High to High Dimensional Multivariate Mixture Regression

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Idea

Goal: Correctly cluster observations & regress in high dimensional X & Y.

- $Y_{n\times q}$ Matrix of responses
- $X_{n\times p}$ Design matrix
- $A_{p\times q}$ Coefficient matrix (sparse in p)
- k clusters

$$f\left(\boldsymbol{y}_i \mid \boldsymbol{x_i}; \boldsymbol{\theta}\right) = \Sigma_{k=1}^{K} \pi_k \mathcal{N}_q\left(\boldsymbol{y_i}; \boldsymbol{x_i} A_k, \Sigma_k\right)$$

- Parameter space $\theta = \{\pi_k, A_k, \Sigma_k; k = 1 \ldots K\}$ solved by general EM using SARRS to compute A_k.

SARRS

- Excellent performance, even in high dimension (> 5000)
- Computationally very fast

Algorithm 1: Subspace Assisted Regression with Row Sparsity (SARRS)

Input: Observed response matrix Y, design matrix X,
rank r, initial matrix $V_{(0)}$ and penalty function $\rho(\cdot;\lambda)$ with penalty level λ.

Output: Estimated coefficient matrix $\widehat{A}$.

1 Group penalized regression

$$B_{(1)} = \underset{B\in\mathbb{R}^{p\times r}}{\arg\min} \left\{ \|YV_{(0)} - XB\|_F^2/2 + \rho(B;\lambda) \right\},$$

2 Compute the left singular vectors of $XB_{(1)}$, denoted by $U_{(1)}$.

3 Compute the right singular vectors of $U_{(1)}U_{(1)}'Y$, denoted by $V_{(1)}$.

4 Group penalized regression

$$B_{(2)} = \underset{B\in\mathbb{R}^{p\times r}}{\arg\min} \left\{ \|YV_{(1)} - XB\|_F^2/2 + \rho(B;\lambda) \right\},$$

5 Compute the estimated coefficient matrix by $\widehat{A} = B_{(2)}V_{(1)}'$.

Figure 1: "SARRS Main Algorithm"

HTH Mixture Algorithm

- Initialize: $\pi_k^{(0)} = \frac{n_k^{(0)}}{n}$
- Randomly initialize observations into k clusters

While not converged ($m = 1, \ldots, M$) do:

- for $k = 1, \ldots, K$ apply SARRS on all observations in $C_k^{(m-1)}$ to obtain $A_k^{(m)}$, $\Sigma_k^{(m)}$
- compute $\mu_{ik}^{(m)} = \mathcal{N}_p\left(\boldsymbol{y_i}; A_k^{(m)}\boldsymbol{x_i}, \Sigma_k^{(m)}\right)$
- $C_k^{(m)} = \{i | \text{ML component k}\}$
- $\pi_k^{(m)} = \frac{n_k^{(m)}}{n}$

HTH Mixture Algorithm

- Empirically, HTH Mixture reaches local maximum quickly
- Need to determine method for efficiently exploring the likelihood space with different random initialization.

Likelihood Space Exploration Idea 1

- Mimic the idea of chains from MCMC
- In parallel, run large number of chains and select the one which reaches the largest likelihood.
- This method works well, although not the most efficient way to explore the space.

Likelihood Space Exploration Idea 2

- To more efficiently explore the space, when a local maximum is reached, perturb the initialized state by a proportion p (e.g. 20%) and rerun.

Data Simulation

- X_k consists of iid random vectors sample from $MVN(\mathbf{0}, \Sigma_k)$
- Σ_k diagonal
- Noise matrix $Z_k \in \mathbb{R}^{n \times q}$ has iid $N(0, \sigma^2)$ entries
- $A_k = \begin{pmatrix} b_k B_{0_k} B_{1_k} \\ 0 \end{pmatrix}$
  - with $b > 0$, $B_0 \in \mathbb{R}^{s \times r}$, $B_1 \in \mathbb{R}^{r \times q}$
- $Y_k = X_k A_k + Z_k$

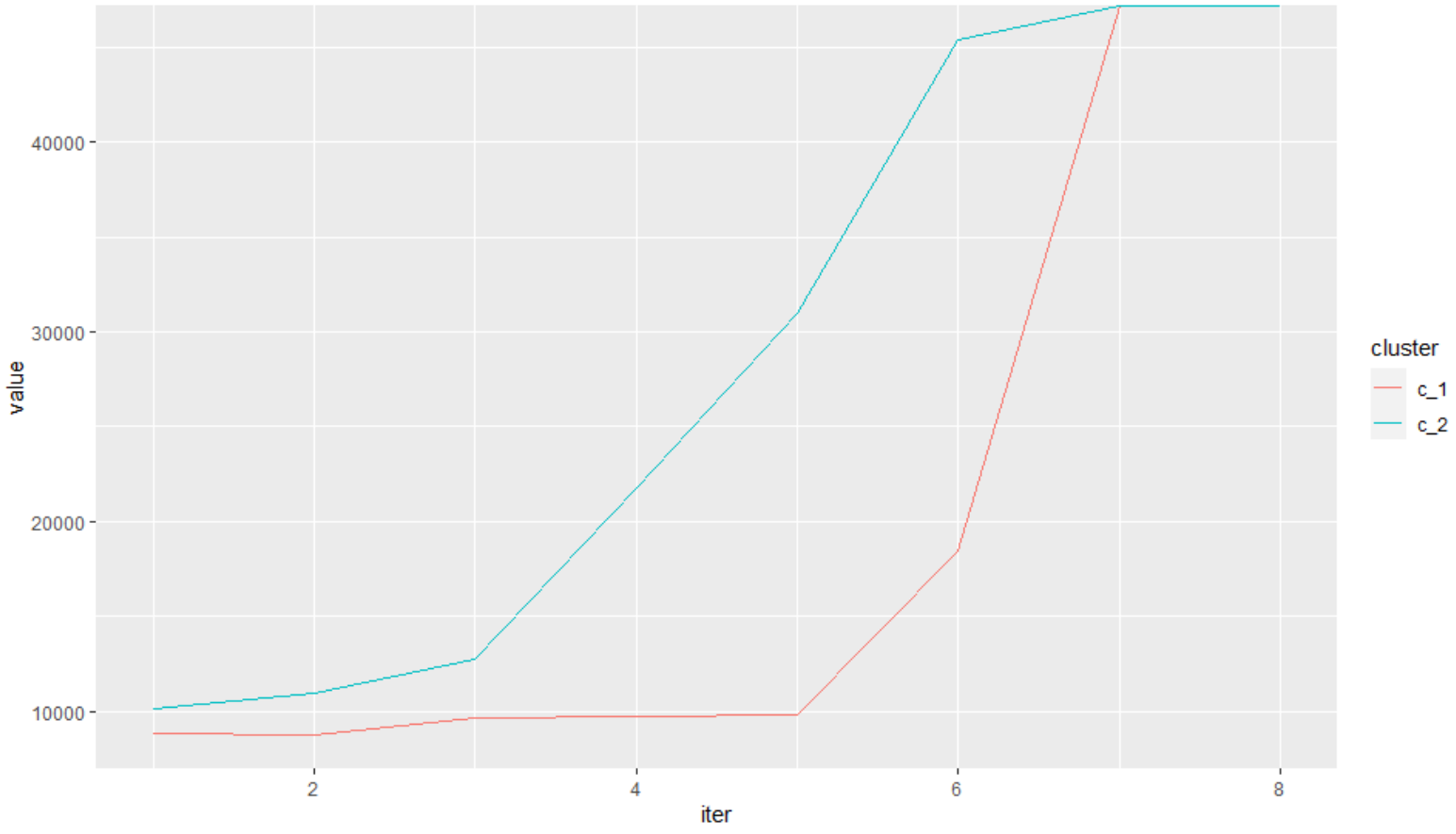
Finally, combine X & Y

Simulation

- N: $50 - 400$
- s: $5 - 20$
- rank: $1 - 2$
- B: 1
- $p = m = 1000$
- Perturb: 20%
- Cluster with equal probability
- K: 2
- σ: 1
- CHains: 500

Results

- HTH algorithm consistently reaches local maximum



Results

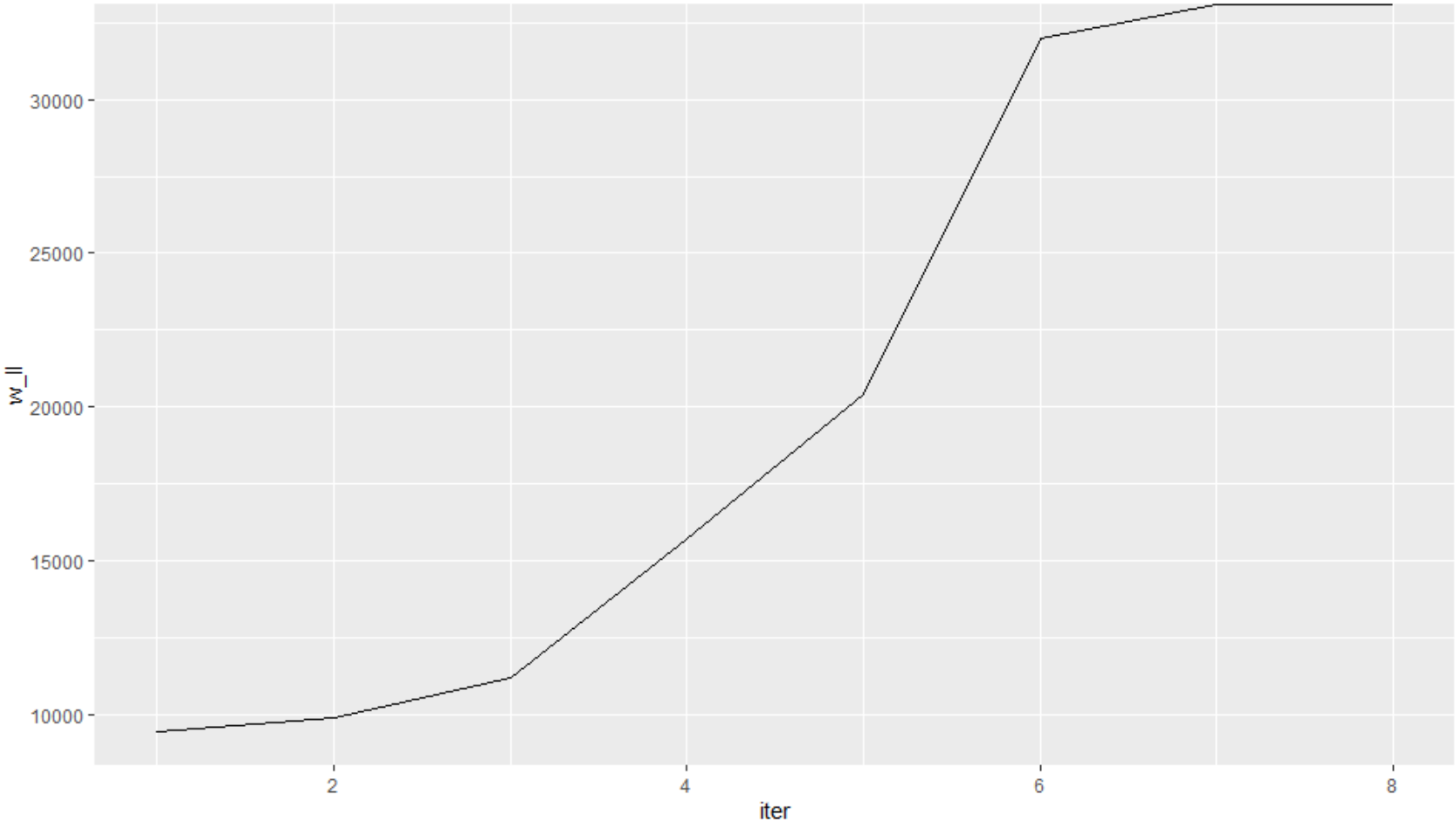
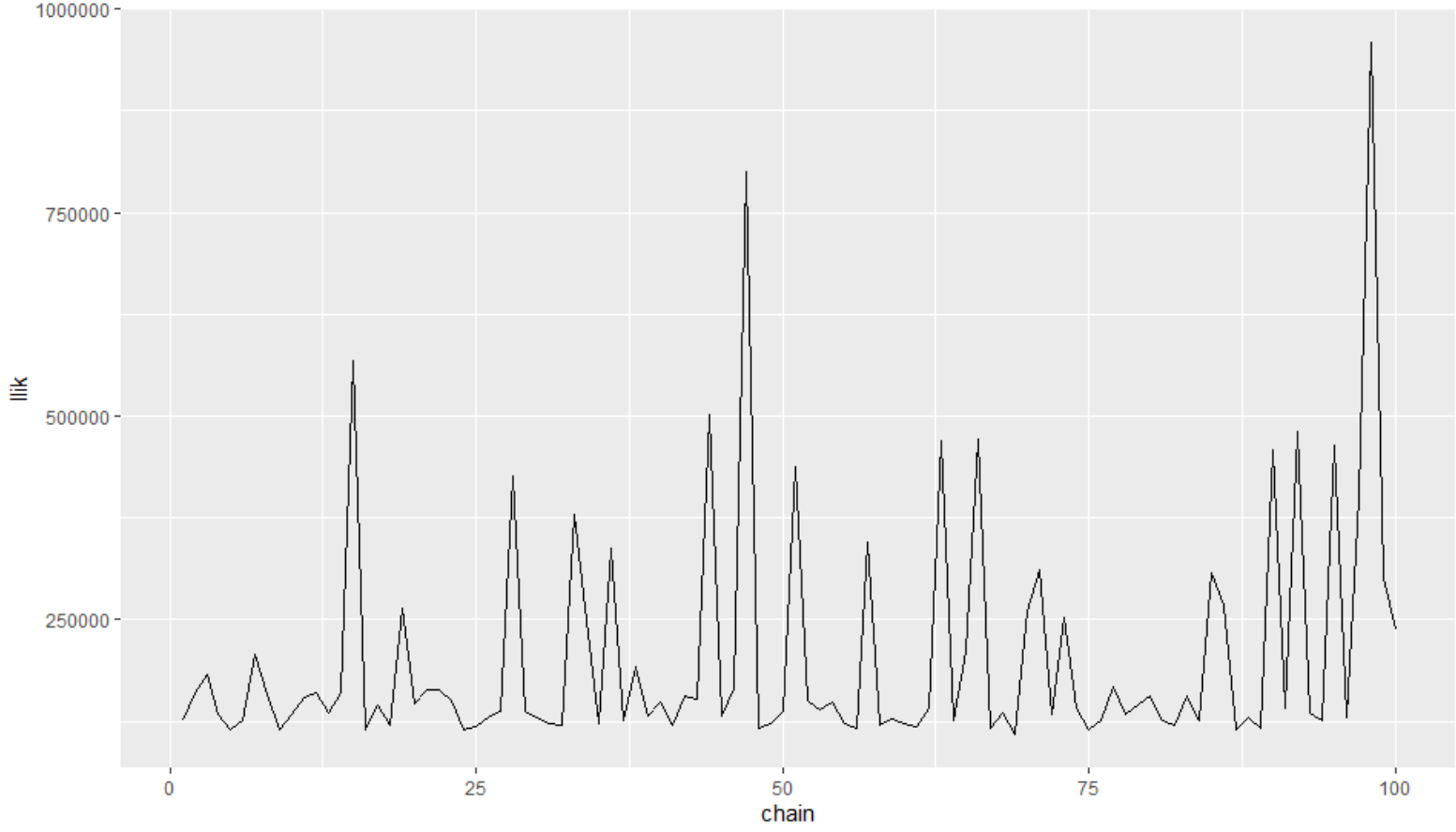


Figure 2: Weighted Likelihood

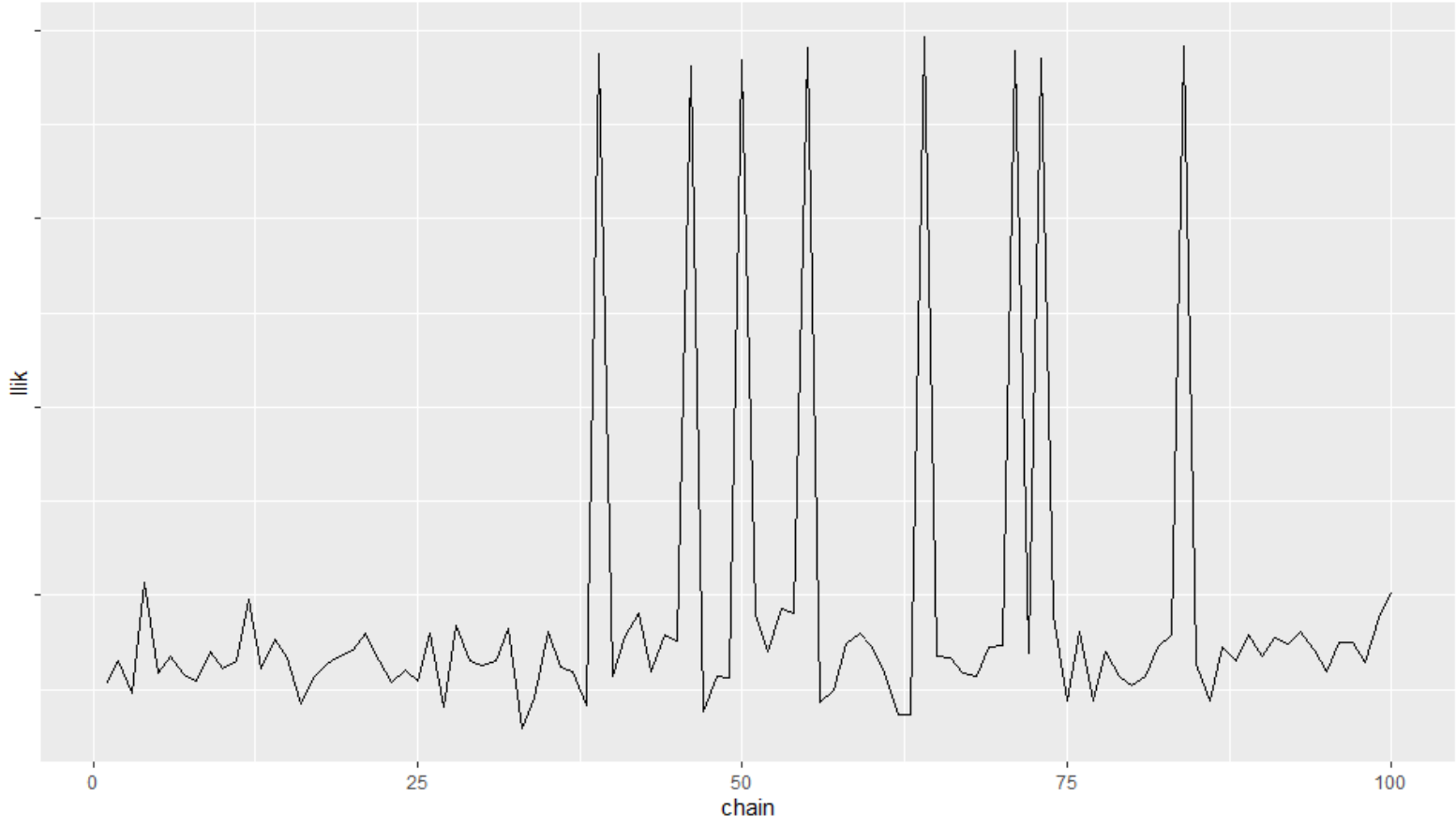
Results

- Idea 1 $\rightarrow$ random initialization each time



Results

- Idea 2 $\rightarrow$ perturb local maximum
- Appears to be more efficient



Results

N	s	R	hthmix	kmeans
50	5	1	0.90	0.70
100	5	1	1.00	0.66
200	5	1	1.00	0.51
400	5	1	1.00	0.54
50	10	1	0.84	0.62
100	10	1	0.92	0.50
200	10	1	1.00	0.66
400	10	1	1.00	0.52
50	20	1	0.80	0.72
100	20	1	0.80	0.53
200	20	1	0.98	0.68
400	20	1	1.00	0.51

Results

N	s	R	hthmix	kmeans
50	5	2	1.00	0.64
100	5	2	1.00	0.72
200	5	2	1.00	0.52
400	5	2	1.00	0.64
50	10	2	0.86	0.58
100	10	2	1.00	0.55
200	10	2	1.00	0.53
400	10	2	1.00	0.68
50	20	2	0.84	0.64
100	20	2	0.78	0.53
200	20	2	1.00	0.71
400	20	2	1.00	0.65

Performance

- In simulated data, current algorithm clusters well (perfectly in most cases given enough chains)
- Challenges:
  - Likelihood space is explored inefficiently, sometimes requires large number of chains
  - Computationally cumbersome/inefficient