# Bayesian methods for rank and preference data: from recommender systems to cancer genomics

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Thomas Fleischer, Vessela Kristensen, Ida Scheel,
Elja Arjas, and Arnoldo Frigessi

**Nordic Probabilistic AI School. NTNU, Trondheim, June 5, 2019**

# Outline

# Key collaborators

**Original method:**

Øystein Sørensen,
LCBC – UiO

Arnoldo Frigessi,
OCBE – UiO & BigInsight

Elja Arjas,
OCBE – UiO & Univ. Of Helsinki

**Extensions:**

Qinghua Liu,
math - UiO

Derbachew Asfaw,
Univ. of Hawassa, Ethiopia

Marta Crispino,
INRIA, Grenoble, France

**Cancer Genomics:**

Manuela Zucknick,
OCBE - UiO

Vessela Kristensen, UiO & OUS

Thomas Fleischer, OUS

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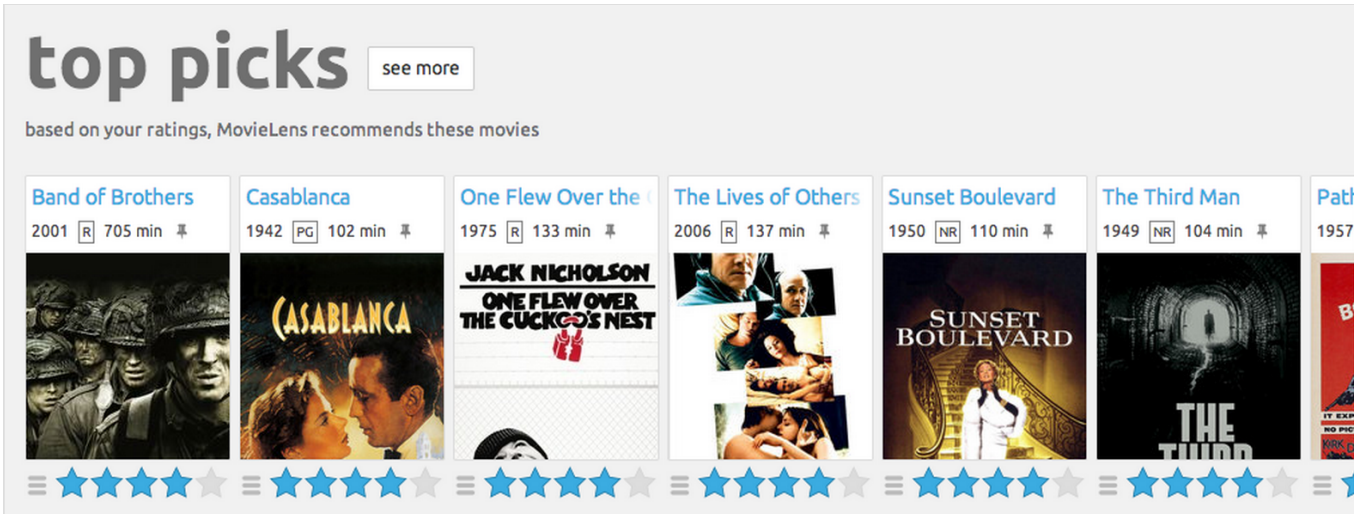

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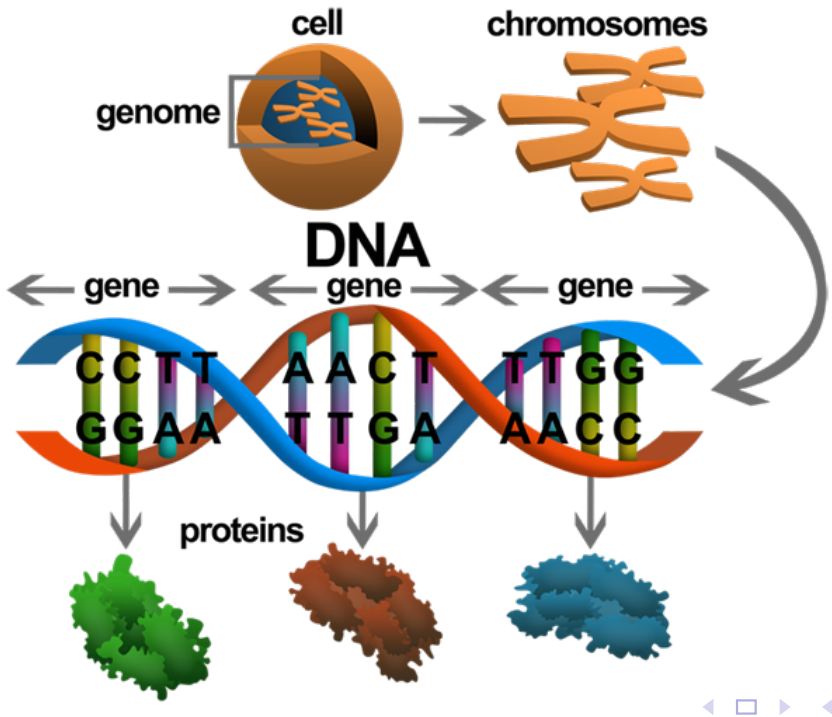

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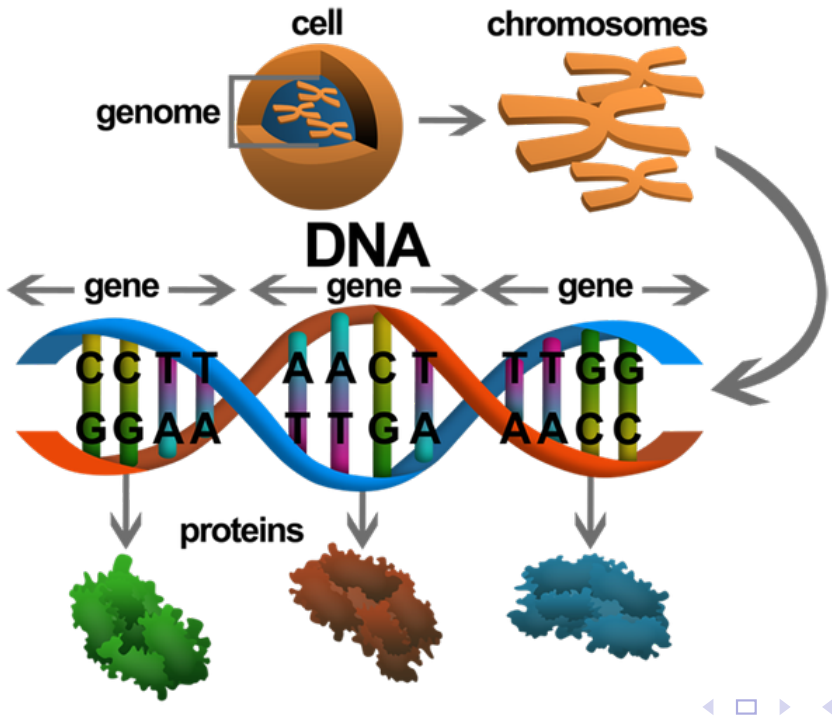
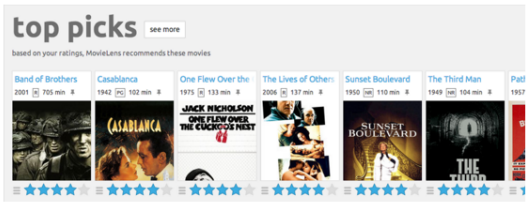


# Building blocks of a preference learning framework

sugar intake / taste / healthy

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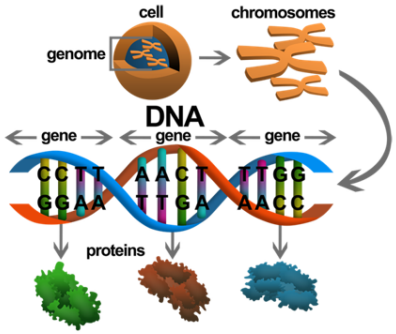


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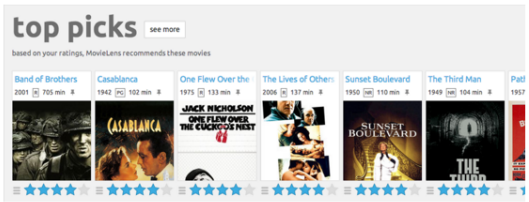


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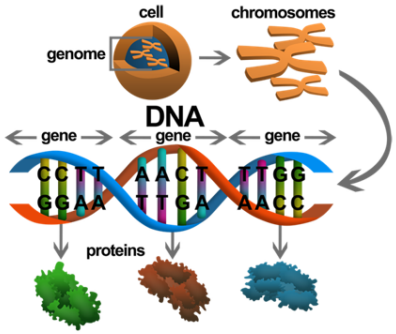


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1. Set of ordered items
   - according to an unknown feature
   - not necessarily complete ranking
2. Who provides the ordering?
   A set of assessors expressing their preference about items (as panels, users, patients, ...)

# Where to use this? Recommender Systems

**Challenges / opportunities:**

- messy data, typical of internet-user activities (rating, clicking, ...)
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- prone to non trivial generalizations (on-line inference, inconsistencies, covariates, ...)

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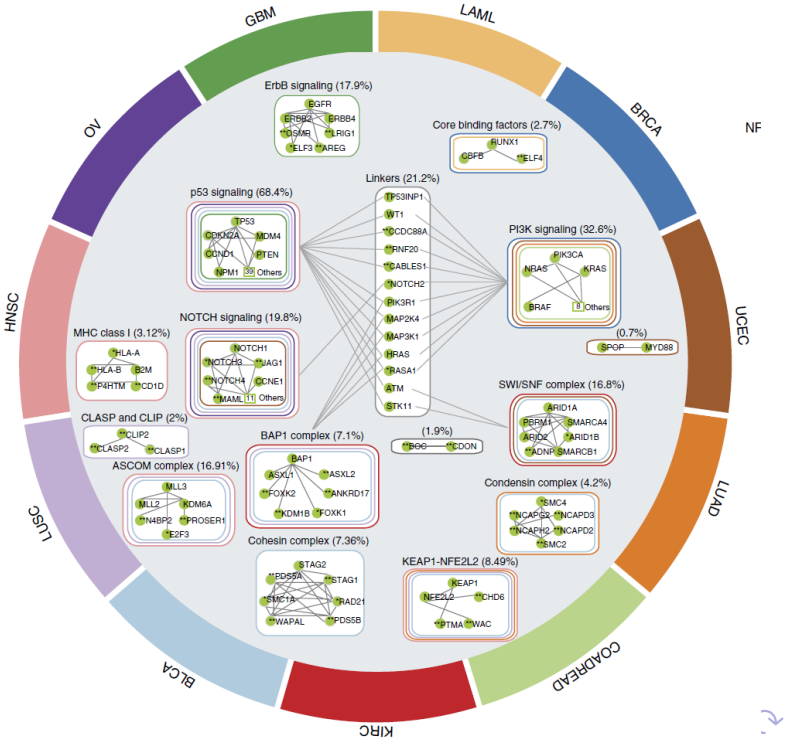
## Is cancer tissue-specific?

However, molecular disease mechanisms are known to be part of the development of diverse cancers across different tissues. Examples:

- **TP53 mutation:** serous ovarian, serous endometrial, basal-like breast cancers;
- **ERBB2-HER2 mutation/amplification:** subsets of glioblastoma, breast, gastric, serous endometrial, bladder and lung cancers.



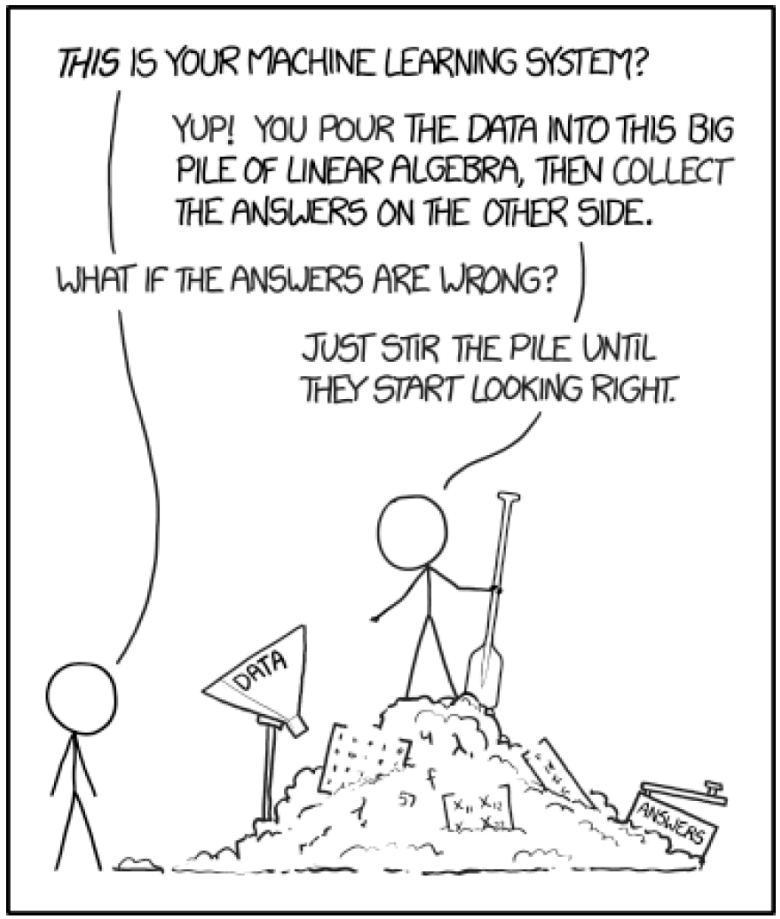
# Why model-based data analysis?

For the current problem-solving task:

- formalize reality in simple terms (good initial description of our beliefs)
- easy to control complexity (look into the box)
- neat probabilistic interpretations of the results

For the future:

- real applications are born to pass, models live forever
- sufficiently general to apply to a diversity of situations



# Ingredients for Preference Data

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A set of **items**, to be evaluated...

...and a pool of **assessors** to evaluate them

# Objectives

1. aggregate, merge, summarize multiple rankings to estimate the **consensus ranking** across the assessors, and discover shared patterns and structures

| | | | | | | |
|---|---|---|---|---|---|---|
| 1 | 1 | 1 | 3 | 2 | 3 | 3 |
| 2 | 3 | 2 | 1 | 1 | 2 | 1 |
| 3 | 2 | 3 | 2 | 3 | 1 | 2 |

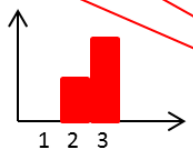


| |
|---|
| ? |
| ? |
| ? |

# Objectives

2 in case of **incomplete rankings** or preferences, predict the ranks of the missing items for each assessor

| | | | | | | |
|---|---|---|---|---|---|---|
| 1 | 1 | 1 | 3 | 2 | 3 | 3 |
| 2 | 3 | ? | 1 | 1 | ? | 1 |
| 3 | 2 | ? | 2 | 3 | ? | 2 |




| |
|---|
| ? |
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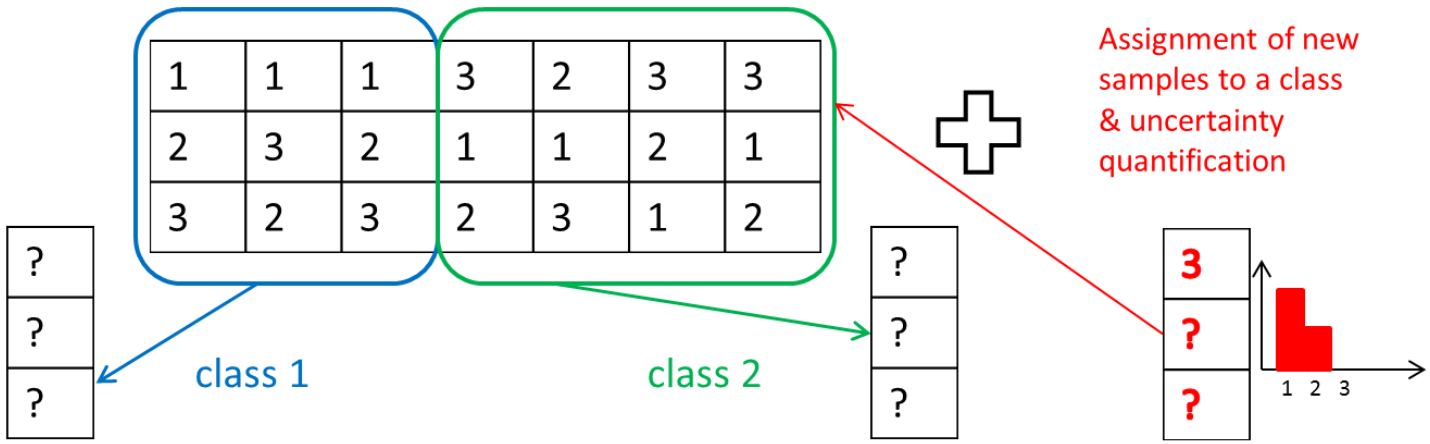
uncertainty quantification

# Objectives

3 partition the assessors into **classes**, each sharing a consensus ranking of the items, and classify new assessors to a class



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2. **preference learning methods:** methods for learning the individual rankings, when they are not readily available from the data, in order to perform personalized recommendations. Examples: the Hierarchical Bradley-Terry (HBT) model (Crispino & Frigessi, 2018, draft), which is based on the BT model. Collaborative Filtering (CF), which is grounded on matrix factorization techniques, and only infers on personal preferences (Koren et al. 2009).

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- See Liu et al. (2019a) for a review of possible alternative approaches to preference learning, with extensive comparisons of the Bayes Mallows performance with competitive methods on the very famous "potato data".

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**Setting:**

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- we consider the **Mallows model** (Mallows 1957)

# Mallows model (Mallows 1957)

Non-uniform joint distributions for $\mathbf{R}$ on $\mathcal{P}_n$, of the form

$$P(\mathbf{R}|\alpha, \boldsymbol{\rho}) = Z_n(\alpha, \boldsymbol{\rho})^{-1} \exp\{-(\alpha/n) d(\mathbf{R}, \boldsymbol{\rho})\} 1_{\mathcal{P}_n}(\mathbf{R}),$$

where:

- $\boldsymbol{\rho} \in \mathcal{P}_n$ is a location parameter,
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If $d(\cdot, \cdot)$ is right-invariant, the normalizing constant does not depend on $\boldsymbol{\rho}$:

$$Z_n(\alpha) = \sum_{\mathbf{R} \in \mathcal{P}_n} \exp\{-(\alpha/n) d(\mathbf{R}, \mathbf{P})\}$$

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- Other examples are the Hamming distance, the Ulam distance and the Cayley distance (Marden 1995:pp. 23-27).

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- Probabilistic statements about $\boldsymbol{\rho}$ and $\alpha$ are based on the joint posterior:

$$P(\boldsymbol{\rho}, \alpha | \mathbf{R}_1, \ldots, \mathbf{R}_N) \propto Z_n(\alpha)^{-N} \exp\left\{ -\alpha \left[ n^{-1} \sum_{j=1}^{N} d(\mathbf{R}_j, \boldsymbol{\rho}) + \lambda \right] \right\}.$$

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$$\min\left\{1, \frac{P_L(\boldsymbol{\rho}|\boldsymbol{\rho}')\pi(\boldsymbol{\rho}')}{P_L(\boldsymbol{\rho}'|\boldsymbol{\rho})\pi(\boldsymbol{\rho})} \exp\left[-\frac{\alpha}{n}\sum_{j=1}^{N}\left\{d\left(\mathbf{R}_j, \boldsymbol{\rho}'\right) - d\left(\mathbf{R}_j, \boldsymbol{\rho}\right)\right\}\right]\right\},$$

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$$\min\left\{1, \frac{P_L(\boldsymbol{\rho}|\boldsymbol{\rho}')\pi(\boldsymbol{\rho}')}{P_L(\boldsymbol{\rho}'|\boldsymbol{\rho})\pi(\boldsymbol{\rho})} \exp\left[-\frac{\alpha}{n}\sum_{j=1}^{N}\left\{d\left(\mathbf{R}_j, \boldsymbol{\rho}'\right) - d\left(\mathbf{R}_j, \boldsymbol{\rho}\right)\right\}\right]\right\},$$

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$$\min\left\{1, \frac{Z_n(\alpha)^N \pi(\alpha')\alpha'}{Z_n(\alpha')^N \pi(\alpha)\alpha} \exp\left[-\frac{(\alpha' - \alpha)}{n}\sum_{j=1}^{N} d\left(\mathbf{R}_j, \boldsymbol{\rho}\right)\right]\right\},$$

   where $\sigma_\alpha^2$ can be tuned to obtain a desired acceptance ratio.

# Metropolis-Hastings scheme: further details

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   This term can be computed efficiently, since most elements of $\boldsymbol{\rho}$ and $\boldsymbol{\rho}'$ are equal. If $\rho_i = \rho_i'$ for $i \in E \subset \{1, \ldots, n\}$, each MCMC iteration involves computations only on $E^c$, making the algorithm scalable with $n$.

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   This term is computationally heavy, and is thus approximated off-line.

# Off-line computation of $Z_n(\alpha)$

$Z_n(\alpha)$ is known for some choices of $d(\cdot,\cdot)$ and $n$ (see Vitelli et al. (2018)).

In all other cases, we propose the following **importance sampling (IS)** scheme to obtain an off-line approximation of

$$Z_n(\alpha) = \sum_{\mathbf{R}\in\mathcal{P}_n} \exp\left\{\frac{-\alpha}{n} d(\mathbf{R},\mathbf{P})\right\}$$

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5. Interpolate the values of $\hat{Z}_n(\alpha)$ obtained for each $\alpha$ on the grid, so to obtain a smooth estimate to be used in the MCMC.

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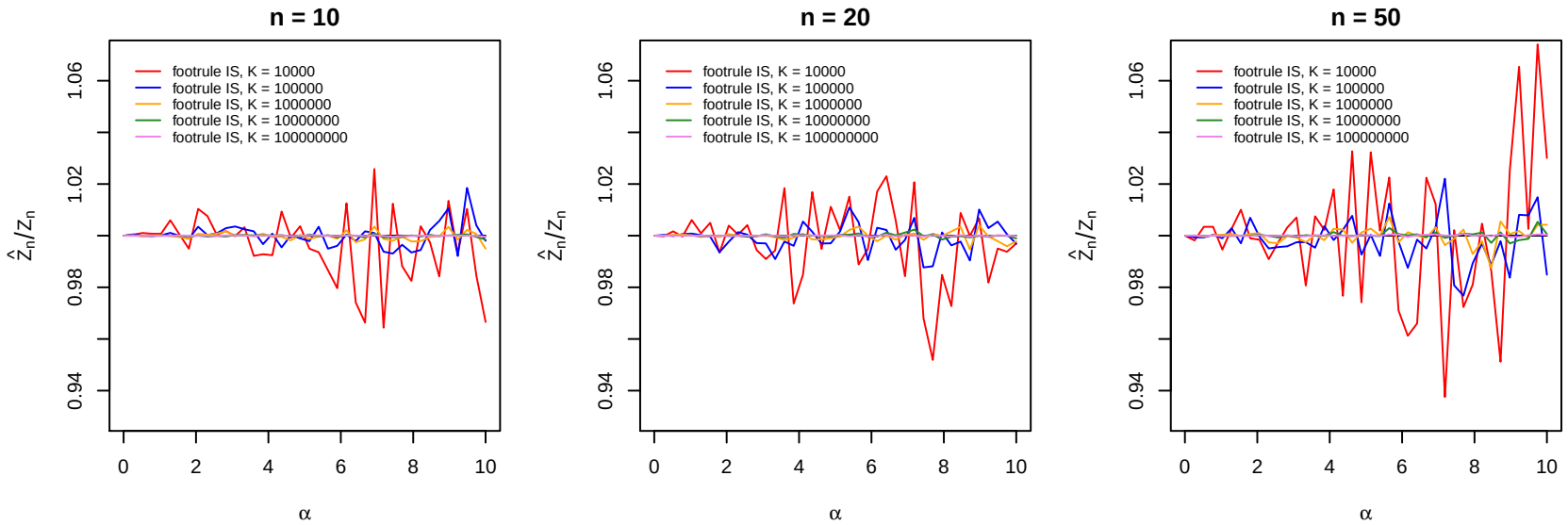
Note 3. A good alternative to the IS construction, for large $n$, is the asymptotic off-line approximation $Z_{lim}(\alpha)$ given in Mukherjee (2016) for $n \to \infty$.

# Testing the importance sampler

Ratio of the approximate partition function computed via IS to the exact:



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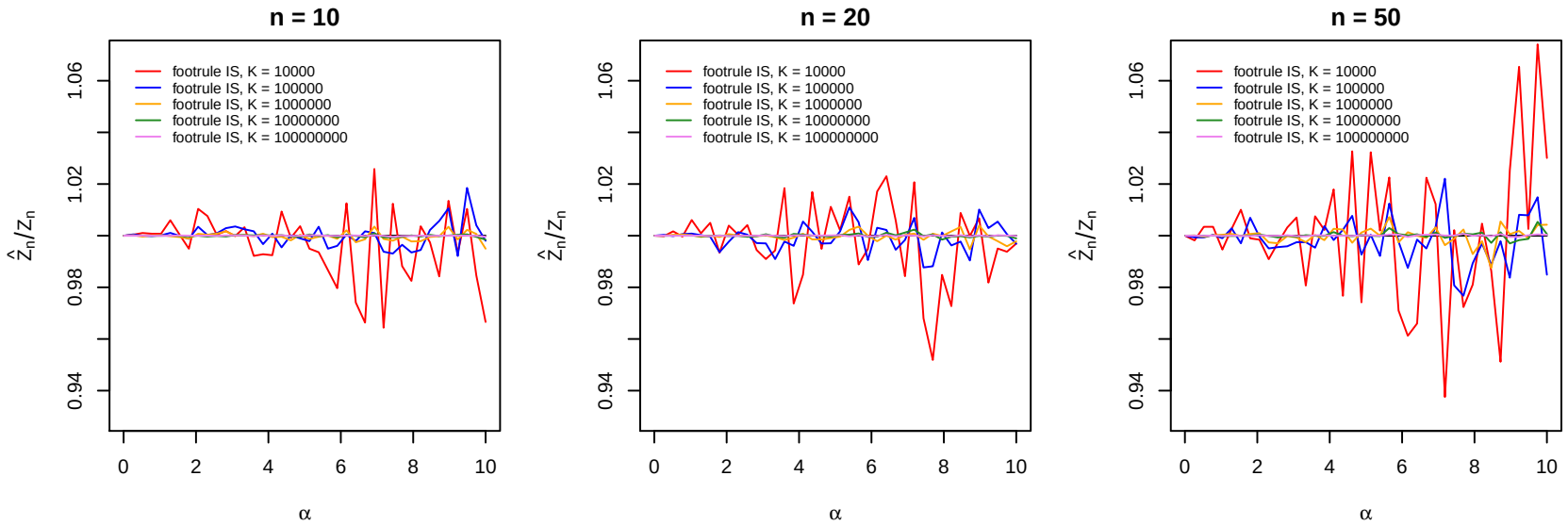


Maximum relative error between the current and the previous $K$:

| $K$ | $10^2$ | $10^3$ | $10^4$ | $10^5$ | $10^6$ | $10^7$ | $10^8$ |
|---|---|---|---|---|---|---|---|
| $n = 75$ | 152.036 | 0.921 | 0.373 | 0.084 | 0.056 | 0.005 | 0.004 |
| $n = 100$ | 67.487 | 1.709 | 0.355 | 0.187 | 0.045 | 0.018 | 0.004 |

# Effect of the approximation of $Z_n(\alpha)$ on inference

**Proposition 1.** The previous M-H algorithm using $\hat{Z}_n(\alpha)$ instead of $Z_n(\alpha)$ converges to the posterior distribution proportional to

$$\frac{1}{\hat{C}(\mathbf{R})}\pi(\boldsymbol{\rho})\pi(\alpha)\hat{Z}_n(\alpha)^{-N}\exp\left\{-\frac{\alpha}{n}\sum_{j=1}^{N}d(\mathbf{R}_j,\boldsymbol{\rho})\right\}, \tag{1}$$

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Hence, things should be just fine for reasonable values of $K$, $n$, and $N$

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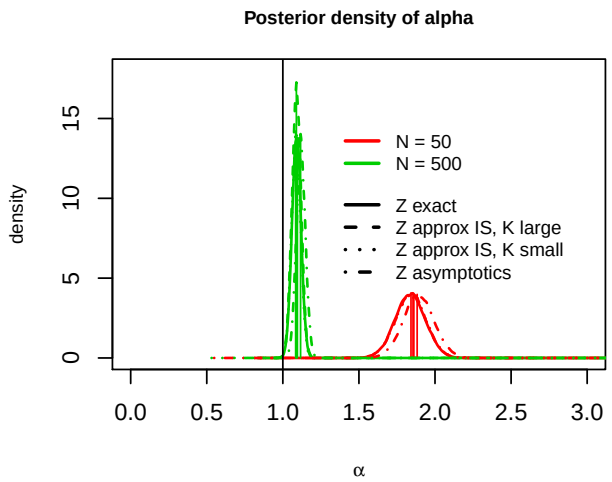


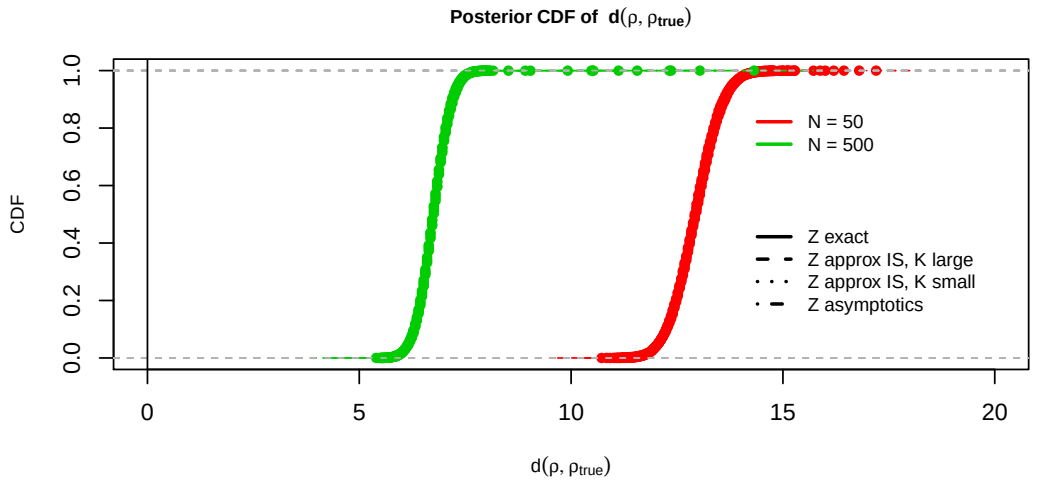


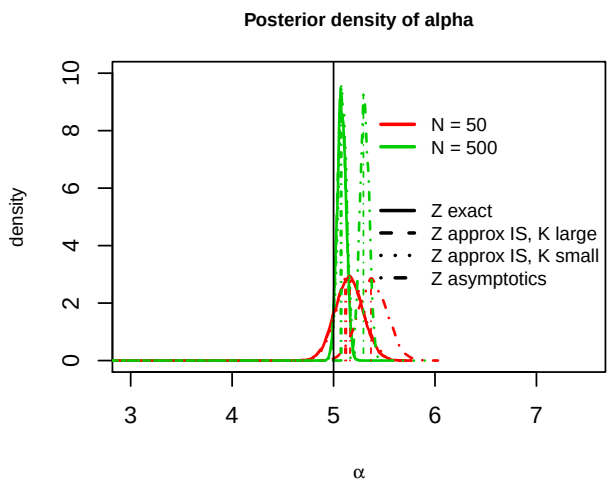


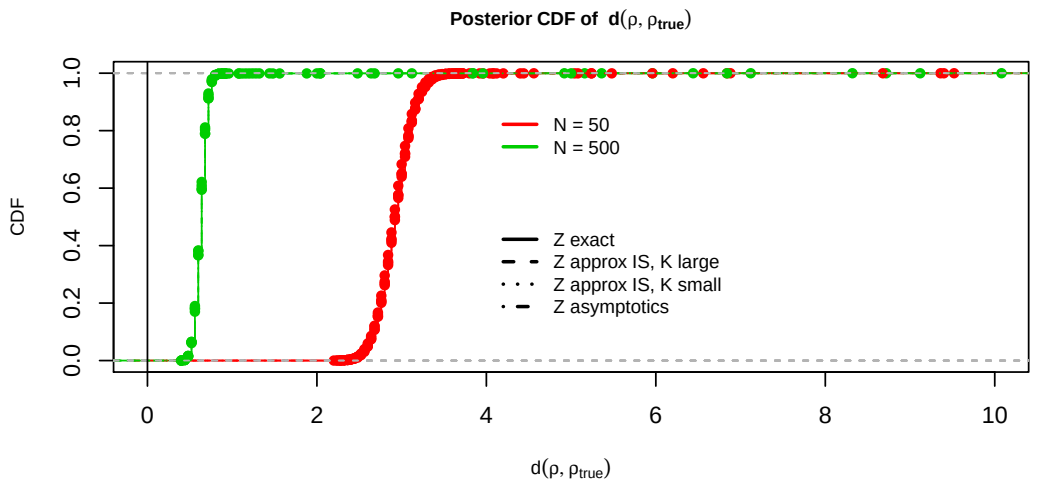

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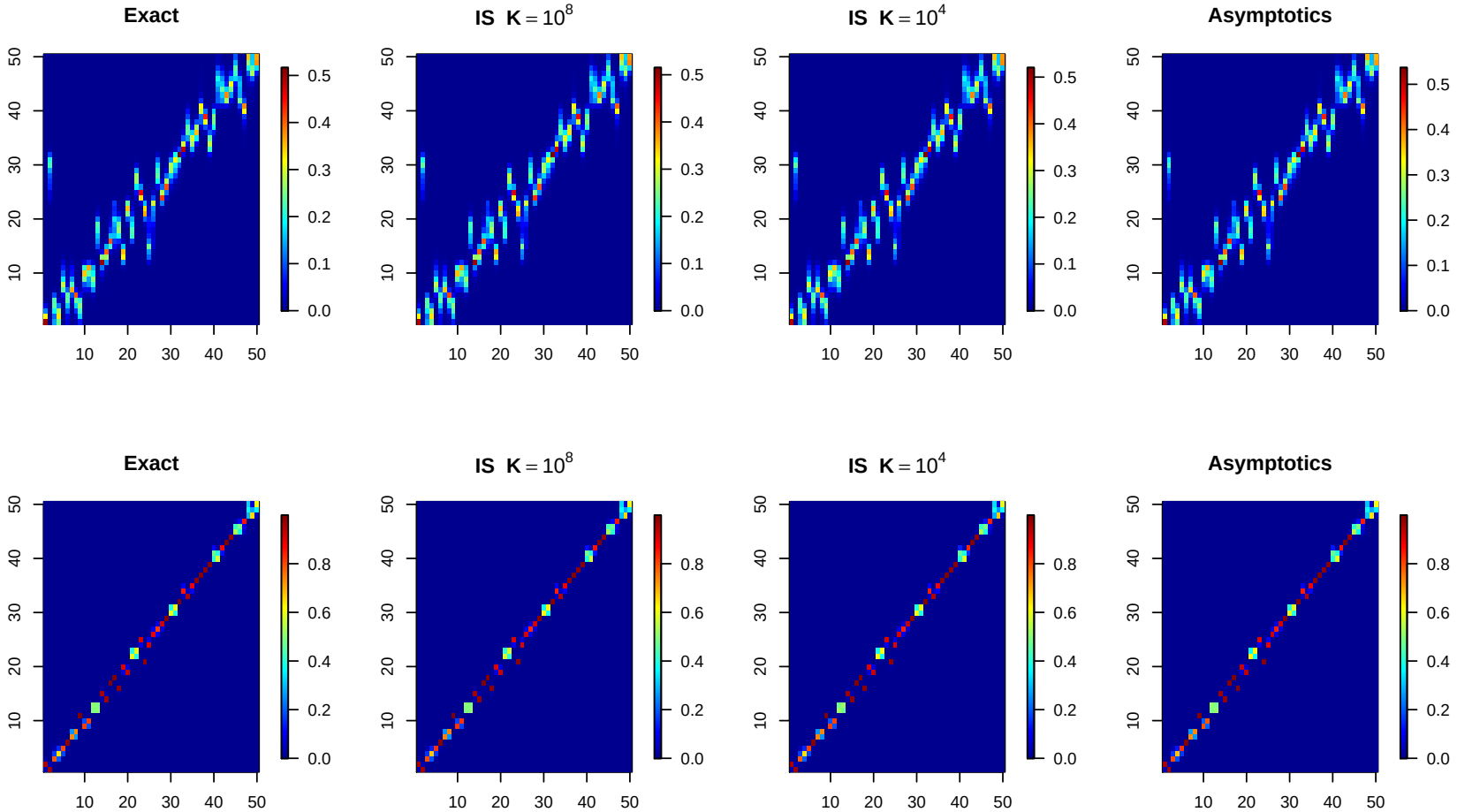

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Partial rankings can be handled easily in the Bayesian framework, by applying **data augmentation** techniques: estimating the lacking ranks consistently with the partial observations. Let $\tilde{\mathbf{R}}_1, \ldots, \tilde{\mathbf{R}}_N$ be the augmented rankings, the MCMC alternates between two steps:

1. update the parameters given the augmented rankings (basic Mallows model)
$$P(\boldsymbol{\rho}, \alpha | \tilde{\mathbf{R}}_1, \ldots, \tilde{\mathbf{R}}_N);$$
2. sample the augmented ranks from a Mallows model given the current parameter values
$$P(\tilde{\mathbf{R}}_1, \ldots, \tilde{\mathbf{R}}_N | \boldsymbol{\rho}, \alpha; \mathbf{R}_1, \ldots, \mathbf{R}_N).$$

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Pairwise preferences can also be handled via data augmentation. Suppose to observe the following preferences for assessor $j$: $\mathbf{R}_j = \{A > B, B > C, D > C\}$. Then, inside the MCMC

1. compute the associated **transitive closure**

$$tc_j = \mathbf{R}_j \cup \{A > C\}$$

2. sample $\tilde{\mathbf{R}}_j \in \mathcal{P}_n$ consistent with $tc_j$.

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Note. Label switching is handled via post-hoc re-ordering of MCMC outputs.

# R package BayesMallows

This is just to say: the package implementing the method (with all extensions) is finally on CRAN! Pretty easy to use...

## short example:

```
library(BayesMallows)
load("../../data/valeriv/pancancer/data/Ciriello2013.Rdata")
fitMallows <- compute_mallows(rankings = R, nmc = 1.1e7,
n_clusters = 2:20, include_wcd = TRUE, logz_estimate = estimate)
plot_elbow(fitMallows)
```

**Note:** See Sørensen et al. (2019) for more details on the implementation.

# MovieLens Data

**Data characteristics:**

- $n = 200$ most rated movies
- $N = 6004$ users who rated (not equally) at least 3 movies
- each user compared an average of 30.2 movies
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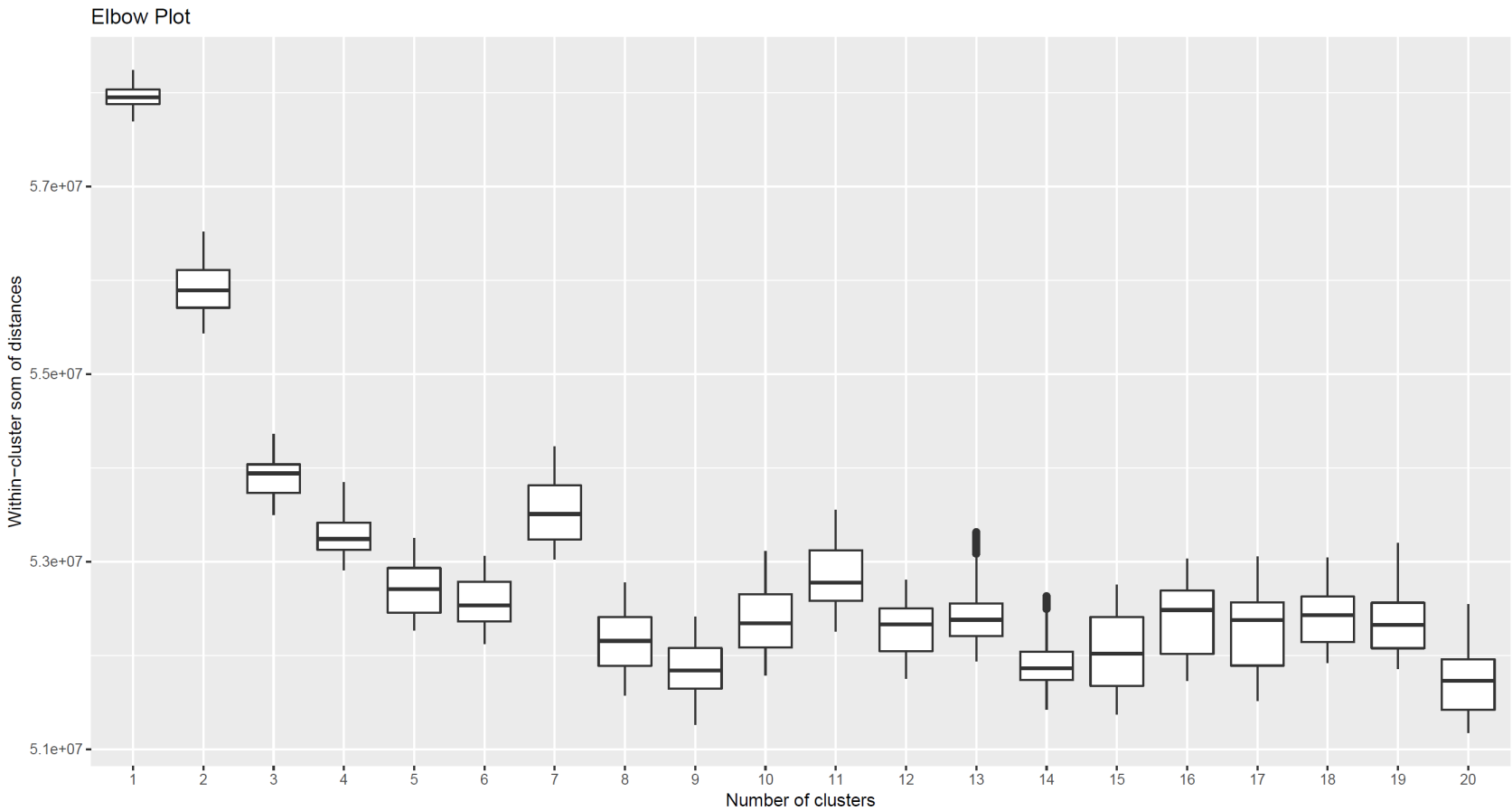
**Strategy:**

- **very sparse incomplete data:**
  use the Mallows model with data augmentation;
- perform **clustering:**
  cannot assume homogeneity across so many assessors!
- run for reasonable $C$ and **a posteriori decide the number of groups;**
- perform **preference prediction** with uncertainty quantification

# Choosing the right $C$ – within-cluster distance from $\rho_c$



# Preference prediction for the model with $C = 9$ clusters

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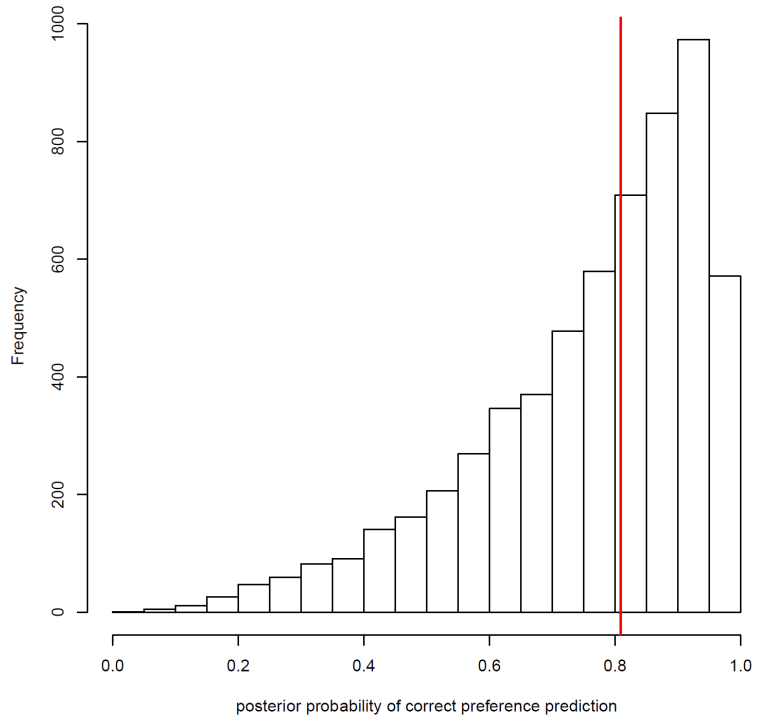
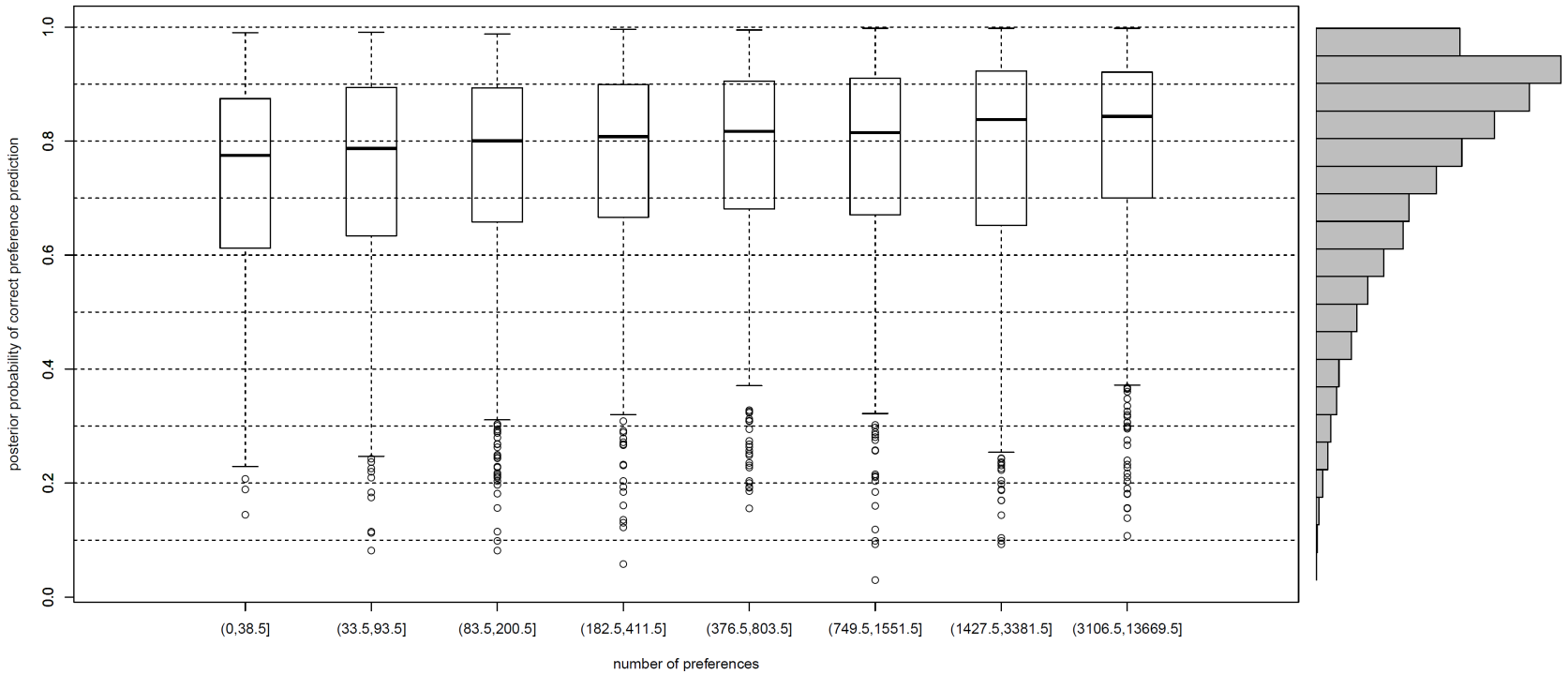
- compute the posterior probability of guessing the discarded preference **right**
- plot these posterior probabilities for all assessors $\rightarrow$
  the median across assessors is 0.809 for the model with 9 groups; moreover 89 % of these probabilities were higher than 0.5



# Preference prediction for the model with $C = 9$ clusters

We can also inspect the same posterior predictive probabilities stratifying on **how many preferences the assessor was giving**



# Meta-analysis of differential gene expression

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- Little agreement among gene lists found by independent studies comparing the same conditions leads to difficulties in finding a consensus list over all available studies. This situation raises the question of whether a consensus top list over all available studies can be found.
- Biologists are often concerned with the few most relevant genes in the specific context of the pathology, to set in place further more detailed lab experiments.

# Meta-analysis of differential gene expression

**Benchmark for meta-analysis:** five studies comparing **prostate cancer patients** with healthy controls (Dhanasekaran et al. 2001; Luo et al. 2001; Singh et al. 2002; True et al. 2006; Welsh et al. 2001). The top-25 lists from each study contained 89 genes in total.

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| 2 | AMACR | 0.59 | 0.69 | 0.8 |
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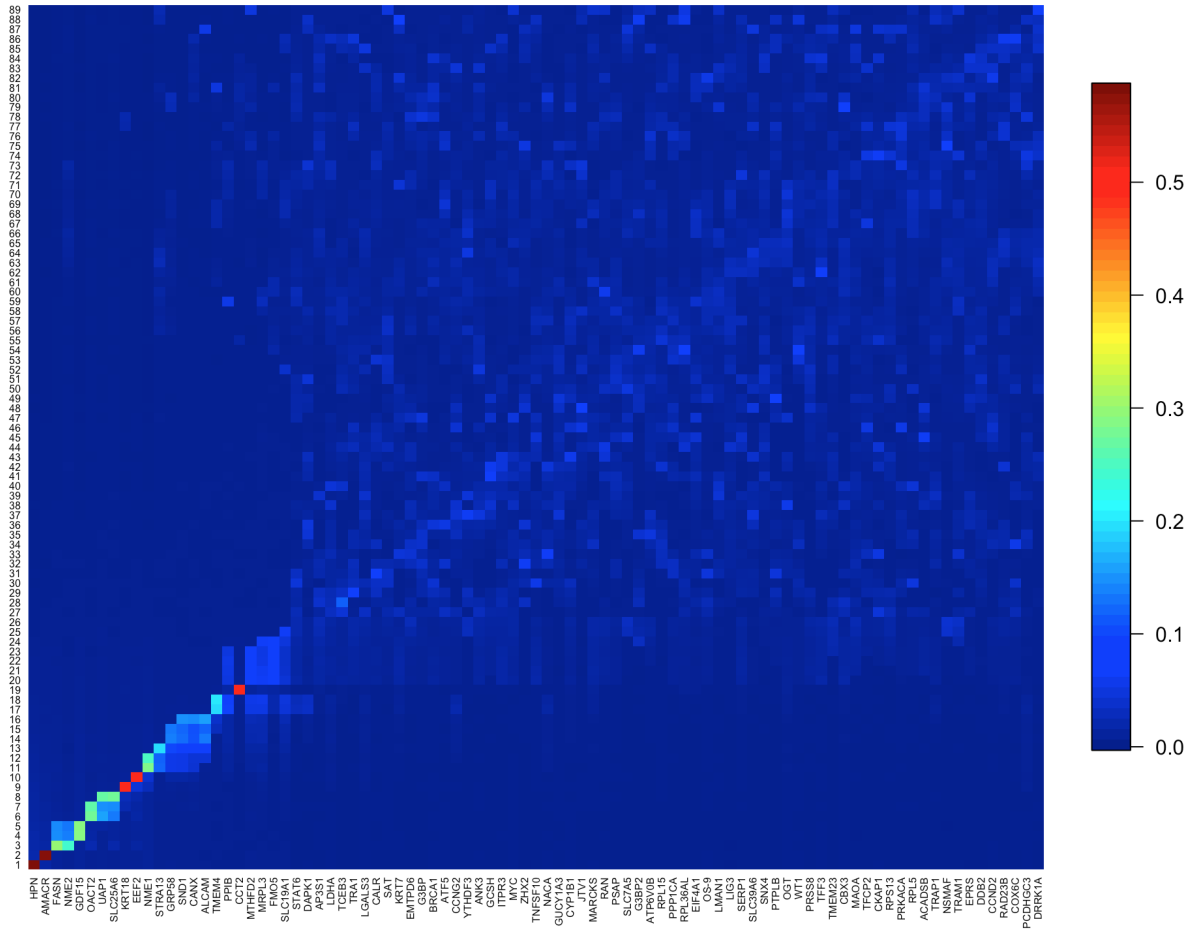
- Like De Conde et al. (2006), Deng et al. (2014), and Lin and Ding (2009), HPN and AMACR are ranked first and second in the MAP consensus ranking.
- If comparing with `RankAggreg` (Pihur et al. 2009), and the aggregation methods implemented in `TopKLists` (Schimek et al. 2015), the same genes are nearly always shared between different top$-k$ lists.

# Meta-analysis of differential gene expression



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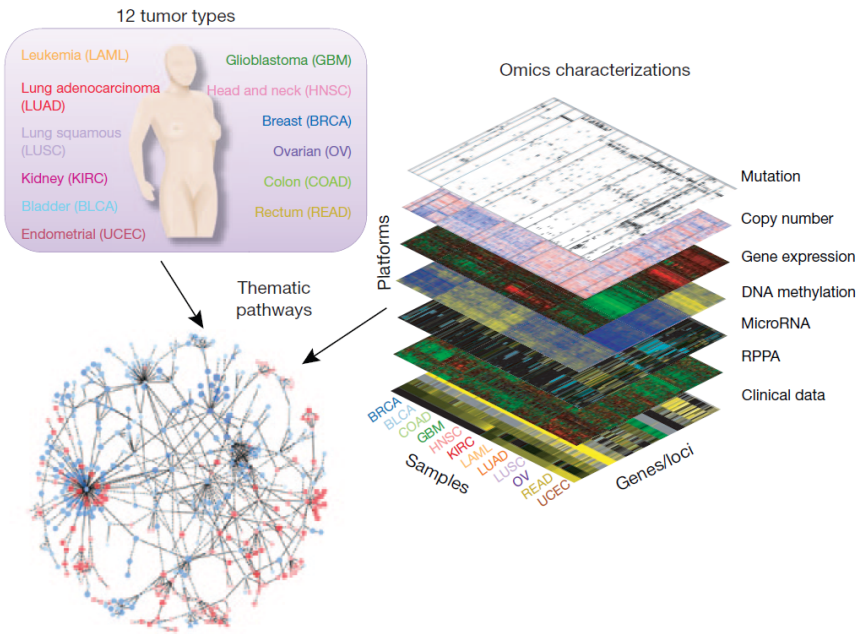
- The Cancer Genome Atlas (TCGA) started in 2006: profiling 10,000 tumour samples from 20 tumour types (`http://www.nature.com/tcga/`): multiple technical platforms; increasingly complete picture of molecular alterations in cancer.



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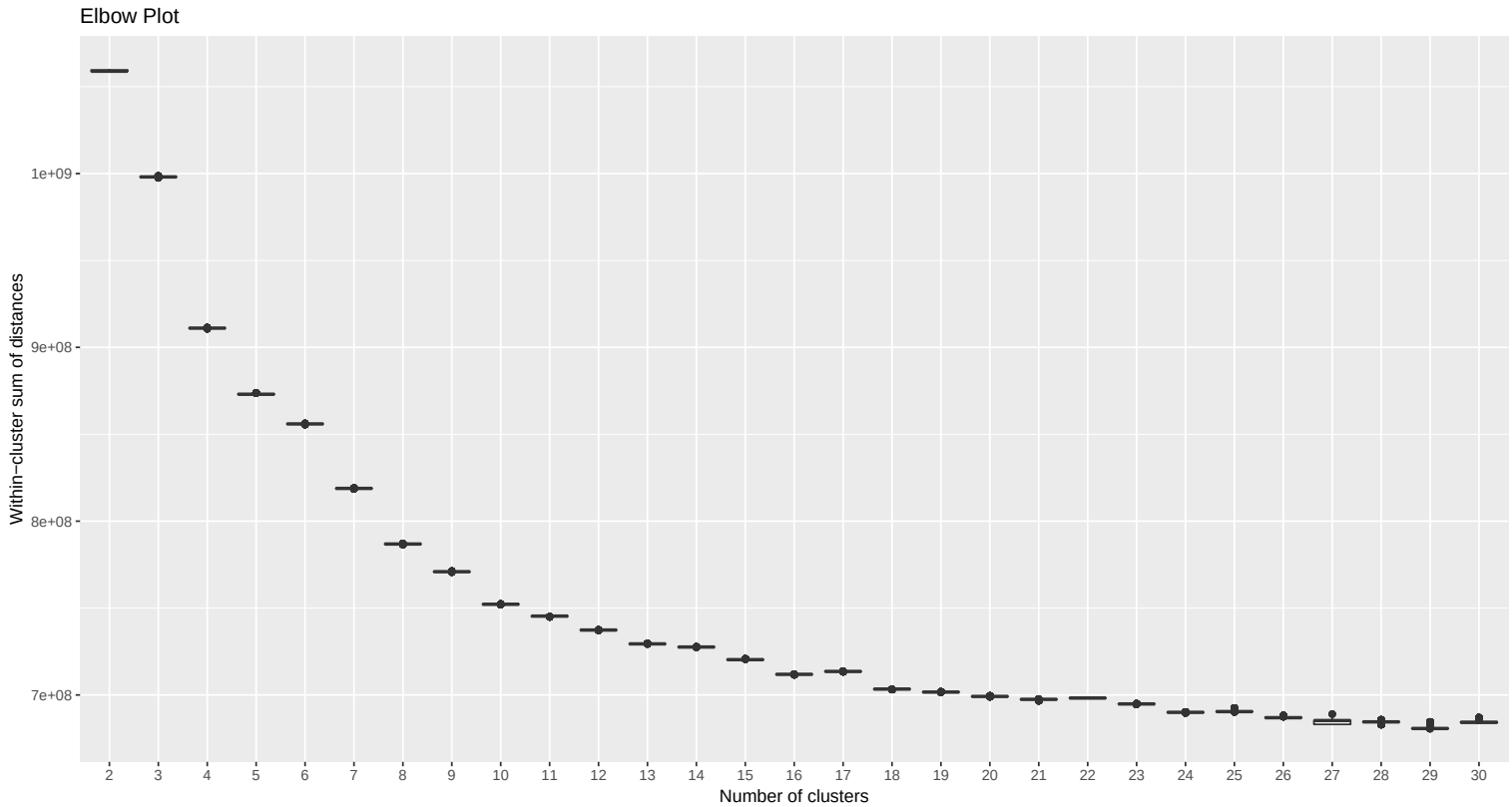
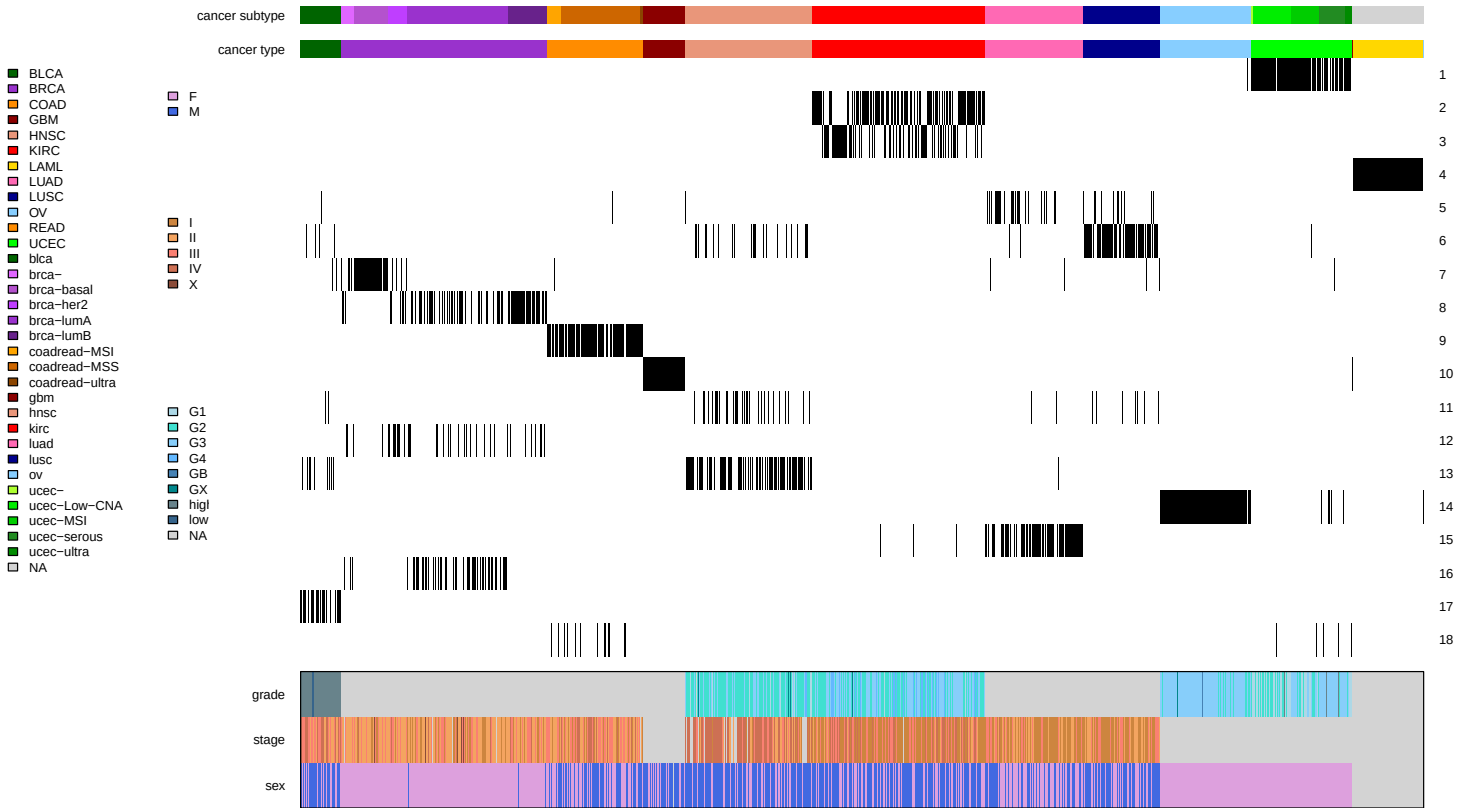
- MCMC setting: we run `BayesMallows` for 1.1 million MCMC iterations, with 1 million burn-in. Use $L^1$ metric (footrule). No missing data; aim: clustering.

# Pan-cancer analysis of TCGA data: number of clusters



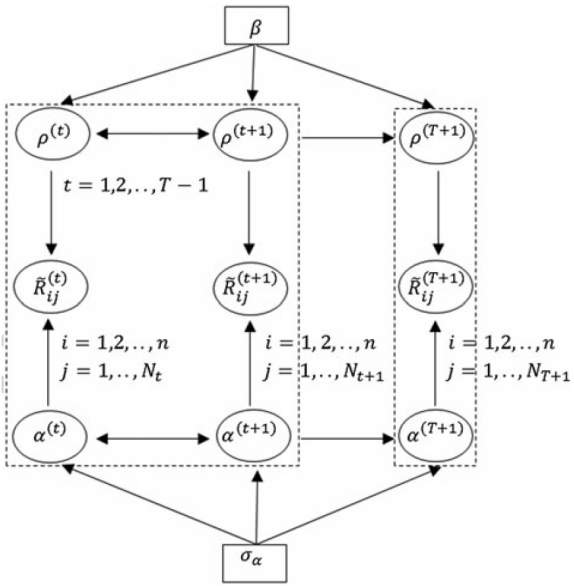

Vitelli et al. (2019)

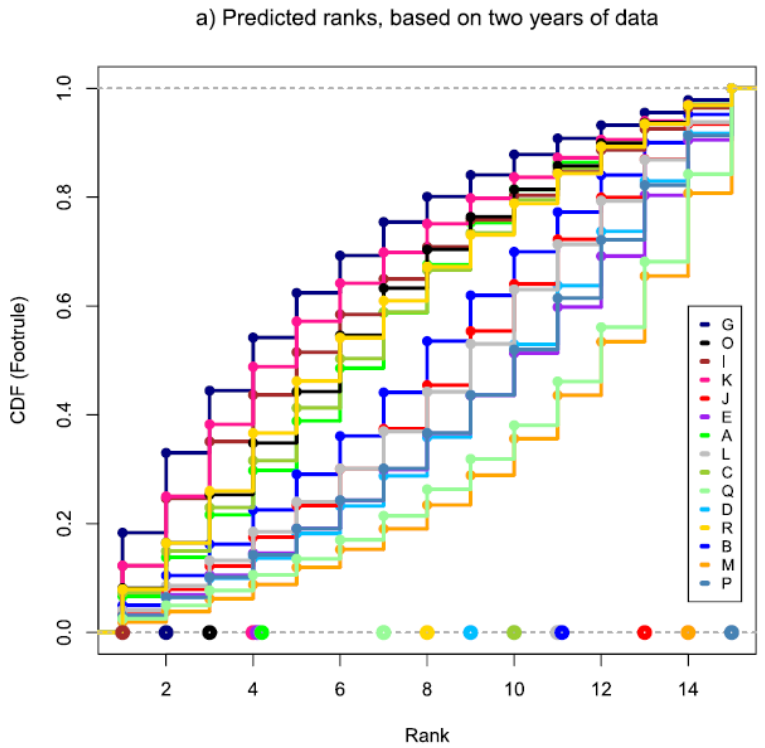
# Pan-cancer analysis of TCGA data: 18 clusters




Vitelli et al. (2019)

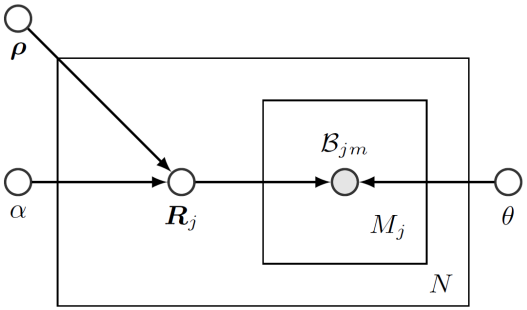
# Time dependency: students along school years

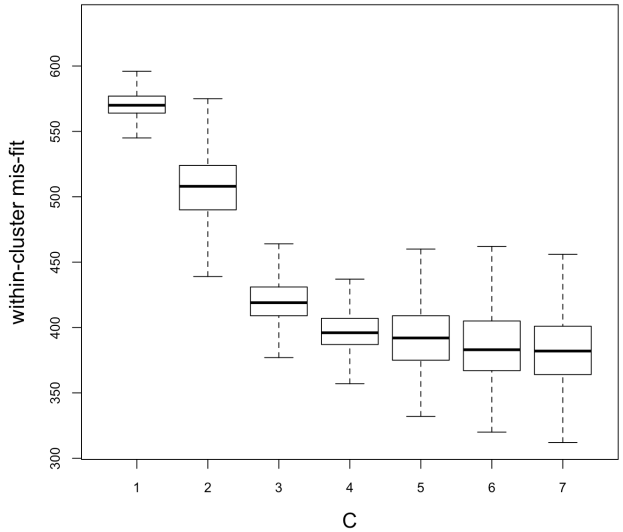


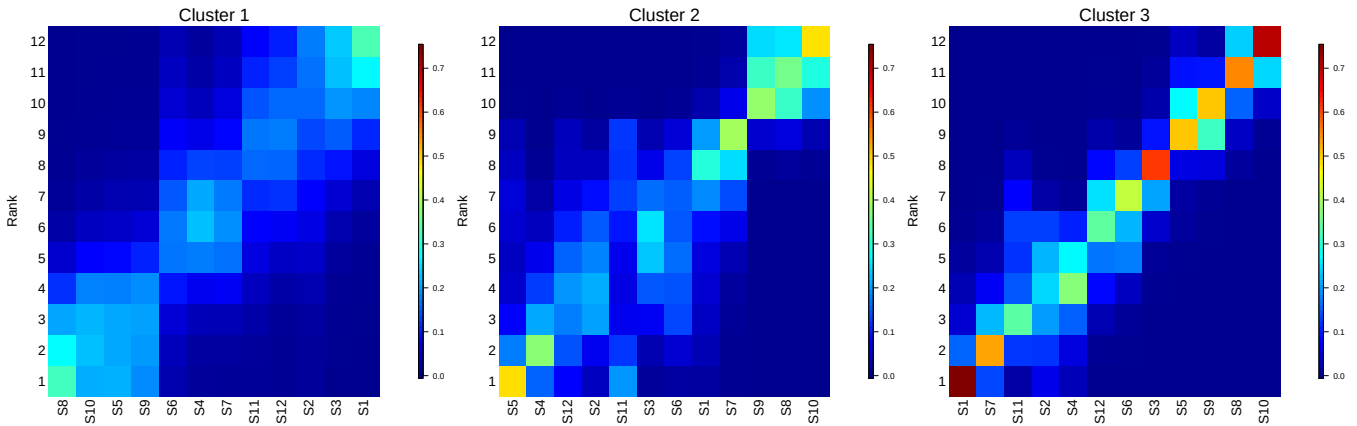




Asfaw et al. (2017)

# Inconsistent preferences: users' contradictions



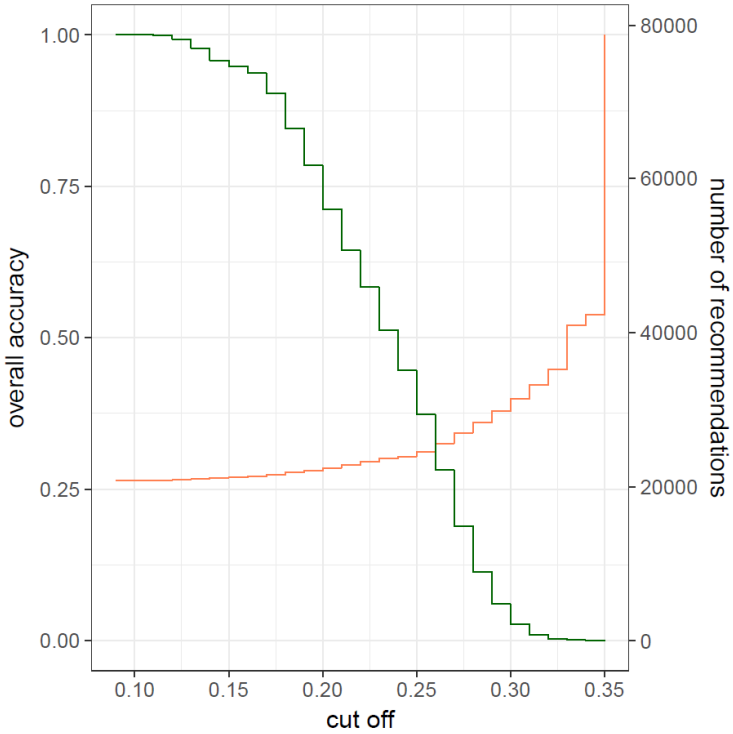




Crispino et al. (2019)

# Mallows for high-dimensional clicking data

- Clicking dataset from the Norwegian Broadcasting Company (NRK).
- Data characteristics: $n = 200$ (most popular clicks); selected users who have at least 13 clicks; randomly remove 10 clicks per user for prediction purposes.
- Uncertainty in results matters!




Liu et al. (2019b)

# Items selection

Why is this relevant?

- it reduces the dimension of the space where the ranks live (ease of computation);
- it allows for automatically selecting the items that are "relevant enough" to be included in the distance computation (better modeling);
- and it enforces a better distinction between noisy and relevant items (better interpretation).

All these aspects, I feel, have a quite substantial importance in genomics applications.

## Machine learning inspired approach

- find a quick-and-rough pre-ordering of the items (ex. Borda);
- define a sufficiently large "buffer" $L$ of items depending on how many we are interested in (ex. $L = 50$ if we aim at estimating top-20 ranks);
- run subsequent analyses on batches of $2L$ items, by fixing the first $L$ in the pre-ordering and merging them with the next $L$-dimensional batch with increasingly lower rank in the pre-ordering;
- (hopefully) prove that the posterior probability of an item way down in the ordering appearing in the top ranks is decreasing.

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## Model-based approach

Include a variable selection step directly in the model definition, by directly defining a variable including/excluding items.

# Multi-platform analysis

Consider rankings from various genomic layers: gene expressions, copy number variation, protein levels, miRNAs, methylation, and so on.

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2. use the prior to enforce a link among the layers, possibly following the underlying biology. Advantage: can follow the dogma model; disadvantage: implementation less straightforward.
3. identify one common ranking combining the information across layers, and then fit the Mallows model as if we had only one layer. Possibility: rank on the basis of a higher dimensional distance metric, one dimension for each layer, differently weighting the layers to model the "biological importance". Question: results sensitivity to the choice of the metric?

# Open points & directions worth exploring

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# Thanks for your attention!

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