.182 seconds
SALSO (12)	1.5649	1.552 seconds
M & S (comp)	1.5829	0.673 seconds
M & S (avg)	1.5858	0.733 seconds
Draws	1.9108	0.555 seconds
W & G	7.2197	41.6 hours
L & G	—	—

Wrapping Up

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 violate constraint
 - 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

Way to Improve the Method?

Modified method:

1. Build up a full structure from an empty structure
 - Periodically reallocate items (a la Step 2) in the as-of-yet incomplete structure.
2. Improve the full structure
3. Do it for many random permutations

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 *latent features*.
- SALSO is a *stochastic search* method involving a *series of micro optimizations*.
- Status:
 - Well-developed for *clusterings*. Implemented in the “sdols” package on CRAN.
 - Initial version for *feature allocations* in the “sdols” package.
 - Want to apply to other structures, e.g., *networks*.
- Can we pick a representative observation?
- Summarizes other than point estimates?