

Supplementary Material

main document

A compositional model to assess expression changes from single-cell RNA-seq data

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Synthetic Data

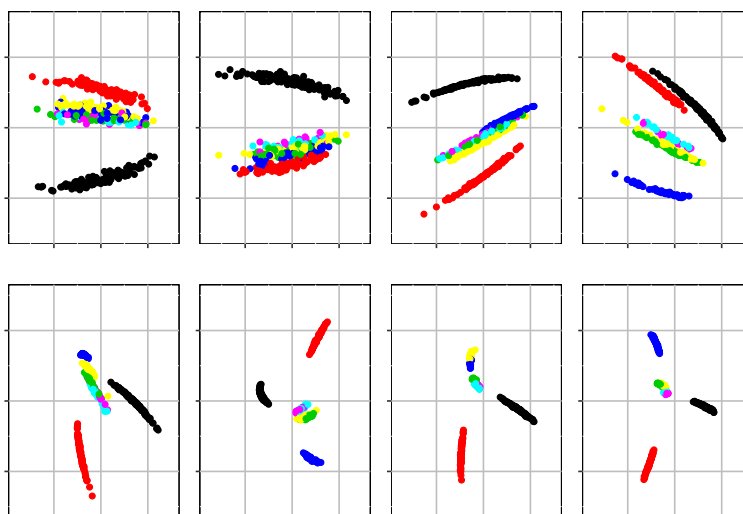


Fig 1: first two principal components of transcripts under different parameters for simulated data. Different parameters resulted in different degree of separation of subtypes. We have 4 different settings for hyper-parameters of simulation, each setting has 2 replicates

Data sets

EBSeq

Data set	Conditions	Number of cells/condition	Organism	Ref	K
GSE52529	T0 vs T24	96,96	human	(?)	6
GSE57872	patient1 vs patient2	192,96	human	(?)	7
GSE48968-GPL13112	BMDC (2h LPS stimulation) vs 6h LPS	96,96	mouse	(?)	8
GSE60749-GPL13112	serum + LIF vs 2i + LIF	90,94	mouse	(?)	3
GSE74596	NKT1 vs NTK2	46,68	mouse	(?)	5
EMTAB2805	G1 vs G2M	95,96	mouse	(?)	7
GSE71585-GPL13112	Gad2tdTpositive vs Cux2tdTnegative	80,140	mouse	(?)	7
GSE64016	G1 vs G2	91,76	human	(?)	8
GSE79102	patient1 vs patient2	51, 89	human	?	4
GSE45719	16-cell stage blastomere vs mid blastocyst cell	50, 60	mouse	(?)	5
GSE63818	Primordial Germ Cells, develop- mental stage: 7 week gestation vs Somatic Cells, developmental stage: 7 week gestation	40,26	mouse	(?)	6
GSE75748	DEC vs EC	64, 64	human	(?)	9
GSE84465	neoplastic cells vs non-neoplastic cells	546, 664	human	(?)	9

TABLE 1
datasets used for comparisons of DD analysis under different methods

Suppose we have K subtypes, let $X_g^I = X_{g,1}^I, \dots, X_{g,S_1}^I$ denote transcripts at gene g from subtype $I, I = 1, \dots, K$. In the EBSeq model it assumed that counts within subtype I are distributed as Negative Binomial: $X_{g,s}^I | r_{g,s}, q_g^I \sim NB(r_{g,s}, q_g^I)$ Where

$$P(X_{g,s}^I | r_{g,s}, q_g^I) = \binom{X_{g,s} + r_{g,s} - 1}{X_{g,s}} (1 - q_g^I)^{X_{g,s}} (q_g^I)^{r_{g,s}}$$

and $\mu_{g,s}^I = r_{g,s}(1 - q_g^I)/q_g^I$; $\sigma_{g,s}^I = r_{g,s}(1 - q_g^I)/(q_g^I)^2$.

The EBSeq model assumed a prior distribution on $q_g^I : q_g^I | \alpha, \beta^{I_g} \sim \text{Beta}(\alpha, \beta^{I_g})$. The hyperparameter α is shared by all the isoforms and β^{I_g} is I_g specific. We further assume that $r_{g,s} = r_{g,0} * l_s$ where $r_{g,0}$ is an isoform specific parameter common across subtypes and $r_{g,s}$ depends on it through the sample-specific normalization factor l_s

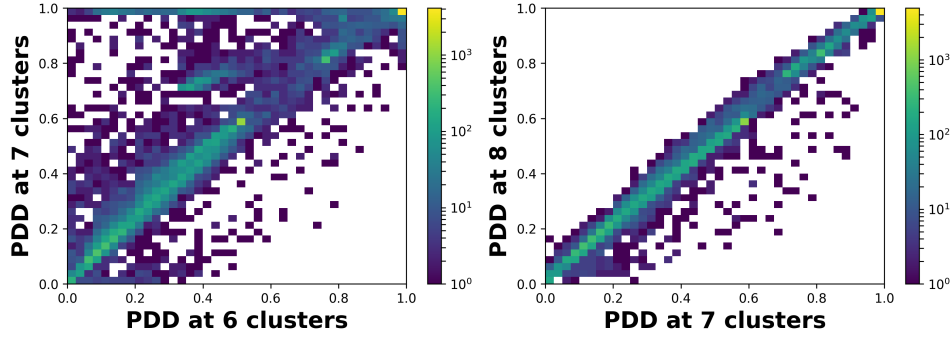


Fig 2: comparison of posterior probabilities of being DD among different number of subtypes, when we underestimate the number of subtypes, the difference is huge, see PDD between 6 subtypes and 7 subtypes. There is an approximate horizontal line with massive points at the top of left panel, which indicate that we underestimate lots of DD genes due to underestimate the number of subtypes. While in the case when we overestimate the number of subtypes 7 subtypes vs. 8 subtypes, though inflating PDD but the variation of difference is small, from 6 to 8 subtypes the PDD become more linear related.

What we are interested at those K groups comparison is the expression pattern, through EBSeq modeling we are able to obtain posterior probabilities over

$$M_{g,\pi} = \{\theta \in \Theta : \mu_{g,k} = \mu_{g,k'} \iff k, k' \in b, b \in \pi\}.$$

For any partition π of K elements.

For example $K = 3$, there are 5 expression pattern, P_1, P_2, \dots, P_5

$$\begin{aligned} P1 : q_g^1 &= q_g^2 = q_g^3 \\ P2 : q_g^1 &= q_g^2 \neq q_g^3 \\ P3 : q_g^1 &\neq q_g^2 = q_g^3 \\ P4 : q_g^1 &= q_g^3 \neq q_g^2 \\ P5 : q_g^1 &\neq q_g^2 \neq q_g^3 \text{ and } q_g^1 \neq q_g^3 \end{aligned}$$

Under the assumption that two groups I and J share the same q_g we can pool the counts from the two groups by viewing them come from same distribution i.e. $X_g^{I,J} | r_{g,s}, q_g \sim NB(r_{g,s}, q_g)$, $q_g | \alpha, \beta^{I_g} \sim Beta(\alpha, \beta^{I_g})$

and obtained the prior predictive function $f_0^{I_g}(X_g^{I,J}) = \int_0^1 P(X_g^{I,J} | r_{g,s}, q_g) * P(q_g | \alpha, \beta^{I_g}) dq_g = \left[\prod_{s=1}^S \binom{X_{g,s} + r_{g,s} - 1}{X_{g,s}} \right] \frac{\text{Beta}(\alpha + \sum_{s=1}^S r_{g,s}, \beta^{I_g} + \sum_{s=1}^S X_{g,s})}{\text{Beta}(\alpha, \beta^{I_g})}$. Consequently, we have prior predictive function for $P1, \dots, P5$ as

$$\begin{aligned} g_1^{I_g}(X_g^{1,2,3}) &= f_0^{I_g}(X_g^{1,2,3}) \\ g_2^{I_g}(X_g^{1,2,3}) &= f_0^{I_g}(X_g^{1,2}) f_0^{I_g}(X_g^3) \\ g_3^{I_g}(X_g^{1,2,3}) &= f_0^{I_g}(X_g^1) f_0^{I_g}(X_g^{2,3}) \\ g_4^{I_g}(X_g^{1,2,3}) &= f_0^{I_g}(X_g^{1,3}) f_0^{I_g}(X_g^2) \\ g_5^{I_g}(X_g^{1,2,3}) &= f_0^{I_g}(X_g^1) f_0^{I_g}(X_g^2) f_0^{I_g}(X_g^3) \end{aligned}$$

Then the marginal distribution of counts $X_g^{1,2,3}$ is $\sum_{k=1}^5 p_k g_k^{I_g}(X_g^{1,2,3})$, where proportion parameters p_k satisfying $\sum_{k=1}^5 p_k = 1$ and are estimated by EM algorithm. Thus, the posterior probability of an expression pattern k is obtained by:

$$\frac{p_k g_k^{I_g}(X_g^{1,2,3})}{\sum_{k=1}^5 p_k g_k^{I_g}(X_g^{1,2,3})}$$

modalclust

Product Partition Model Let $X = (X_1, X_2, \dots, X_n)$ be n one dimension observed data, given a partition for the data $\pi = \{S_1, \dots, S_q\}$, where S_i are disjoint subsets of $\{1, 2, \dots, n\}$ and $\bigcup_{i=1}^q S_i = \{1, 2, \dots, n\}$. The likelihood for X satisfying such partition is

$$p(X|\pi) = \prod_{i=1}^q f(X_{S_i})$$

where X_{S_i} is the vector of observations corresponding to the items of component S_i , The component likelihood $f(X_S)$ is defined for any non-empty component S and can take any form. The partition π is the only parameter we are interested at. Any other parameters that may have been involved in the model have been integrated over their prior.

The prior distribution for a partition π is also taken as a product form. We use the partition that maximize the posterior $p(\pi|X) \propto p(X|\pi)p(\pi)$ as the estimated clustering of X .

Dahl demonstrated by some choice of f and prior of π , we can reduce the time complexity of finding the MAP partition from factorial(n) to $O(n^2)$?, And the crucial condition for f is that if X_{S_1} and X_{S_2} are overlapped in the sense that $\min\{X_{S_2}\} < \max\{X_{S_1}\} < \max\{X_{S_2}\}$ or $\min\{X_{S_1}\} < \max\{X_{S_2}\} < \max\{X_{S_1}\}$, $X_{S_1^*}$ and $X_{S_2^*}$ be the sets of swapping one pair of those overlapped terms and keep the other unchanged. Then $f(X_{S_1})f(X_{S_2}) \leq f(X_{S_1^*})f(X_{S_2^*})$. Under such condition, we know that possible MAP candidates must be those partition that for any two subgroups of data, all the data from subgroup1 has to be either greater or smaller than all the data from subgroup2.

In Poisson-Gamma Model we assuming:

$$\begin{aligned} X_i|\pi, \lambda &\sim \text{Poisson}(X_i|\lambda_1\mathbf{I}\{i \in S_1\} + \dots + \lambda_q\mathbf{I}\{i \in S_q\}) \\ \pi &\sim p(\pi) \\ \lambda_j &\sim \text{Gamma}(\alpha_0, \beta_0) \end{aligned}$$

where $p(\pi) \propto \prod_{i=1}^q \eta_0 \Gamma(|S_i|)$. Integrate out λ , $f(X_S)$ is obtained as:

$$f(X_S) = \frac{\beta^\alpha}{(|S| + \beta)^{\sum_{i \in S} X_i + \alpha}} \frac{\Gamma(\sum_{i \in S} X_i + \alpha)}{\Gamma(\alpha)} \frac{1}{\prod_{i \in S} X_i}$$

$f(X_S)$ still satisfying the condition mentioned

PROOF. if X_{S_1} and X_{S_2} are overlapped, without loss of generality, we assume $\min\{X_{S_2}\} < \max\{X_{S_1}\} < \max\{X_{S_2}\}$, and we swap $\max\{X_{S_1}\}$ with $\min\{X_{S_2}\}$ and keep the rest unchanged or we could also swap $\max\{X_{S_1}\}$ with $\max\{X_{S_2}\}$. We denote the new set forming by swap of $\max\{X_{S_1}\}$ with $\min\{X_{S_2}\}$ as S_1^* and S_2^* and swap of $\max\{X_{S_1}\}$ with $\max\{X_{S_2}\}$ as S_1^{**}, S_2^{**} accordingly.

Then we need to show at least one of the following happens

- (1) $f(X_{S_1^*})f(X_{S_2^*}) \geq f(X_{S_1})f(X_{S_2})$
- (2) $f(X_{S_1^{**}})f(X_{S_2^{**}}) \geq f(X_{S_1})f(X_{S_2})$

Let $a = \max\{X_{S_1}\}$, $b = \min\{X_{S_2}\}$ and $c = \max\{X_{S_2}\}$. $h_1 = \sum_{i \in S_1} X_i - a$ and $h_2 = \sum_{i \in S_2} X_i - b$, n_1 and n_2 are the number of elements in S_1 and S_2 . Then

$$\begin{aligned}
f(X_{S_1^*})f(X_{S_2^*}) &\geq f(X_{S_1})f(X_{S_2}) \\
&\iff \\
\frac{\Gamma(h_1 + a + \alpha)}{(n_1 + \beta)^{h_1 + a + \alpha}} \frac{\Gamma(h_2 + b + \alpha)}{(n_2 + \beta)^{h_2 + b + \alpha}} &\leq \frac{\Gamma(h_2 + a + \alpha)}{(n_2 + \beta)^{h_2 + a + \alpha}} \frac{\Gamma(h_1 + b + \alpha)}{(n_2 + \beta)^{h_1 + b + \alpha}} \\
&\iff \\
\frac{\Gamma(h_1 + a + \alpha)}{\Gamma(h_1 + b + \alpha)} \frac{\Gamma(h_2 + b + \alpha)}{\Gamma(h_2 + a + \alpha)} &\leq \left(\frac{n_1 + \beta}{n_2 + \beta}\right)^{a-b}
\end{aligned}$$

Left hand side of above formula is $\text{LHS}_1 = \frac{(h_1+b+\alpha)\dots(h_1+a-1+\alpha)}{(h_2+b+\alpha)\dots(h_2+a-1+\alpha)}$ by the property of Gamma function and X_i are integer.

Similarly,

$$\begin{aligned}
f(X_{S_1^{**}})f(X_{S_2^{**}}) &\geq f(X_{S_1})f(X_{S_2}) \\
&\iff \\
\frac{\Gamma(h_2 + c + \alpha)}{\Gamma(h_2 + a + \alpha)} \frac{\Gamma(h_1 + a + \alpha)}{\Gamma(h_1 + c + \alpha)} &\leq \left(\frac{n_2 + \beta}{n_1 + \beta}\right)^{c-a}
\end{aligned}$$

Left hand side of above formula is $\text{LHS}_2 = \frac{(h_2+a+\alpha)\dots(h_2+c-1+\alpha)}{(h_1+a+\alpha)\dots(h_1+c-1+\alpha)}$

If $h_1 \leq h_2$, then $\text{LHS}_1 \leq \left(\frac{h_1+a-1+\alpha}{h_2+a-1+\alpha}\right)^{a-b}$ and $\text{LHS}_2 \leq \left(\frac{h_2+c-1+\alpha}{h_1+c-1+\alpha}\right)^{a-b}$

So if $\frac{h_1+a-1+\alpha}{h_2+a-1+\alpha} \leq \frac{n_1+\beta}{n_2+\beta}$ then (12) holds, if $\frac{h_2+c-1+\alpha}{h_1+c-1+\alpha} \leq \frac{n_1+\beta}{n_2+\beta}$ then (13) holds

We multiply those two inequalities, we found that $\frac{h_1+a-1+\alpha}{h_2+a-1+\alpha} * \frac{h_2+c-1+\alpha}{h_1+c-1+\alpha} = \frac{h_1+a-1+\alpha}{h_1+c-1+\alpha} * \frac{h_2+c-1+\alpha}{h_2+a-1+\alpha} \leq 1$ as $c > a$ and $h_1 \leq h_2$ But $\frac{n_1+\beta}{n_2+\beta} * \frac{n_1+\beta}{n_2+\beta} = 1$. At least one equality holds, consequently at least one of (12) and (13) holds.

Similar proof for the case $h_1 > h_2$.

□

Choosing K by validity score:

In order to determine the number of clusters, we consider the change of $validity = \frac{\mathbf{intra}}{\mathbf{inter}}$ defined in ?, where $\mathbf{intra} = \frac{1}{N} \sum_{i=1}^K \sum_{x \in C_i} ||x - z_i||^2$, $\mathbf{inter} = \text{mean}(|z_i - z_j|^2), i = 1, 2, \dots, K-1, j = i+1, \dots, K$ and z_i is the center (medoids) of cluster i . \mathbf{intra} is the average of distance of a point to its corresponding cluster center, which measures the compactness of clusters. We made a small change here, in original paper \mathbf{inter} was defined as minimum distance between medoids, we use average instead for the purpose of getting a smoother quantity. \mathbf{inter} is the average distance of two cluster centers, which measures the separation between clusters. We want to have a small intra-cluster distance and a big inter-cluster distance, consequently we want to minimize the $validity$. From empirical study, we constantly observe a monotone decreasing relation between number of clusters and $validity$. However this quantity stabilize when K is sufficiently large. The stopping rule for searching K is when $|validity_K - \min(validity_K)| < \epsilon$ is satisfied.

Randomized k-means

0.1. *simulation.* We random generate one-dimensional data X from a mixture of 5 normal distributions with different means and same variance. We compare clustering results between random weighting and bayesian clustering with Dirichlet process as prior in terms of posterior probabilities that two elements belong to the same class given the whole data and adjusted rand index comparing to the underlying true class label (Fig 12).

0.2. *empirical study.* **Double Dirichlet Model:**

On the double Dirichlet masses, using notation as in Section 2.3 we have density functions:

$$p_{\pi}(\phi, \psi) = q_{\pi}(\Phi_{\pi}, \Psi_{\pi}) \prod_{b \in \pi} [p(\tilde{\phi}_b) p(\tilde{\psi}_b)]$$

with

$$q_{\pi}(\Phi_{\pi}, \Psi_{\pi}) = \frac{\Gamma(\sum_{b \in \pi} \beta_b)}{\prod_{b \in \pi} \Gamma(\beta_b)} \left[\prod_{b \in \pi} \Phi_b^{\beta_b-1} \right] 1[\Phi_{\pi} = \Psi_{\pi}]$$

and

$$p(\tilde{\phi}_b) = \frac{\Gamma(\sum_{k \in b} \alpha_k)}{\prod_{k \in b} \Gamma(\alpha_k)} \prod_{k \in b} \tilde{\phi}_k^{\alpha_k-1}, \quad p(\tilde{\psi}_b) = \frac{\Gamma(\sum_{k \in b} \alpha_k)}{\prod_{k \in b} \Gamma(\alpha_k)} \prod_{k \in b} \tilde{\psi}_k^{\alpha_k-1}.$$

Proofs:

LEMMA 1. *If π_2 is not refinement of π_1 then $A_{\pi_1} \cap A_{\pi_2}$ is a lower dimensional subset of A_{π_2}*

Proof of lemma 1

PROOF. Let V denote the orthogonal space of $\phi - \psi$, when $(\phi, \psi) \in A_{\pi_1} \cap A_{\pi_2}$, and $\dim(A_{\pi_1} \cap A_{\pi_2}) = \dim(\phi - \psi) + \dim(\psi) = 2K - \dim(V) - 1$. Also let $\pi_1 = \{b_1^1, \dots, b_s^1\}$, $\pi_2 = \{b_1^2, \dots, b_t^2\}$. The corresponding vectors are v_1^1, \dots, v_s^1 and v_1^2, \dots, v_t^2 . We claim there must be a $b_i^1 \in \pi$ whose corresponding v_i^1 is linear independent with v_1^2, \dots, v_t^2 . If not, for every v_i^1 there exists $\alpha_1^i, \dots, \alpha_t^i$ such that

$$v_i^1 = \sum_{j=1}^t \alpha_j^i v_j^2 \quad (*)$$

If $b_j^2 \cap b_i^1 \neq \emptyset$, then multiply v_j^2 on both sides of (*), we obtain $v_i^1 * v_j^2 = \alpha_j^i (v_j^2)^2$, as v_j^2 are orthogonal vectors, and $v_i^1 * v_j^2 > 0$ implies $\alpha_j^i > 0$. Consider $x = f(b_j^2 \setminus b_i^1)$, we have $x * v_i^1 = 0$ and we multiply x on both sides of (*) to obtain $\alpha_j^i v_j^2 * x = 0$, thus x must be zero vector and $b_j^2 \setminus b_i^1 = \emptyset$, which implies $b_j^2 \subset b_i^1$. That is to say when $b_j^2 \cap b_i^1 \neq \emptyset$, b_j^2 must be subset of b_i^1 . So b_i^1 is union of some blocks in π_2 . Which implies π_2 is refinement of π_1 , contradiction.

Consequently there exists $b \in \pi_1$ with $v(b)$ linear independent with $v(b')$, $b' \in \pi_2$. $\dim(V)$ is at least $N(\pi_2) + 1$, $\dim(A_{\pi_1} \cap A_{\pi_2}) < \dim(A_{\pi_2})$ \square

Proof of property 8

PROOF. by lemma 1, it is easy to verify. \square

As the density of DDM is computed by product or ratio over bunches of gamma function and gamma function is not easy to direct work on it and derive limiting theorem. To proof theorem 4 and 5, we need a crucial lemma which gave us an approximation to the gamma function, namely

LEMMA 2. *For $x \geq 1$, $x^{a(x-1)-c} \leq \Gamma(x) \leq x^{b(x-1)-c}$, where $c = 0.577215\dots$ is the Euler-Mascheroni constant and $a = (\pi^2/6 - c)/2, b = 1$.*

PROOF. By (?), we have $x^{a(x-1)-c} < \Gamma(x) < x^{b(x-1)-c}$ for $x > 1$ and now we added the case when $x = 1, \Gamma(x) = 1$ so that both sides will include the equality case. \square

We have another lemma and theorem 4 and 5 are just proportion of the lemma

LEMMA 3. If $(\phi, \psi) \in A_{\pi_1} \cap A_{\pi_2}$, then

$$\begin{aligned} \frac{\omega_{\pi_1}^{post}}{\omega_{\pi_2}^{post}} &\xrightarrow[n \rightarrow \infty]{a.s.} 0 \quad \text{if } N(\pi_1) < N(\pi_2) \\ \frac{\omega_{\pi_1}^{post}}{\omega_{\pi_2}^{post}} &\xrightarrow[n \rightarrow \infty]{d} v \quad \text{if } N(\pi_1) = N(\pi_2) \end{aligned}$$

v is a gamma distributed random variable

PROOF. Recall $\omega_{\pi}^{post} \propto p_{\pi}(t^1 | t_{\pi}^1, y) p_{\pi}(t^2 | t_{\pi}^2, y) p_{\pi}(t_{\pi}^1, t_{\pi}^2 | y) \omega_{\pi}$. and RHS = $f(\pi_1, \pi_2, t^1, t^2, \alpha, \beta) g(\pi_1, \pi_2, \alpha, \beta, n_1, n_2)$

where

Recall $t^1 \sim \text{multinomial}(n_1, \phi), t^2 \sim \text{multinomial}(n_2, \psi)$.

\square

Proof of theorem 4 and theorem 5

PROOF. Given the condition that $\alpha_k = 1, \forall k$ and $\beta_b = \sum_{k \in b} \alpha_k$, recall $p(A_{\pi} | y, z) = \sum_{\pi' \in \text{RF}(\pi)} J(y, z, \pi')$ and $J(y, z, \pi) = \frac{1}{c'} \prod_{b \in \pi} \frac{\Gamma(\beta_b + t_b^1 + t_b^2)}{\Gamma(N(b) + t_b^1) \Gamma(N(b) + t_b^2)} \frac{\Gamma(N(b))}{\Gamma(2N(b))}$

Assuming there are K subgroups, since n_1 and n_2 goes to infinite at same rate, for simplicity we assume $n_1 = n_2$, and the multiplicity term $\frac{\Gamma(N(b))}{\Gamma(2N(b))}$ in $J(y, z, \pi)$ remains finite for any π . To demonstrate limiting

$t^1 \sim \text{multinomial}(\phi), t^2 \sim \text{multinomial}(\psi)$ $t_b^1 = \sum_{i \in b} z_i^1$ and $t_b^2 = \sum_{i \in b} z_i^2$, so $t_b^1 \sim \text{binomial}(n, \Phi_b)$ and $t_b^2 \sim \text{binomial}(n, \Psi_b)$, where $\Phi_b = \sum_{i \in b} \phi_i$ and $\Psi_b = \sum_{i \in b} \psi_i$. Let $f(n, b) = \frac{\Gamma(\beta_b + t_b^1 + t_b^2)}{\Gamma(\beta_b + t_b^1) \Gamma(\beta_b + t_b^2)}$, then

$$J(z^1, z^2, \pi) \propto \prod_{b \in \pi} f(n, b)$$

$\log f(n, b) = \log(\Gamma(\beta_b + t_b^1 + t_b^2)) - \log(\Gamma(\beta_b + t_b^1)) - \log(\Gamma(\beta_b + t_b^2))$, notice that t_b^1, t_b^2 and β_b are integers, and when x is integer, $\Gamma(x)$ is the factorial of $(x - 1)$. We have $\log f(n, b) = \log((\beta_b + t_b^1 + t_b^2 - 1)!) - \log((\beta_b + t_b^1 - 1)!) - \log((\beta_b + t_b^2 - 1)!) - \log((\beta_b + t_b^1 - 1)!) - \log((\beta_b + t_b^2 - 1)!) \approx (\beta_b + t_b^1 + t_b^2 - 1) \log(\beta_b + t_b^1 + t_b^2 - 1) - (\beta_b + t_b^1 - 1) \log(\beta_b + t_b^1 - 1) - (\beta_b + t_b^2 - 1) \log(\beta_b + t_b^2 - 1) + O(\log(n))$.

Plug into $f(n, b)$ we have:

$$\log f(n, b) \approx (\beta_b + t_b^1 - 1) \log(1 + \frac{t_b^2}{\beta_b + t_b^1 - 1}) + (\beta_b + t_b^2 - 1) \log(1 + \frac{t_b^1}{\beta_b + t_b^2 - 1}) + O(\log(n))$$

as $\beta_b \log(\beta_b + t_b^1 + t_b^2 - 1) \sim O(\log(n))$ and by law of large number and slusky's theorem, $\log(1 + \frac{t_b^2}{\beta_b + t_b^1 - 1}) \rightarrow \log(1 + \frac{\Psi_b}{\Phi_b})$, $\log(1 + \frac{t_b^1}{\beta_b + t_b^2 - 1}) \rightarrow \log(1 + \frac{\Phi_b}{\Psi_b})$ a.s. and $\frac{\log f(n, b)}{n} \rightarrow \Phi_b \log(1 + \frac{\Psi_b}{\Phi_b}) + \Psi_b \log(1 + \frac{\Phi_b}{\Psi_b})$ a.s. We have:

$$\frac{\log(\prod_{b \in \pi} f(n, b))}{n} \rightarrow \sum_b [\Phi_b \log(1 + \frac{\Psi_b}{\Phi_b}) + \Psi_b \log(1 + \frac{\Phi_b}{\Psi_b})] \quad a.s.$$

To find the maxima (Φ, Ψ) , we fix Ψ and let $C = \frac{\log(\prod_{b \in \pi} f(n, b))}{n} + \lambda(\sum_{b \in \pi} \Phi_b - 1)$, we have $\frac{\partial C}{\partial \Phi_b} = \log(1 + \frac{\Psi_b}{\Phi_b}) + \lambda$, stationary point is $\Phi_b = \Psi_b, \forall b$. and for the hessian matrix $\frac{\partial^2 C}{\partial \Phi_b^2} = -\frac{\Psi_b}{\Phi_b^2 + \Phi_b \Psi_b} < 0$ and $\frac{\partial^2 C}{\partial \Phi_b \partial \Phi_{b'}} = 0$, if $b \neq b'$, that is to say the hessian matrix is a diagonal matrix with every diagonal elements to be negative, so it is negative definite, and our objective function is concave. The maxima is the stationary point $\Phi = \Psi$. And when $\Phi = \Psi$, $\frac{\log(\prod_{b \in \pi} f(n, b))}{n} = 2 \ln(2)$ a constant not dependent on partition π and Φ . That is to say if $(\phi, \psi) \in A_{\pi_1} \cap A_{\pi_2}$ and $(\phi, \psi) \notin A_{\pi_3}$. Then we would have $\lim_{n \rightarrow \infty} \frac{\log(\prod_{b \in \pi_1} f(n, b))}{n} = \lim_{n \rightarrow \infty} \frac{\log(\prod_{b \in \pi_2} f(n, b))}{n}$ and $\lim_{n \rightarrow \infty} [\frac{\ln(\prod_{b \in \pi_1} f(n, b))}{n} - \frac{\log(\prod_{b \in \pi_3} f(n, b))}{n}] = c > 0$, which implies:

$$(A) \quad \frac{J(t^1, t^2, \pi_3)}{J(t^1, t^2, \pi_1)} \rightarrow 0 \quad a.s.$$

To investigate the limit of $\frac{J(t^1, t^2, \pi_1)}{J(t^1, t^2, \pi_2)}$, We use inequalities that $\sqrt{2\pi} n^{n+\frac{1}{2}} e^{-n} \leq n! \leq e n^{n+\frac{1}{2}} e^{-n}$ holds for all nonnegative integers n . Plug in $f(n, b)$, we

have:

$$(1) \quad \beta_b + \log\sqrt{2\pi} - 3 + g(n, b) \leq f(n, b) \leq \beta_b - 2\log\sqrt{2\pi} + g(n, b)$$

$$g(n, b) = (\beta_b + t_b^1 - \frac{1}{2})\log(1 + \frac{t_b^2}{\beta_b + t_b^1 - 1}) + (\beta_b + t_b^2 - \frac{1}{2})\log(1 + \frac{t_b^1}{\beta_b + t_b^2 - 1}) - (\beta_b - \frac{1}{2})\log(\beta_b + t_b^1 + t_b^2 - 1)$$

Based on inequalities (1), $\sum_{b \in \pi} f(n, b)$ only differ with $\sum_{b \in \pi} g(n, b)$ by a constant. By Taylor's expansion $\log(1+x) = \log 2 + \frac{1}{2}(x-1) + O((x-1)^2)$, we have $\log(1 + \frac{t_b^2}{\beta_b + t_b^1 - 1}) = \log 2 + \frac{1}{2}(\frac{t_b^1 - t_b^2 + 1 - \beta_b}{\beta_b + t_b^1 - 1}) + O_p((\frac{t_b^1 - t_b^2 + 1 - \beta_b}{\beta_b + t_b^1 - 1})^2)$ and under condition $\Phi_b = \Psi_b, \frac{(t_b^1 - t_b^2 + 1 - \beta_b)^2}{\beta_b + t_b^1 - 1}$ is $O_p(1)$. Plug in $g(n, b)$

$$g(n, b) = \log 2 * t_b^1 + \log 2 * t_b^2 - (\beta_b - \frac{1}{2})\log(\beta_b + t_b^1 + t_b^2 - 1) + O_p(1)$$

and sum up

$$(2) \quad \sum_{b \in \pi} g(n, b) = 2n\log 2 - \sum_{b \in \pi} (\beta_b - \frac{1}{2})\log(\beta_b + t_b^1 + t_b^2 - 1) + O_p(1)$$

Notice that when two partition π_1, π_2 have same number of blocks b and $\Phi_b = \Psi_b, \forall b \in \pi_1 \cup \pi_2$,

$$\begin{aligned} \sum_{b \in \pi_1} g(n, b) - \sum_{b' \in \pi_2} g(n, b') &= \sum_{b' \in \pi_2} (\beta_{b'}' - \frac{1}{2})\log(\beta_{b'}' + t_{b'}^1 + t_{b'}^2 - 1) - \sum_{b \in \pi_1} (\beta_b - \frac{1}{2})\log(\beta_b + t_b^1 + t_b^2 - 1) + \\ &= \sum_{b' \in \pi_2} (\beta_{b'}' - \frac{1}{2})\log(\frac{\beta_{b'}' + t_{b'}^1 + t_{b'}^2 - 1}{n}) - \sum_{b \in \pi_1} (\beta_b - \frac{1}{2})\log(\frac{\beta_b + t_b^1 + t_b^2 - 1}{n}) \\ &+ \sum_{b' \in \pi_2 - \frac{1}{2}} (\beta_{b'}' - \frac{1}{2})\log(n) - \sum_{b \in \pi_1 - \frac{1}{2}} (\beta_b - \frac{1}{2})\log(n) + O_p(1) \\ &= O_p(1) + \sum_{b \in \pi_1} \frac{1}{2}\log(n) - \sum_{b' \in \pi_2} \frac{1}{2}\log(n) \\ &= O_p(1) \end{aligned}$$

When π_1 and π_2 have same number of blocks,

$$(B) \quad \frac{J(t^1, t^2, \pi_1)}{J(t^1, t^2, \pi_2)} \rightarrow O_p(1) \quad a.s.$$

When π_1 have less blocks than π_2 , $\sum_{b' \in \pi_2} g(n, b') - \sum_{b \in \pi_1} g(n, b) = O_p(\log(n))$

$$(C) \quad \frac{J(t^1, t^2, \pi_1)}{J(t^1, t^2, \pi_2)} \rightarrow 0 \quad a.s.$$

□

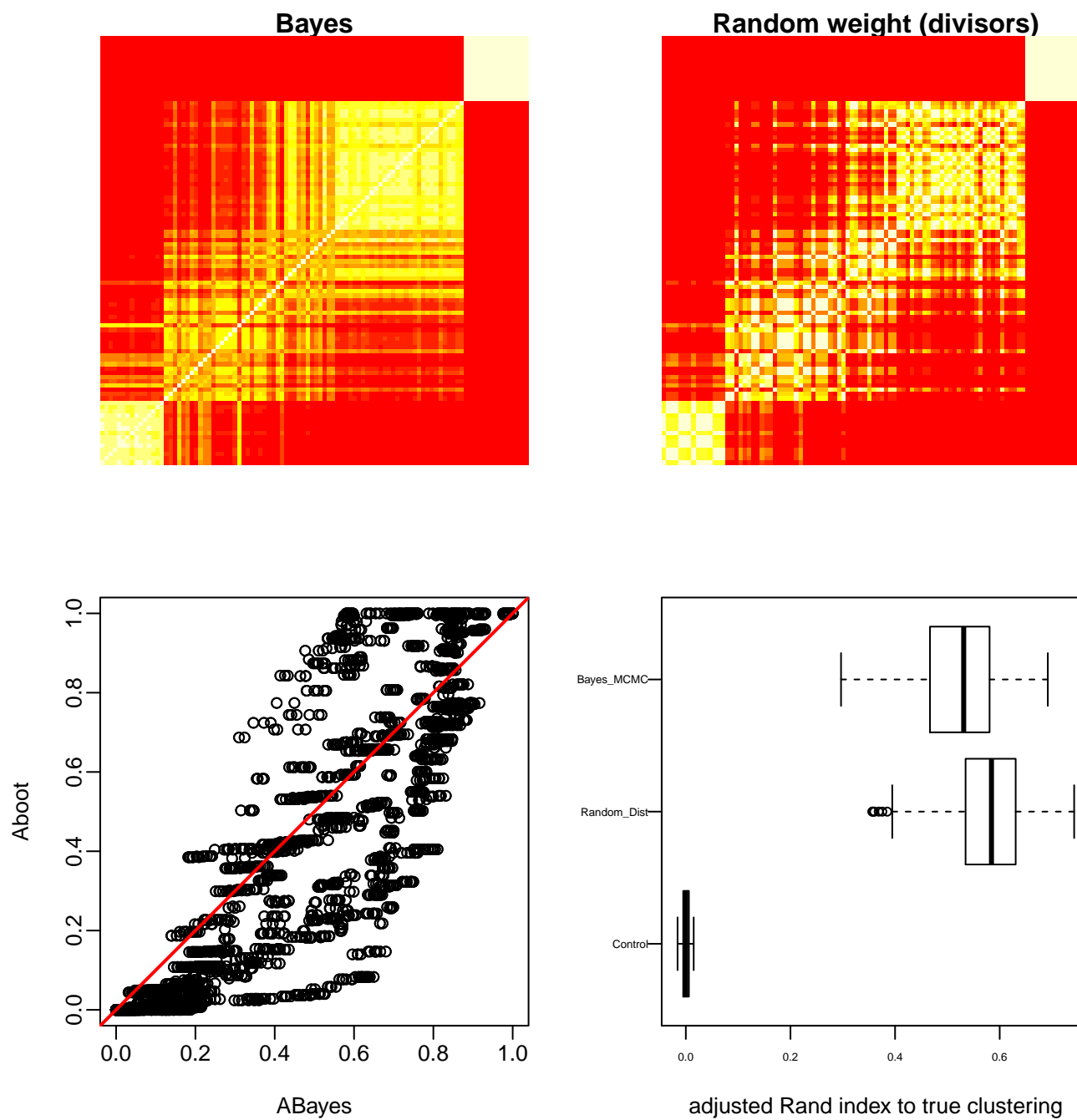


Fig 3: comparison between random weighting scheme and bayesian clustering procedure in terms of posterior probabilities that two elements belong to the same class given the whole data and adjusted rand index comparing to the underlying true class label