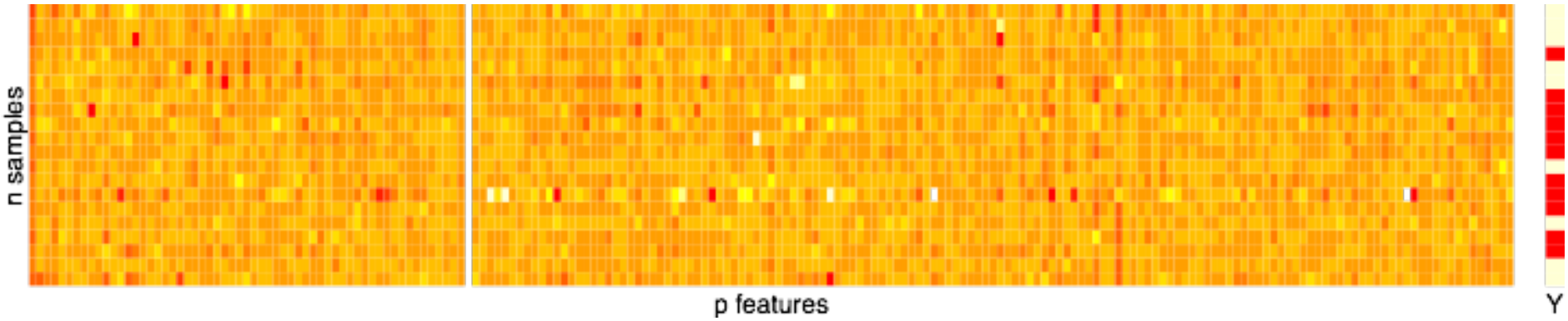
Learning on the symmetric group

Jean-Philippe Vert

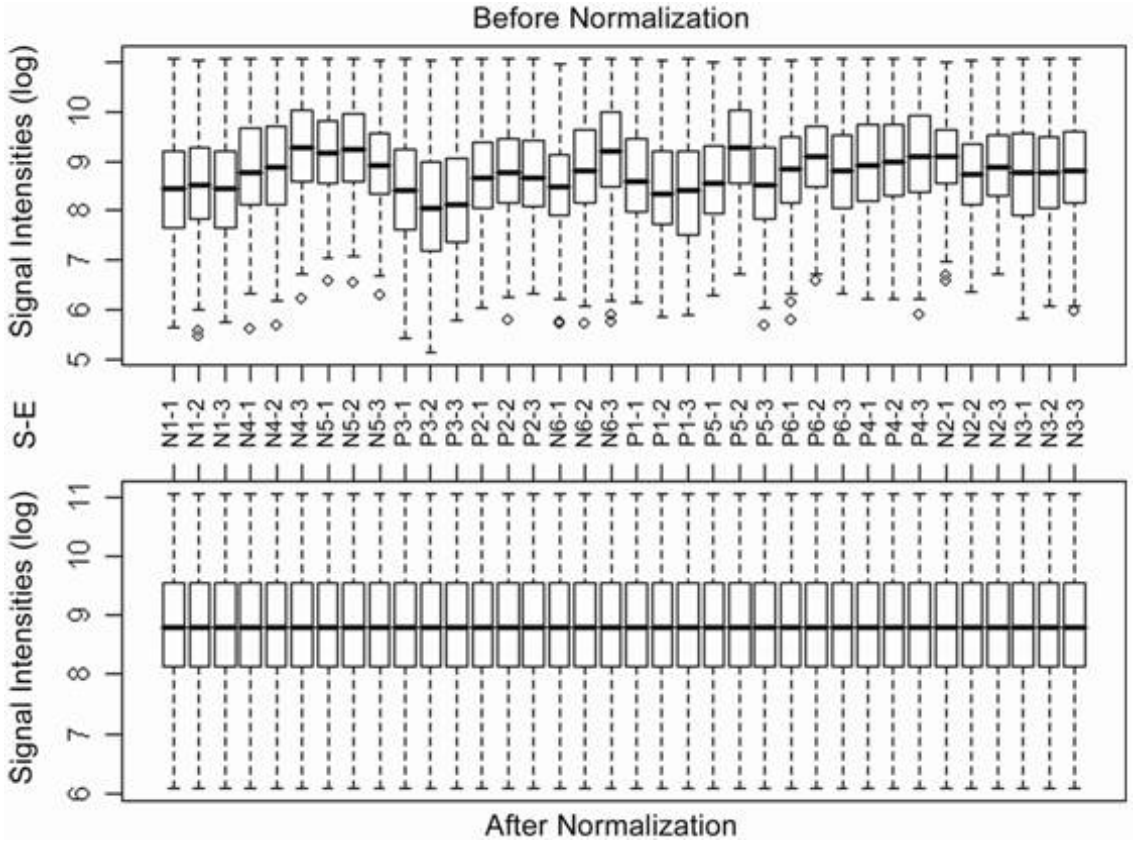
Mathematical methods of modern statistics workshop, CIRM, Luminy, July 13, 2017

Motivation



- X gene expression profile of each patient
- Y survival information of each patient
- $n = 10^2 \sim 10^4$
- $p = 2 \times 10^4$
- Goal: learn to predict Y from X
- But... where does X come from?

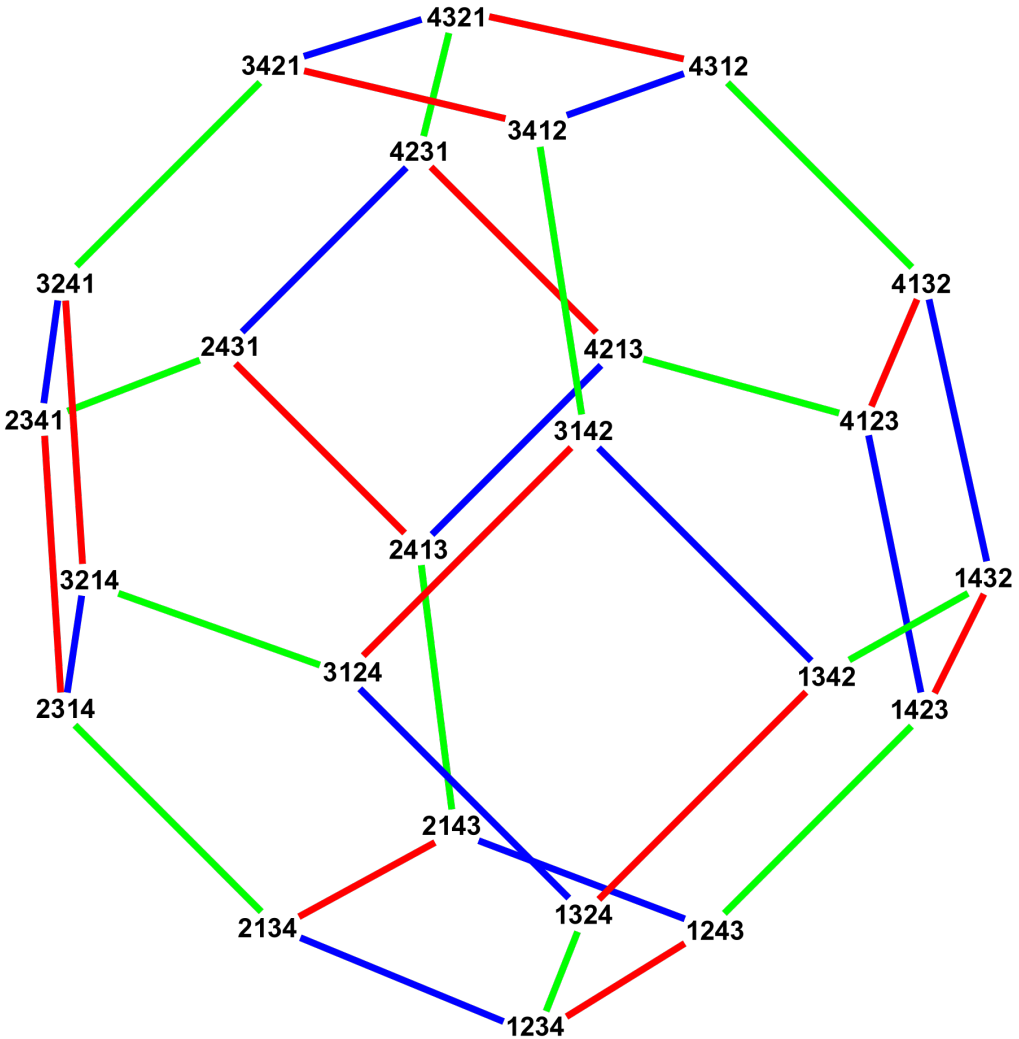
From raw data to X



- Between-sample variability: batch effect, drift over time, ...
- Typical pre-processing: Quantile normalization (per sample)
- Only the relative ordering of features within each sample is used

Learning on the symmetric group

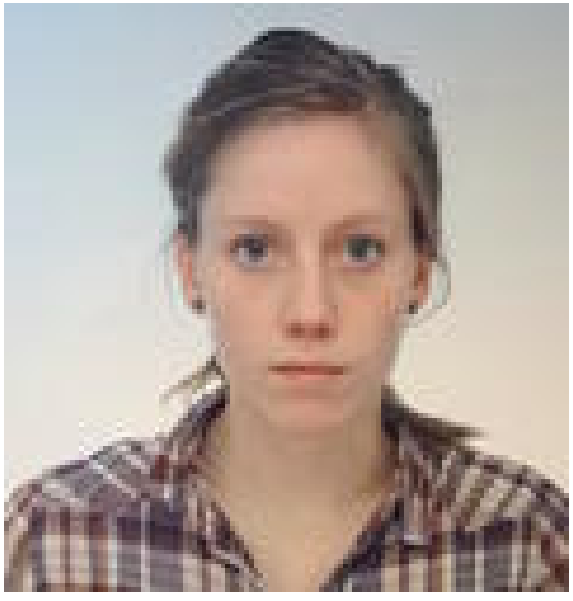
- The symmetric group S_p is the set of permutations of $\{1, \ldots, p\}$
- How to estimate $Y = f(X)$ where $X \in S_p$?



Outline

Outline

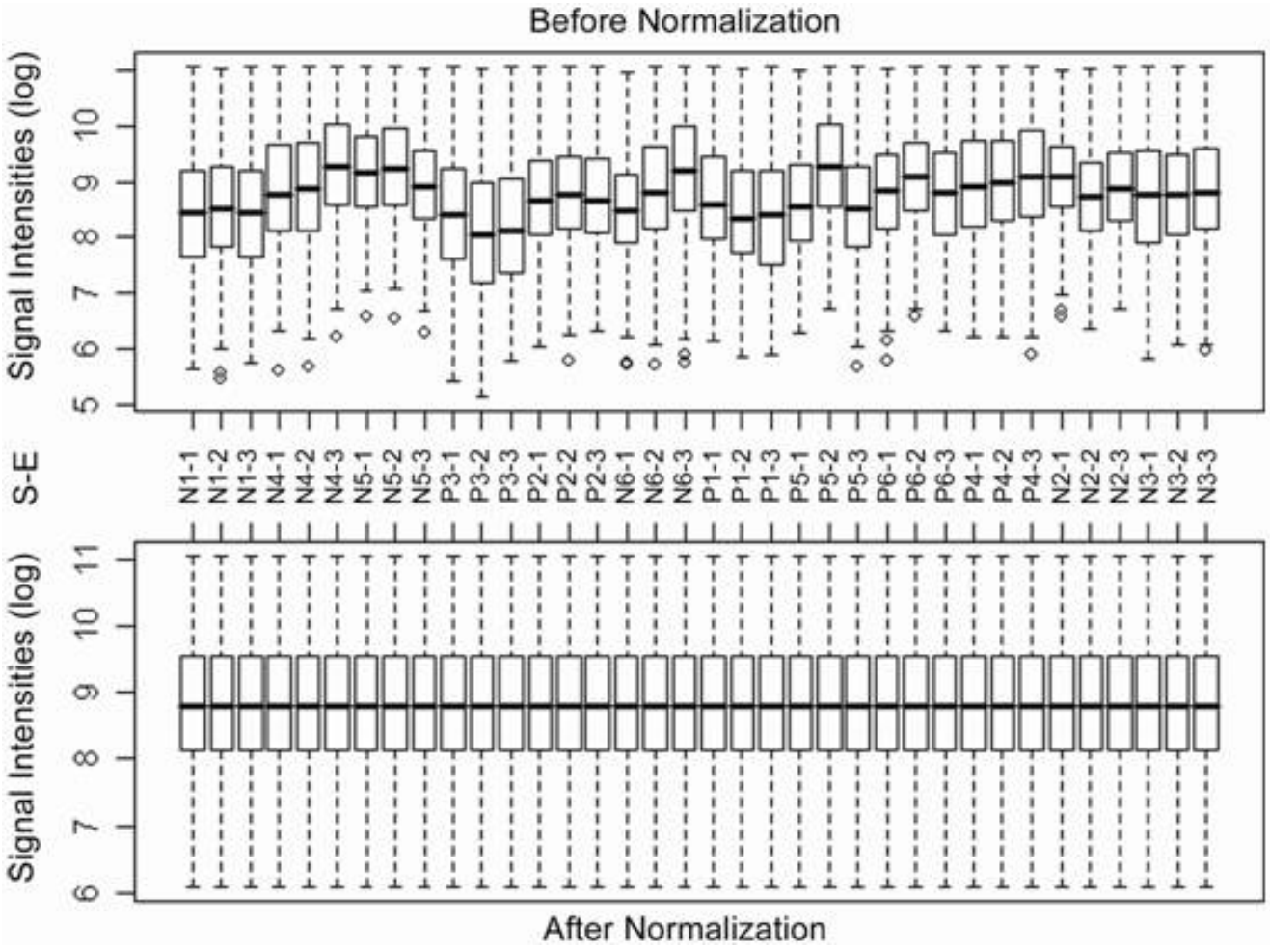
Joint work with



Marine Le Morvan

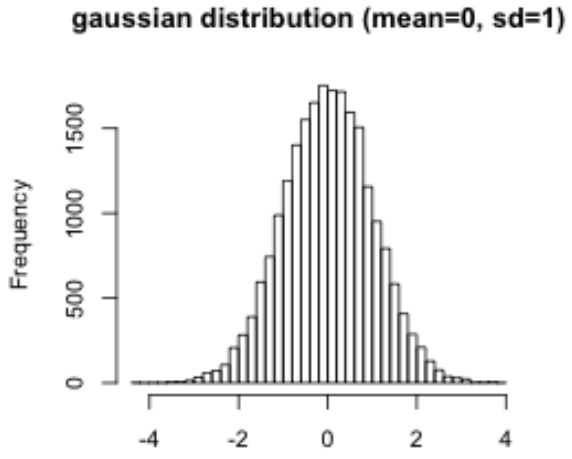
https://arxiv.org/abs/1706.00244

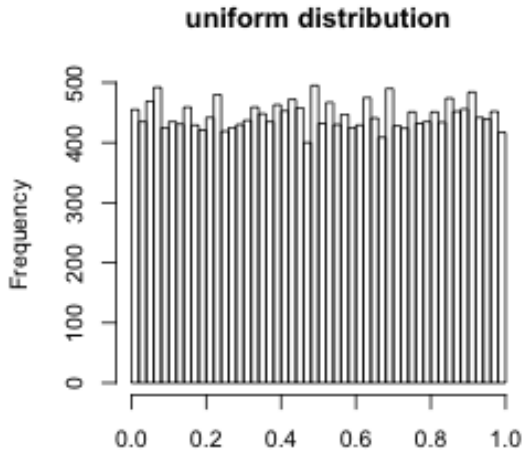
Standard full quantile normalization

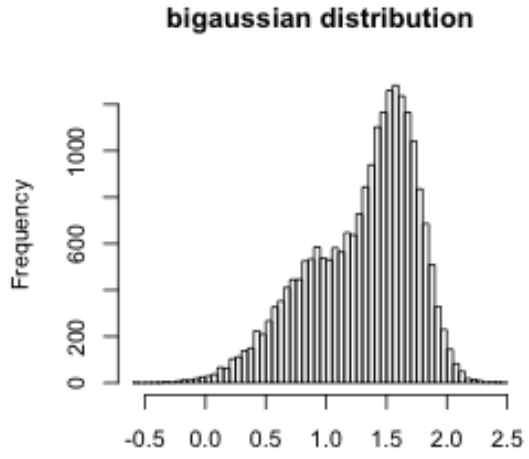


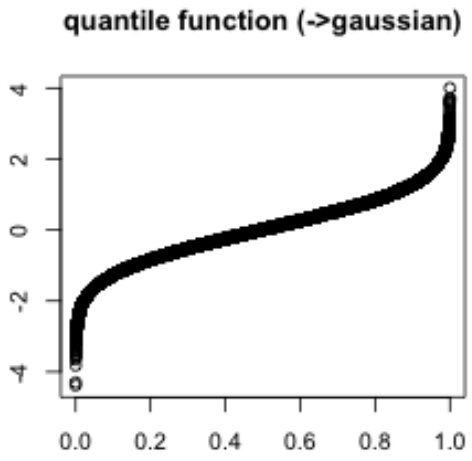
Typically followed by a predictive model $f(X)$ on the normalized data

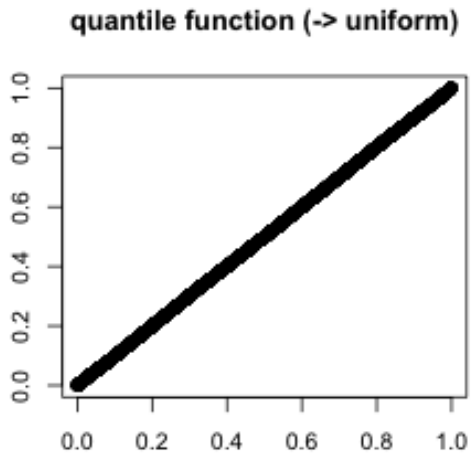
How to choose a "good" target distribution?

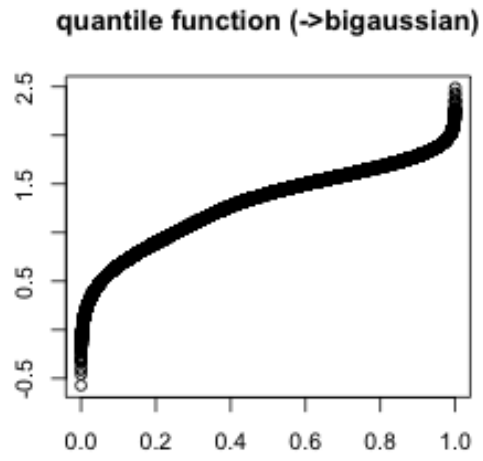






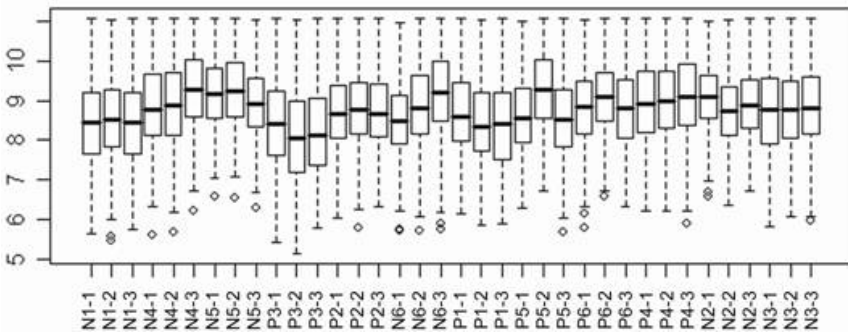




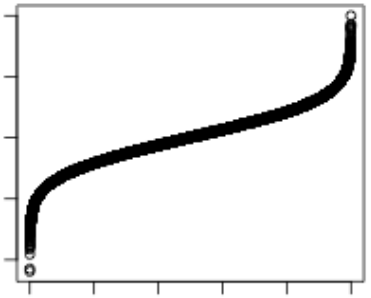


Notations

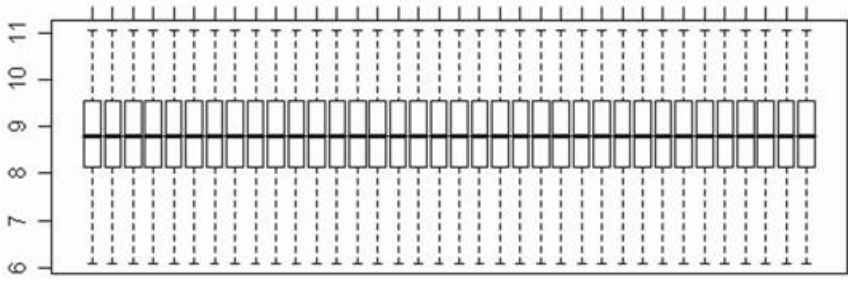
- $x_1, \ldots, x_n \in \mathbb{R}^p$ a set of p-dimensional samples



- $f \in \mathbb{R}^p$ a non-decreasing target distribution (CDF)



- For $x \in \mathbb{R}^p$, let $\Phi_f(x) \in \mathbb{R}^p$ be the data after QN with target distribution f



From QN to supervised QN (SUQUAN)

Standard approaches: learn model after QN preprocessing:

1. Fix f arbitrarily
2. QN all samples to get $\Phi_f(x_1), \ldots, \Phi_f(x_n)$
3. Learn a generalized linear model (w, b) on normalized data:

$$\min_{w,b} \left\{ \frac{1}{n} \sum_{i=1}^{n} \ell_i \left(w^\top \Phi_f(x_i) + b \right) + \lambda \Omega(w) \right\}$$

SUQUAN: jointly learn f and (w, b):

$$\min_{w,b,f} \left\{ \frac{1}{n} \sum_{i=1}^{n} \ell_i \left(w^\top \Phi_f(x_i) + b \right) + \lambda \Omega(w) + \gamma \Omega_2(f) \right\}$$

SUQAN as matrix regression (1/2)

- For $x \in \mathbb{R}^p$, let $\Pi_x \in \mathbb{R}^{p \times p}$ the permutation matrix of x's entries:

$$[\Pi_x]_{ij} = \mathbf{1}\left(x_j \text{ is the } i\text{-th smallest feature}\right)$$

- Quantile normalized x with target distribution f is:

$$\Phi_f(x) = \Pi_x f$$

- Example:

$$x = \begin{pmatrix} 4.5 \\ 1.2 \\ 10.1 \\ 8.9 \end{pmatrix} \quad \Pi_x = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \quad f = \begin{pmatrix} 0 \\ 1 \\ 3 \\ 4 \end{pmatrix}$$

$$\Phi_f(x) = \Pi_x f = \begin{pmatrix} 1 \\ 0 \\ 4 \\ 3 \end{pmatrix}$$

SUQAN as matrix regression (2/2)

- SUQUAN solves

$$\min_{w,b,f} \left\{ \frac{1}{n} \sum_{i=1}^{n} \ell_i \left(w^\top \Phi_f(x_i) + b \right) + \lambda \Omega(w) + \gamma \Omega_2(f) \right\}$$

$$= \min_{w,b,f} \left\{ \frac{1}{n} \sum_{i=1}^{n} \ell \left(w^\top \Pi_{x_i} f + b \right) + \lambda \Omega(w) + \gamma \Omega_2(f) \right\}$$

$$= \min_{w,b,f} \left\{ \frac{1}{n} \sum_{i=1}^{n} \ell \left(< w f^\top, \Pi_{x_i} >_F + b \right) + \lambda \Omega(w) + \gamma \Omega_2(f) \right\}$$

- A particular rank-1 matrix optimization, x is replaced by Π_x
- Non-convex
- Local optimum found by alternatively optimizing f and w

Constraints on f

- Ridge

$$\mathcal{F}_0 = \left\{ f \in \mathbb{R}^p \,:\, \frac{1}{p}\sum_{i=1}^{p} f_i^2 \leq 1 \right\} .$$

- Non-decreasing

$$\mathcal{F}_{\text{BND}} = \mathcal{F}_0 \cap \mathcal{I}_0 \,, \quad \text{where} \quad \mathcal{I}_0 = \{ f \in \mathbb{R}^p \,:\, f_1 \leq f_2 \leq \ldots \leq f_p \}$$

- Non-decreasing and smooth

$$\mathcal{F}_{\text{SPAV}} = \left\{ f \in \mathcal{I}_0 \,:\, \sum_{j=1}^{p-1} (f_{j+1} - f_j)^2 \leq 1 \right\} .$$

SUQUAN-BND and SUQUAN-PAVA

Algorithm 2: SUQUAN-BND and SUQUAN-SPAV

Input: $(x_1, y_1), \ldots, (x_n, y_n), f_{init} \in \mathcal{I}_0, \lambda \in \mathbb{R}$

Output: $f \in \mathcal{I}_0$ target quantile

1: **for** $i = 1$ to n **do**

2: $\quad rank_i, order_i \leftarrow \text{sort}(x_i)$

3: **end for**

4: $w, b \leftarrow \underset{w,b}{\text{argmin}} \frac{1}{n} \sum_{i=1}^{n} \ell_i \left(w^\top f_{init}[rank_i] + b\right) + \lambda ||w||^2$

(standard linear model optimisation)

5: $f \leftarrow \underset{f \in \mathcal{F}_{BND}}{\text{argmin}} \frac{1}{n} \sum_{i=1}^{n} \ell_i \left(f^\top w[order_i] + b\right)$

(isotonic optimisation problem using PAVA as prox)

OR

$f \leftarrow \underset{f \in \mathcal{F}_{SPAV}}{\text{argmin}} \frac{1}{n} \sum_{i=1}^{n} \ell_i \left(f^\top w[order_i] + b\right)$

(smoothed isotonic optimisation problem using SPAV as prox)

- Alternate optimization in *w* and *f*, monotonicity constraint on *f*
- Accelerated proximal gradient optimization for *f*, using the Pool Adjacent Violators Algorithm (PAVA, **?**) or the Smoothed Pool Adjacent Violators algorithm (SPAV, **?**) as proximal operator.

A variant: SUQUAN-SVD

Algorithm 1: SUQUAN-SVD

Input:

$(x_1, y_1), \ldots, (x_n, y_n) \in \mathbb{R}^p \times \{-1, 1\}$

Output: $f \in \mathcal{F}_0$ target quantile

1: $M_{LDA} \leftarrow 0 \in \mathbb{R}^{p \times p}$
2: $n_{+1} \leftarrow |\{i \,:\, y_i = +1\}|$
3: $n_{-1} \leftarrow |\{i \,:\, y_i = -1\}|$
4: **for** $i = 1$ to n **do**
5: Compute Π_{x_i} (by sorting x_i)
6: $M_{LDA} \leftarrow M_{LDA} + \frac{y_i}{n_{y_i}} \Pi_{x_i}$
7: **end for**
8: $(\sigma, w, f) \leftarrow SVD(M_{LDA}, 1)$

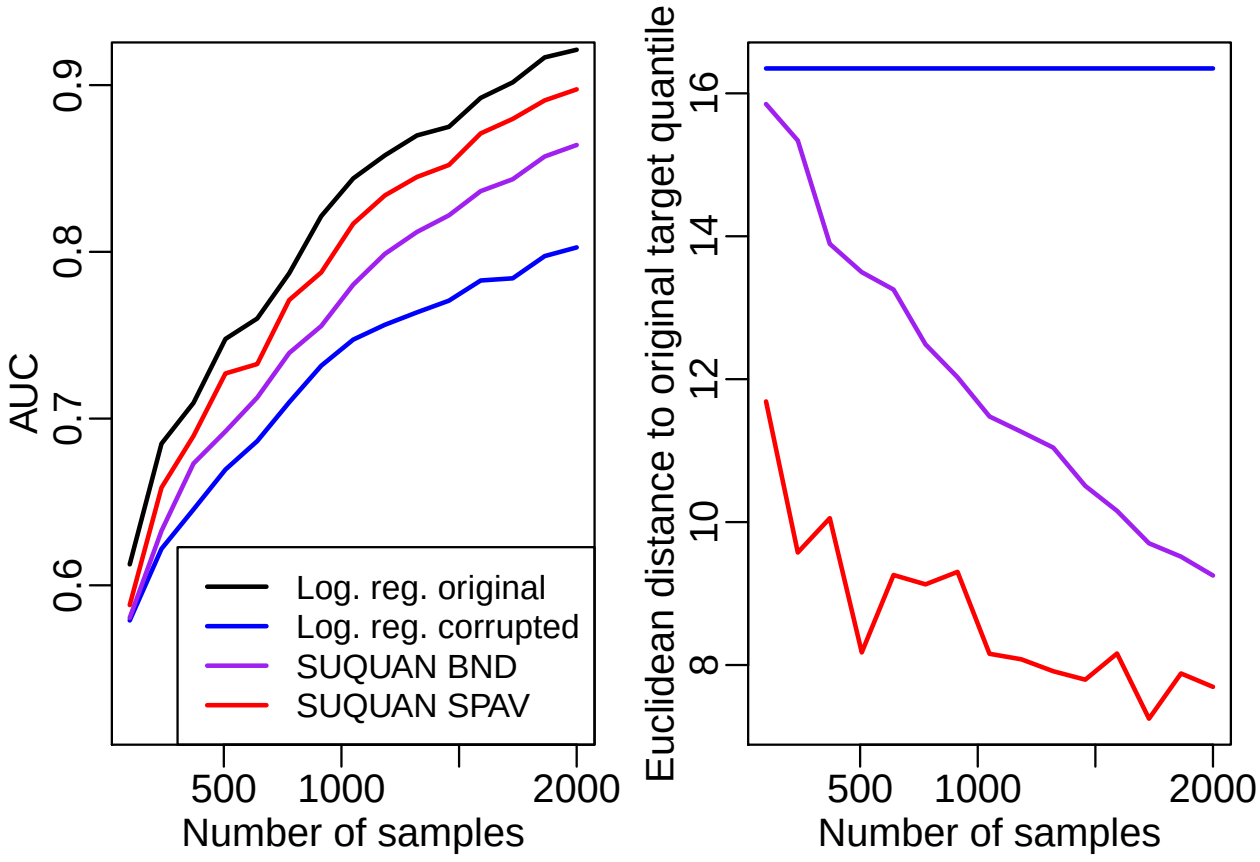
- Ridge penalty (no monotonicity constraint), equivalent to rank-1 regression problem
- SVD finds the closest rank-1 matrix to the LDA solution:

$$M_{LDA} = \frac{1}{n_+} \sum_{i\,:\,y_i=+1} \Pi_{x_i} - \frac{1}{n_-} \sum_{i\,:\,y_i=+1} \Pi_{x_i}$$

- Complexity $O(np\ln(p))$ (same as QN only)

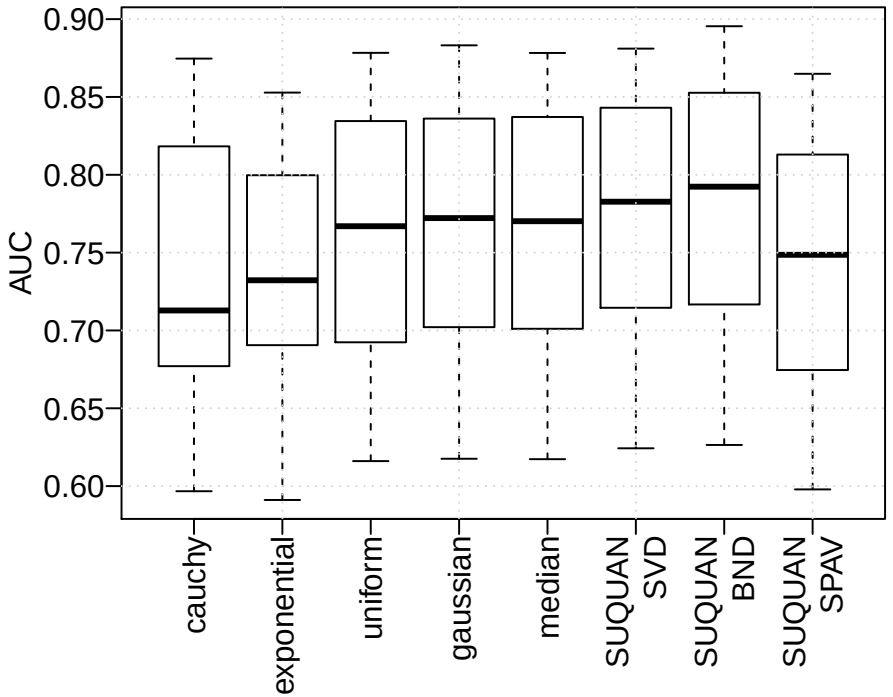
Experiments: Simulations

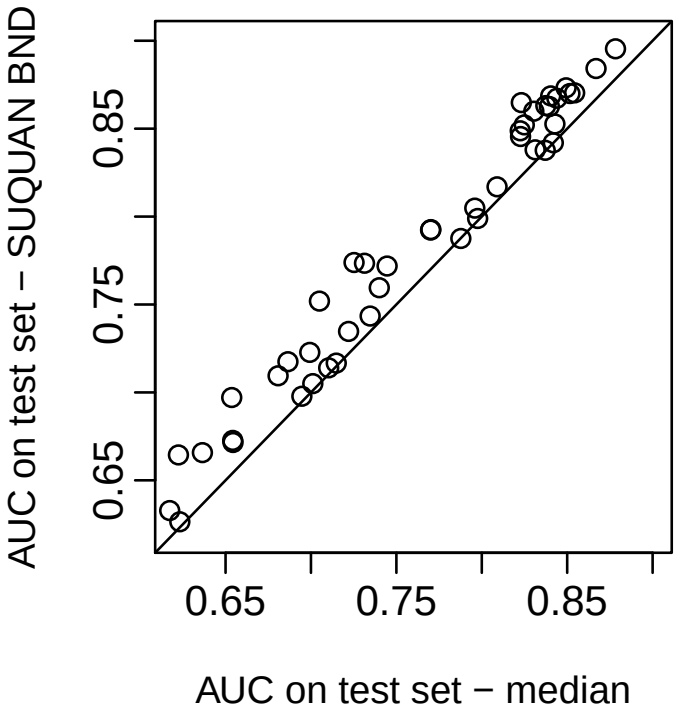
- True distribution of X entries is normal
- Corrupt data with a cauchy, exponential, uniform or bimodal gaussian distributions.
- $p = 1000$, n varies, logistic regression.



Experiments: CIFAR-10

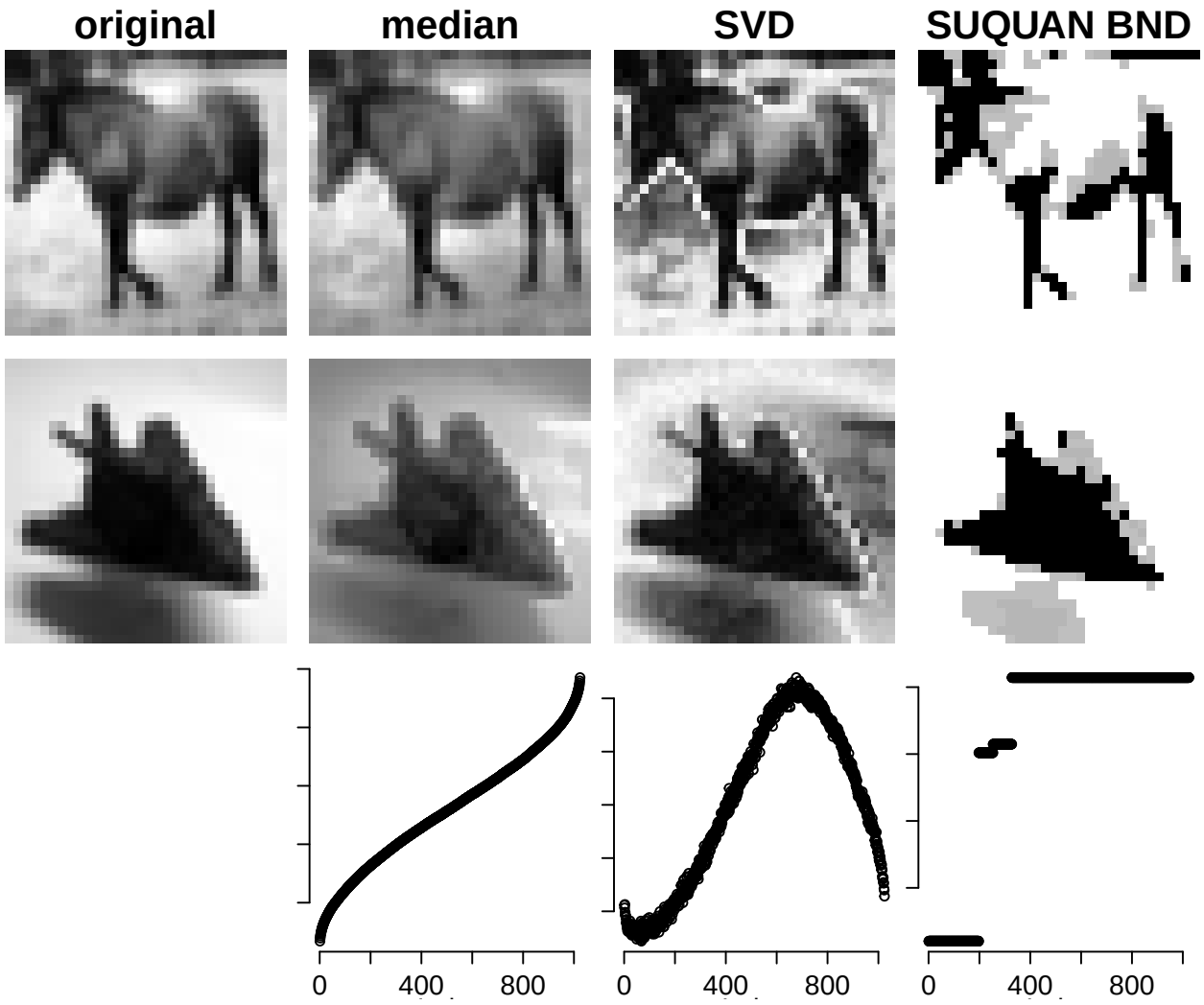
- Image classification into 10 classes (45 binary problems)
- $n = 5,000$ per class, $p = 1,024$ pixels





Experiments: CIFAR-10

- Example: horse vs. plane
- Different methods learn different quantile distributions



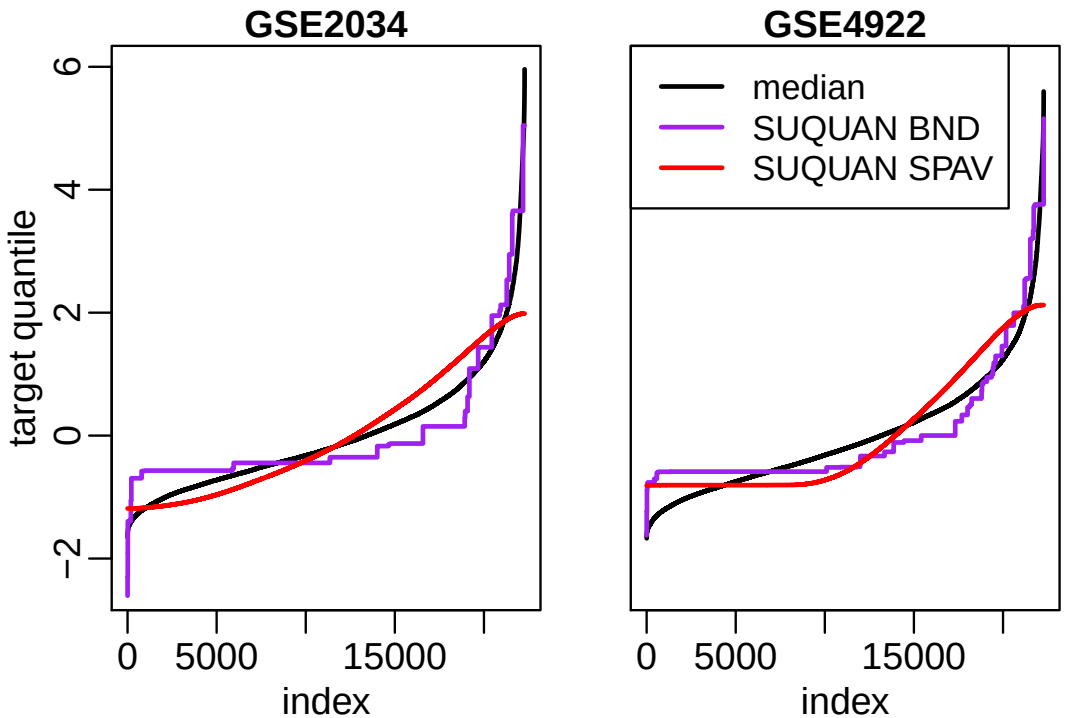
Experiments: gene expression data

- Breast cancer prognosis from gene expression data.
  - X = expression levels of 22,283 genes of the tumour at diagnosis
  - Y = 1 if cancer relapse within 6 years of diagnosis, 0 otherwise
- 4 datasets:

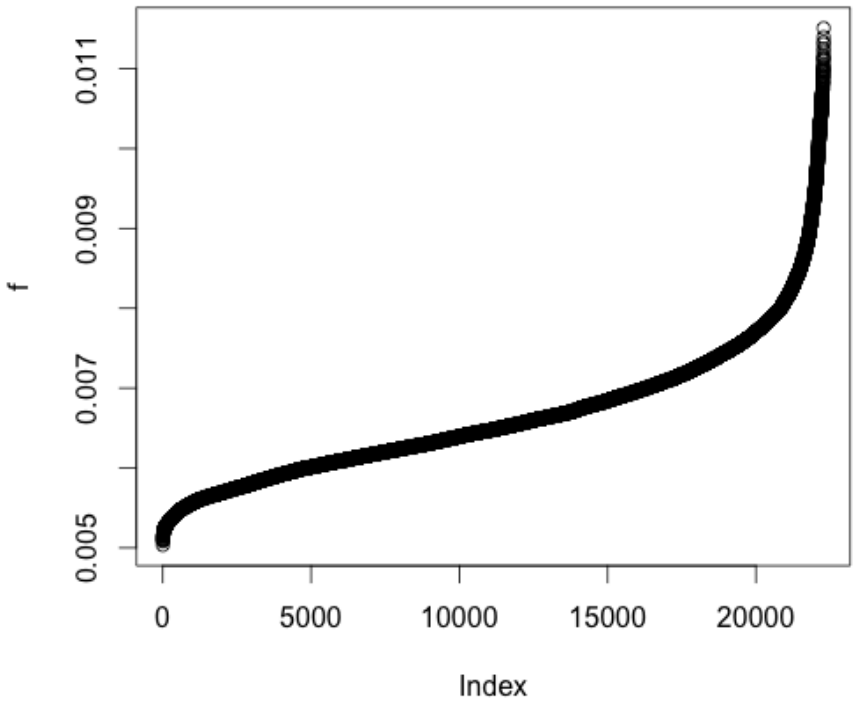
DATASET NAME	# PATIENTS	# POSITIVES	% POSITIVES
GSE1456	141	37	0.26
GSE2034	271	104	0.38
GSE2990	106	32	0.30
GSE4922	225	73	0.32

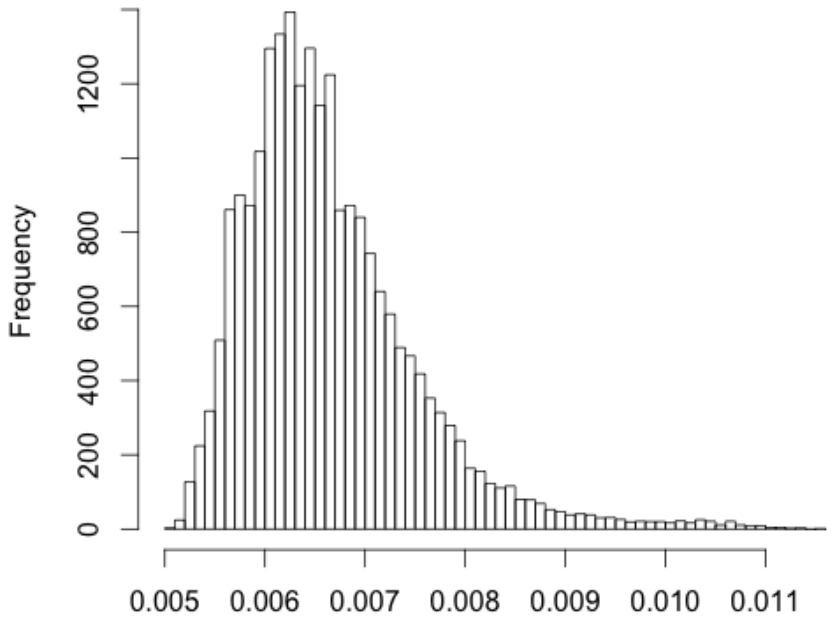
Results: gene expression data

	LOGISTIC REGRESSION							SUQUAN		
	RAW	RMA	CAUCHY	EXP.	UNIF.	GAUS.	MEDIAN	SVD	BND	SPAV
GSE1456	65.94	68.73	59.56	68.86	68.72	69.00	69.06	57.60	**71.44**	69.60
GSE2034	74.52	75.42	61.91	74.53	75.22	**76.45**	74.92	52.61	70.50	76.11
GSE2990	57.01	60.43	54.72	**61.25**	56.25	58.66	59.72	52.51	59.22	59.94
GSE4922	58.52	58.86	55.24	58.81	55.66	60.01	59.18	52.39	**61.82**	61.41
AVERAGE	64.00	65.86	57.86	65.86	63.96	66.03	65.72	53.78	65.75	**66.77**

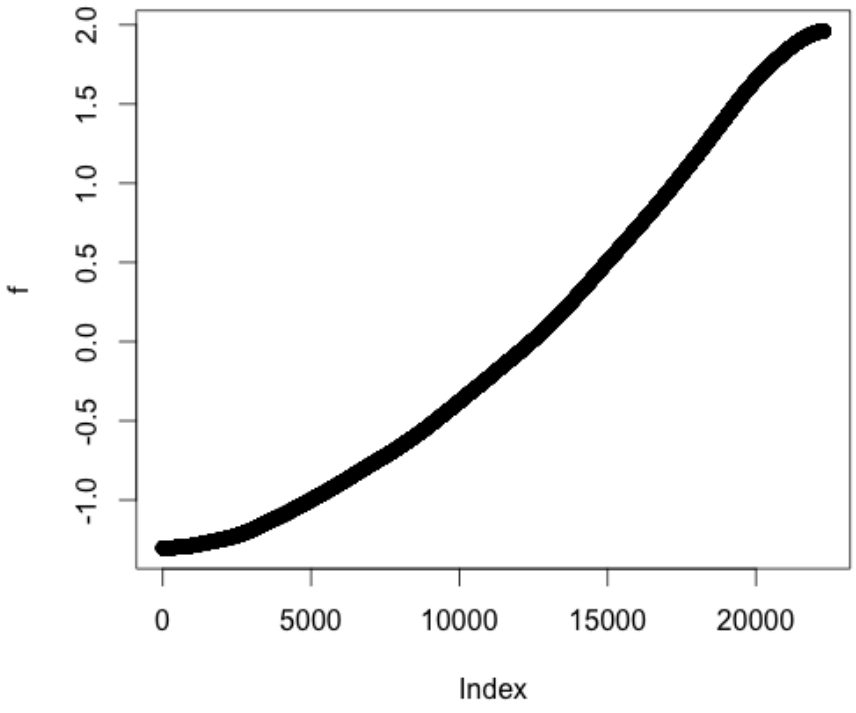


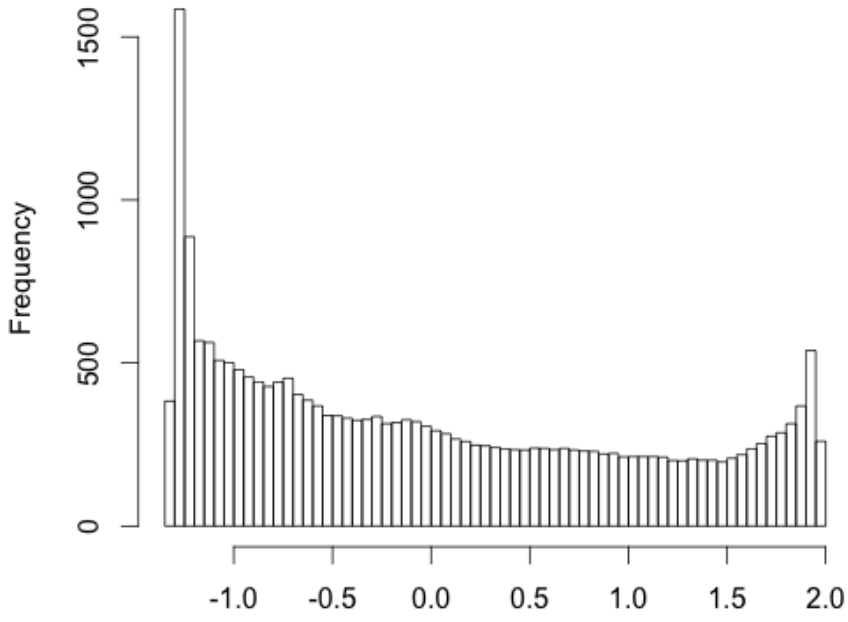
Estimated distribution: iteration=0



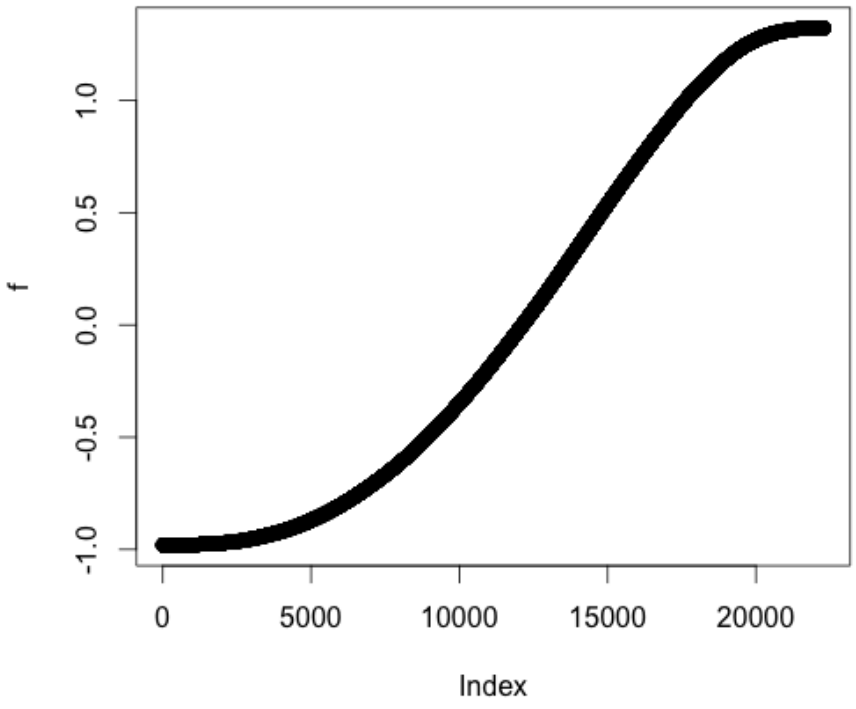


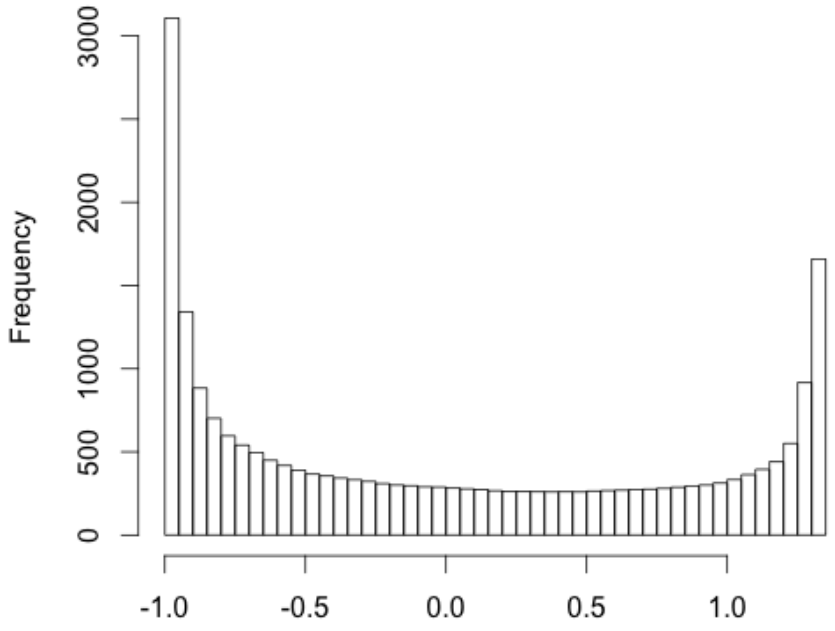
Estimated distribution: iteration=1





Estimated distribution: iteration=2





Outline

Joint work with

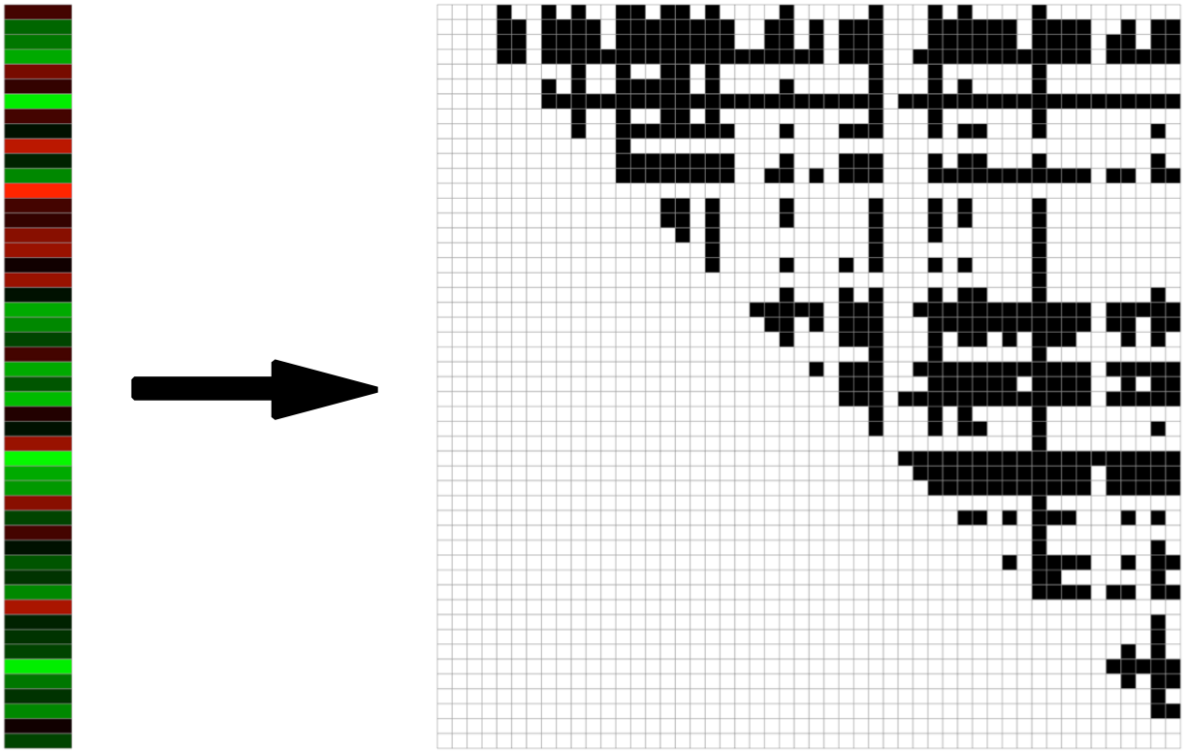
Yunlong Jiao

https://hal.archives-ouvertes.fr/hal-01279273

An idea: all pairwise comparisons

Replace $x \in \mathbb{R}^p$ by $\Phi(x) \in \{0,1\}^{p(p-1)/2}$:

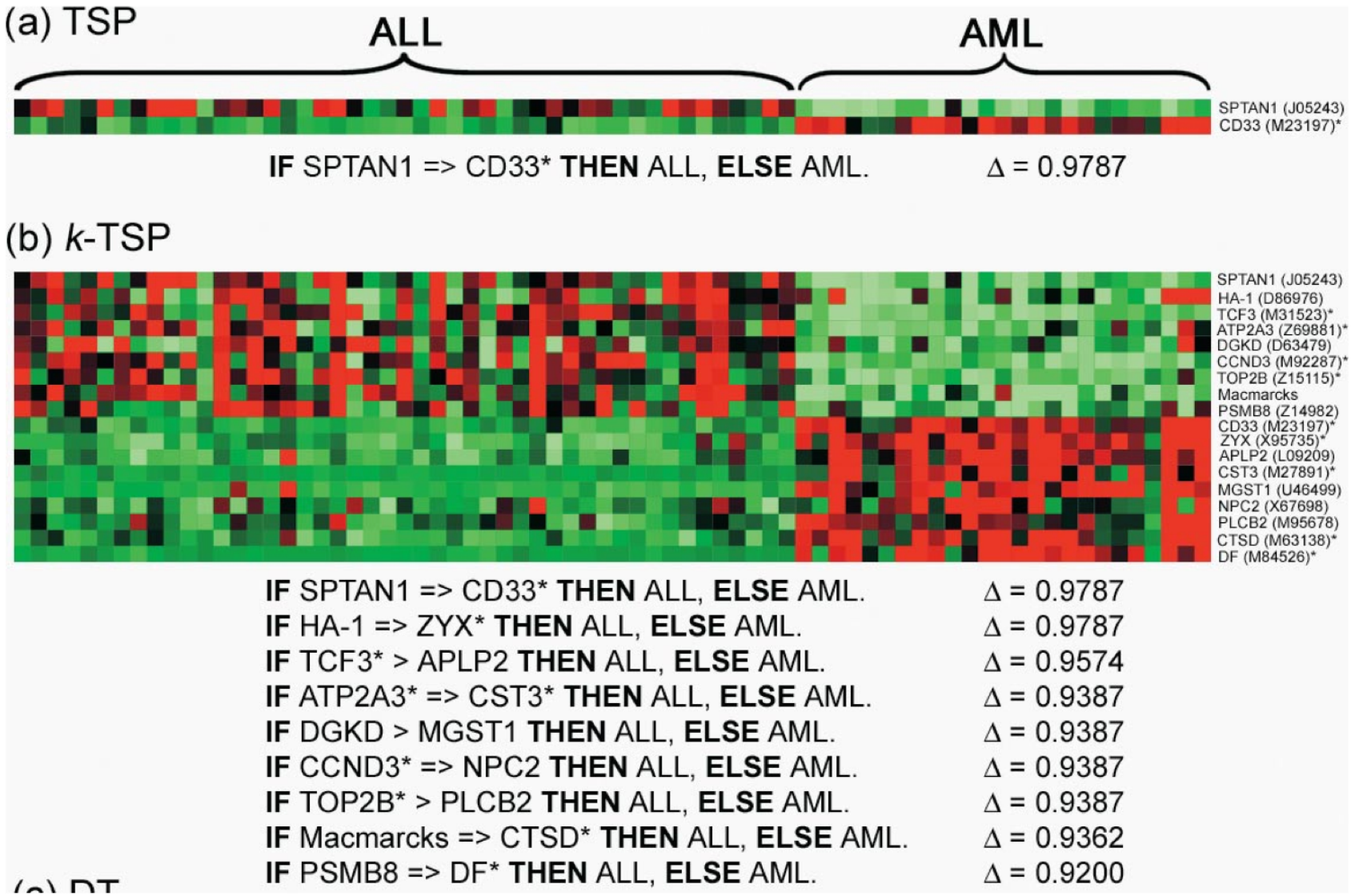
$$\Phi_{i,j}(x) = \begin{cases} 1 & \text{if } x_i \leq x_j\,, \\ 0 & \text{otherwise.} \end{cases}$$



One sample x
p features

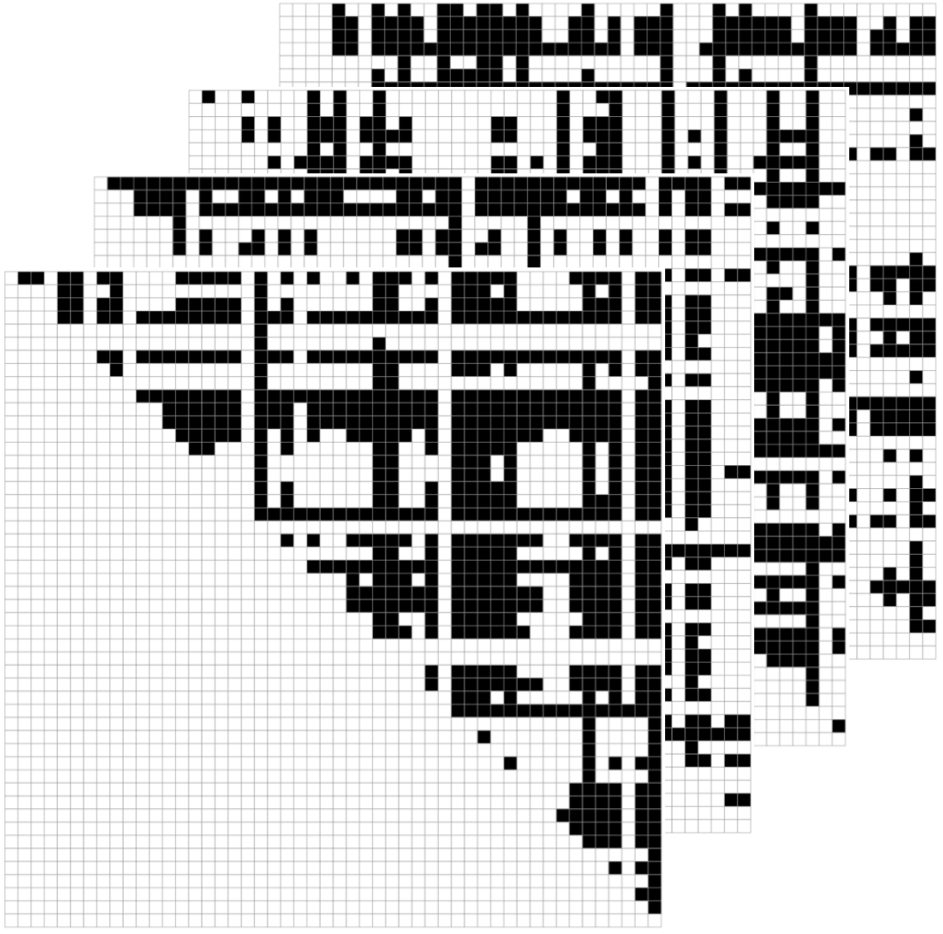
Mapping f(x)
p(p-1)/2 bits

Related work: Top scoring pairs (TSP)



(Geman et al., 2004; Tan et al., 2005; Leek, 2009)

Practical challenge



- Need to store $O(p^2)$ bits per sample
- Need to train a model in $O(p^2)$ dimensions

Kernel trick

Theorem (Wahba, Schölkopf, ...)

Training a linear model over a representation $\Phi(x) \in \mathbb{R}^Q$ of the form:

$$\min_{w \in \mathbb{R}^Q} \frac{1}{n} \sum_{i=1}^{n} \ell(w^\top \Phi(x_i), y_i) + \lambda ||w||^2$$

can be done efficiently, independently of Q, if the kernel

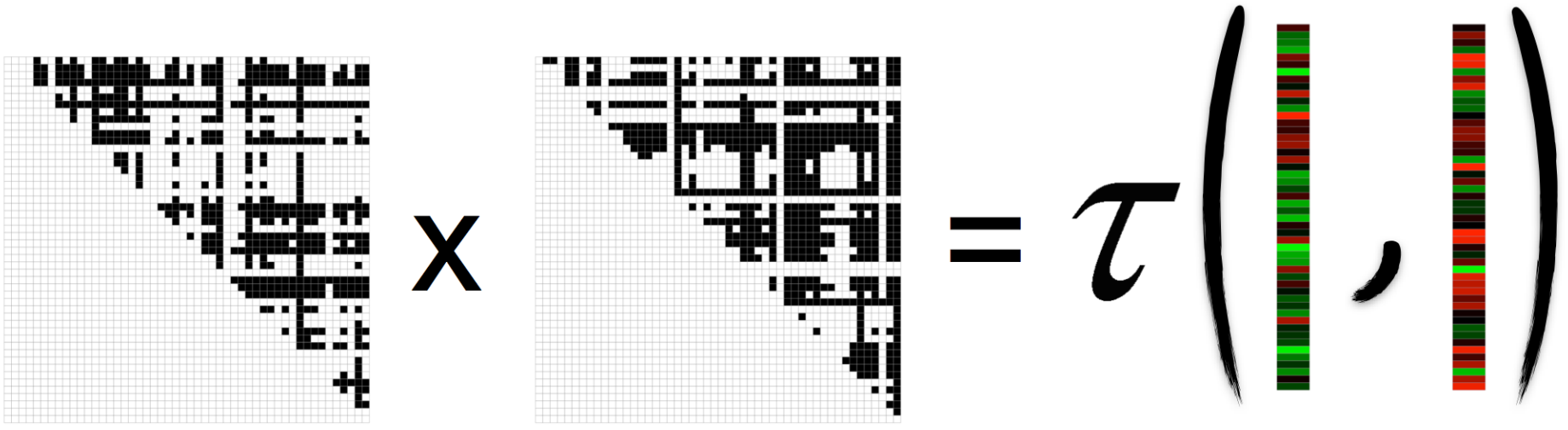
$$K(x, x') = \Phi(x)^\top \Phi(x')$$

can be computed efficiently.

Ex: ridge regression, $O(Q^3 + nQ^2)$ becomes $O(n^3 + n^2 T)$
Other: SVM, logistic regression, Cox model, survival SVM, ...

Kernel trick for us: Kendall's τ

$$\Phi(x)^\top \Phi(x') = \tau(x, x') \quad \text{(up to a scaling)}$$



O(p^2) O(p log(p))

Good news for SVM and kernel methods!

More formally

- For two permutations σ, σ' let $n_c(\sigma, \sigma')$ (resp. $n_d(\sigma, \sigma')$) the number of concordant (resp. discordant) pairs.
- The Kendall kernel (a.k.a. Kendall tau coefficient) is defined as

$$K_\tau(\sigma, \sigma') = \frac{n_c(\sigma, \sigma') - n_d(\sigma, \sigma')}{\binom{p}{2}} .$$

- The Mallows kernel is defined for any $\lambda \geq 0$ by

$$K_M^\lambda(\sigma, \sigma') = e^{-\lambda n_d(\sigma, \sigma')} .$$

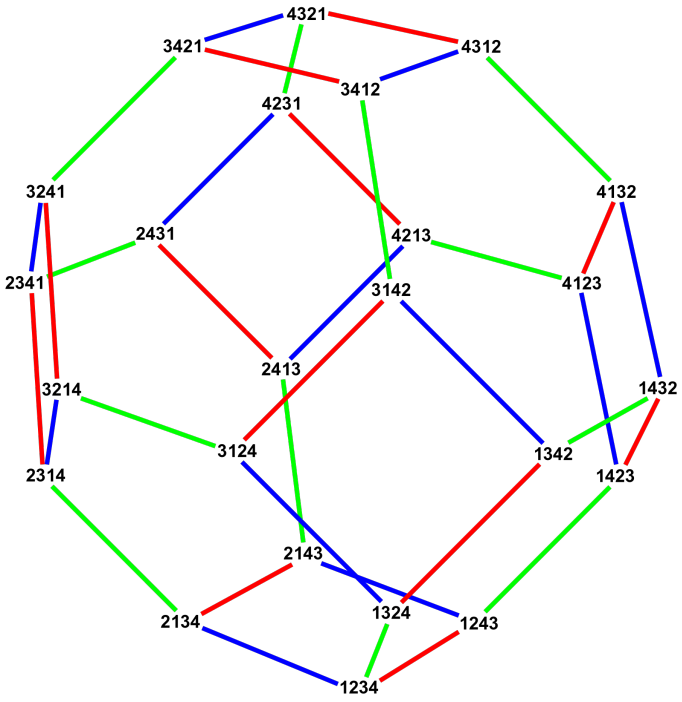
Theorem (Jiao and V., 2015)

The Kendall and Mallows kernels are positive definite.

Theorem (Knight, 1966)

These two kernels for permutations can be evaluated in $O(p \log p)$ time.

Related work



Cayley graph of $\mathbb{S}_4$

- Kondor and Barbarosa (2010) proposed the diffusion kernel on the Cayley graph of the symmetric group generated by adjacent transpositions.
- Computationally intensive ($O(p^p)$)
- Mallows kernel is written as

$$K_M^{\lambda}(\sigma, \sigma') = e^{-\lambda n_d(\sigma,\sigma')},$$

where $n_d(\sigma, \sigma')$ is the shortest path distance on the Cayley graph.

- It can be computed in $O(p \log p)$

Application: supervised classification

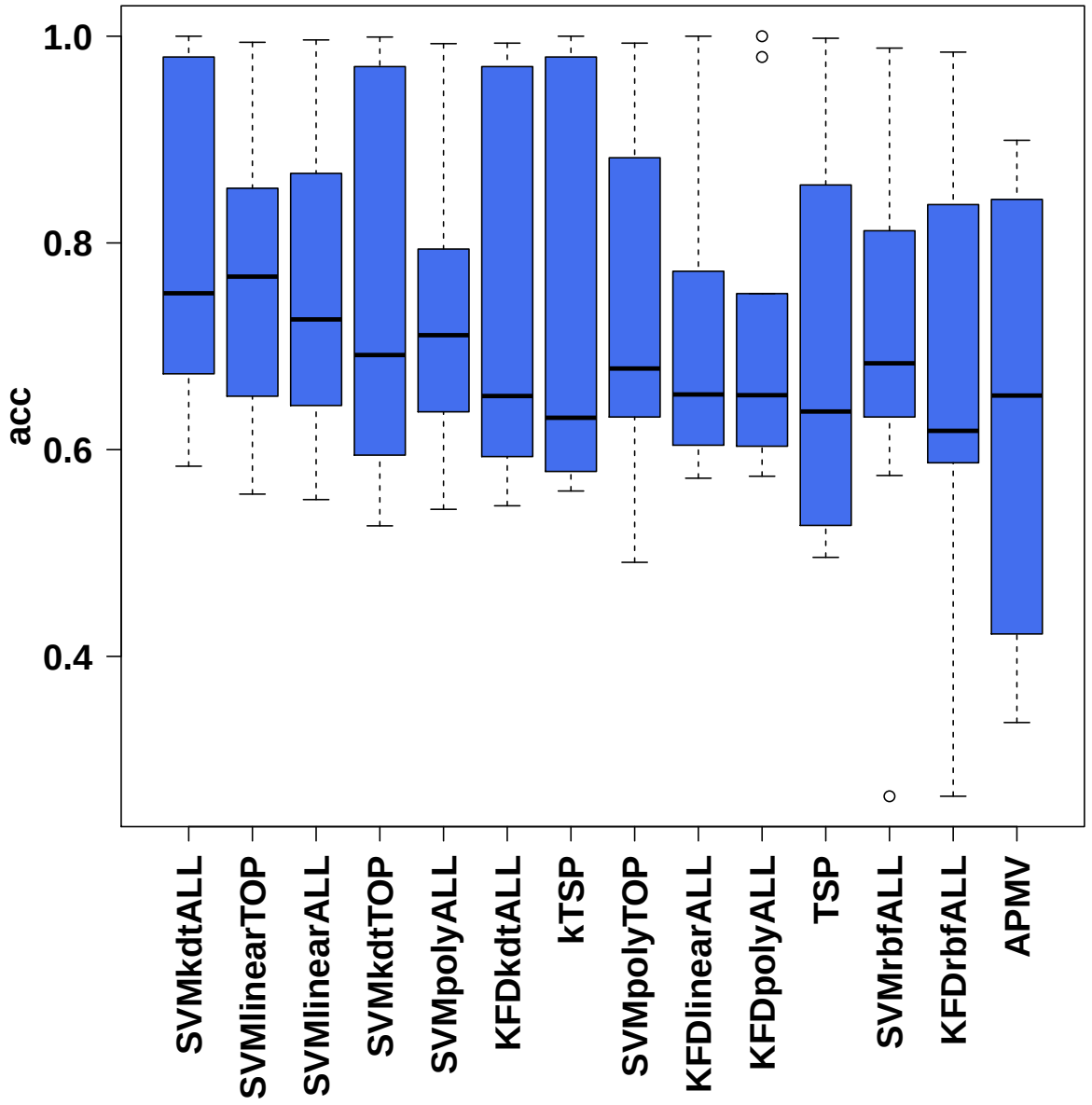
Datasets

Dataset	No. of features	No. of samples (training/test)	
		C_1	C_2
Breast Cancer 1	23624	44/7 (Non-relapse)	32/12 (Relapse)
Breast Cancer 2	22283	142 (Non-relapse)	56 (Relapse)
Breast Cancer 3	22283	71 (Poor Prognosis)	138 (Good Prognosis)
Colon Tumor	2000	40 (Tumor)	22 (Normal)
Lung Cancer 1	7129	24 (Poor Prognosis)	62 (Good Prognosis)
Lung Cancer 2	12533	16/134 (ADCA)	16/15 (MPM)
Medulloblastoma	7129	39 (Failure)	21 (Survivor)
Ovarian Cancer	15154	162 (Cancer)	91 (Normal)
Prostate Cancer 1	12600	50/9 (Normal)	52/25 (Tumor)
Prostate Cancer 2	12600	13 (Non-relapse)	8 (Relapse)

Methods

- Kernel machines Support Vector Machines (SVM) and Kernel Fisher Discriminant (KFD) with Kendall kernel, linear kernel, Gaussian RBF kernel, polynomial kernel.
- Top Scoring Pairs (TSP) classifiers **?**.
- Hybrid scheme of SVM + TSP feature selection algorithm.

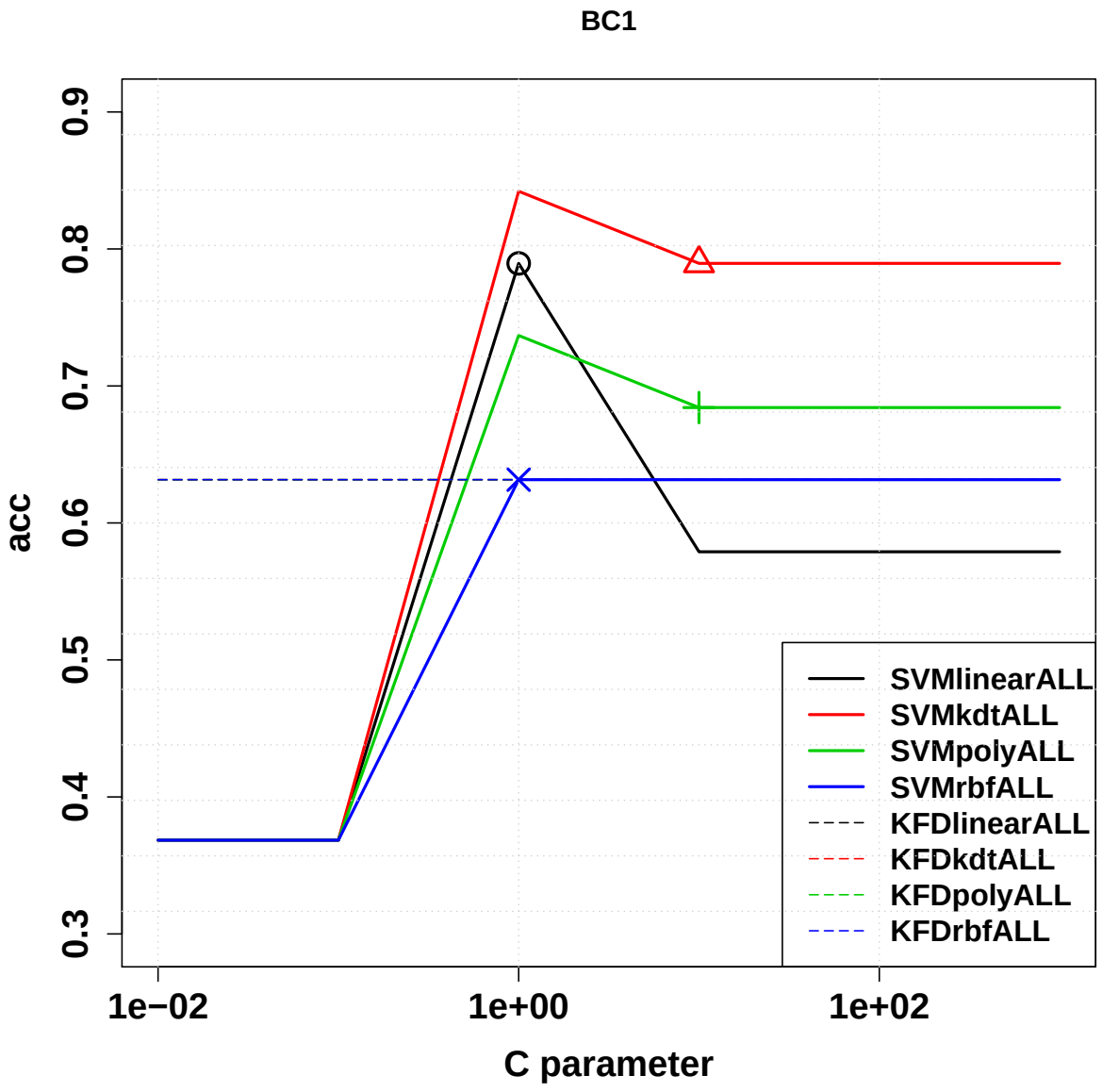
Results



Kendall kernel SVM

- **Competitive accuracy!**
- Less sensitive to regularization parameter!
- No need for feature selection!

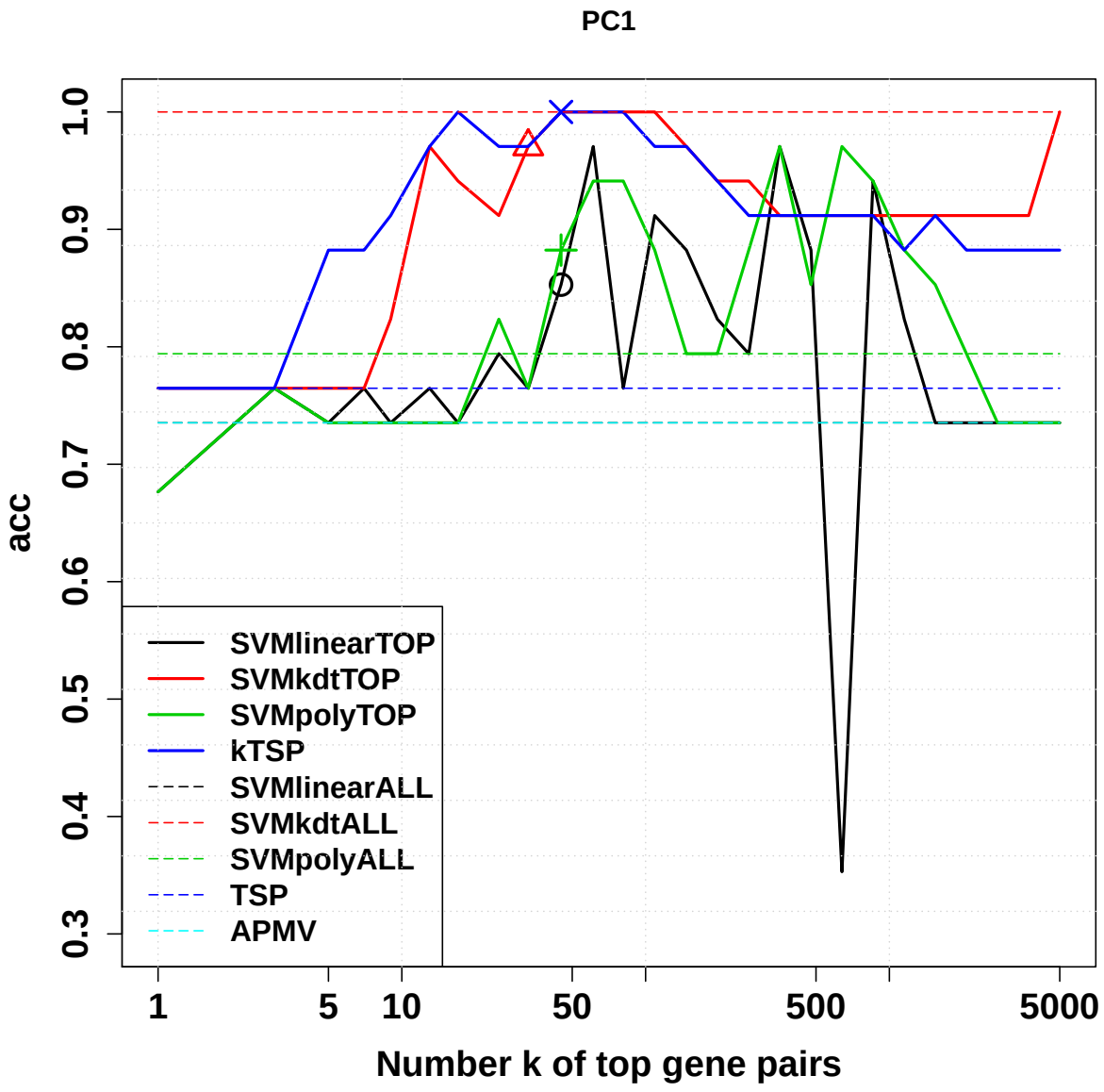
Results



Kendall kernel SVM

- Competitive accuracy!
- **Less sensitive to regularization parameter!**
- No need for feature selection!

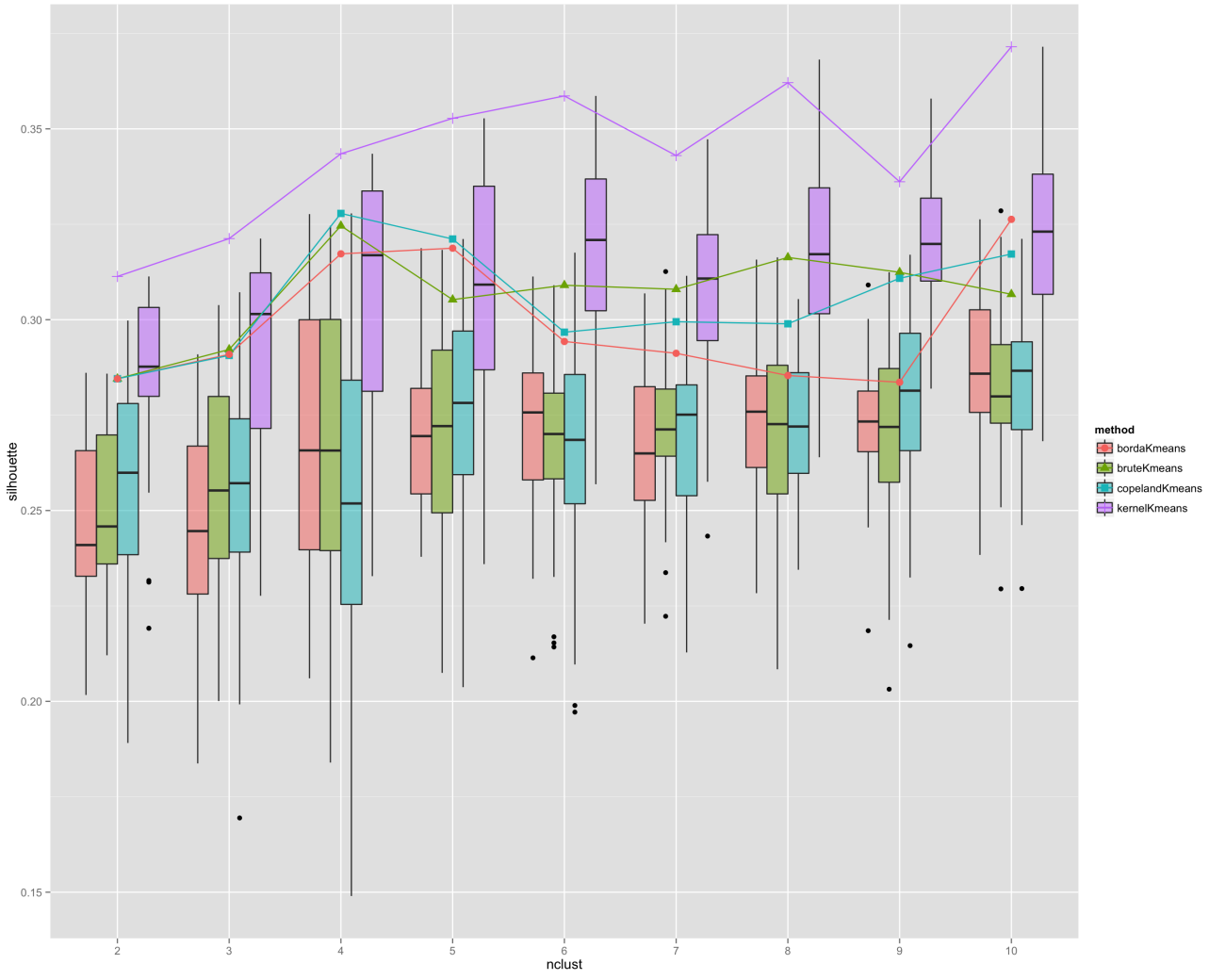
Results



Kendall kernel SVM

- Competitive accuracy!
- Less sensitive to regularization parameter!
- **No need for feature selection!**

Application: clustering



- APA data (full rankings)
- $n = 5738$, $p = 5$
- (new) Kernel k-means vs (standard) k-means in $\mathbb{S}_5$
- Show silhouette as a function of number of clusters (higher better)

Extension to partial rankings

- Two interesting types of partial rankings are interleaving partial ranking

$$x_{i_1} \succ x_{i_2} \succ \cdots \succ x_{i_k}, \quad k \leq n.$$

  and top-k partial ranking

$$x_{i_1} \succ x_{i_2} \succ \cdots \succ x_{i_k} \succ X_{\text{rest}}, \quad k \leq n.$$

- Partial rankings can be uniquely represented by a set of permutations compatible with all the observed partial orders.

Theorem

For these two particular types of partial rankings, the convolution kernel (Haussler, 1999) induced by Kendall kernel

$$K_\tau^\star(R, R') = \frac{1}{|R||R'|} \sum_{\sigma \in R} \sum_{\sigma' \in R'} K_\tau(\sigma, \sigma')$$

can be evaluated in $O(k \log k)$ time.

Extension to partial rankings

- Two interesting types of partial rankings are interleaving partial ranking

$$x_{i_1} \succ x_{i_2} \succ \cdots \succ x_{i_k}, \quad k \leq n.$$

  and top-k partial ranking

$$x_{i_1} \succ x_{i_2} \succ \cdots \succ x_{i_k} \succ X_{\text{rest}}, \quad k \leq n.$$

- Partial rankings can be uniquely represented by a set of permutations compatible with all the observed partial orders.

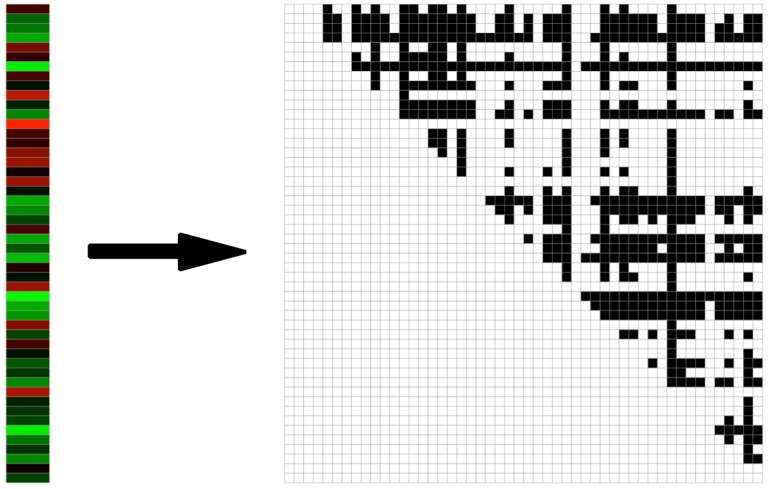
Theorem

For these two particular types of partial rankings, the convolution kernel (Haussler, 1999) induced by Kendall kernel

$$K_\tau^\star(R, R') = \frac{1}{|R||R'|} \sum_{\sigma \in R} \sum_{\sigma' \in R'} K_\tau(\sigma, \sigma')$$

can be evaluated in $O(k \log k)$ time.

Extension to smoother, continuous representations



One sample x
p features

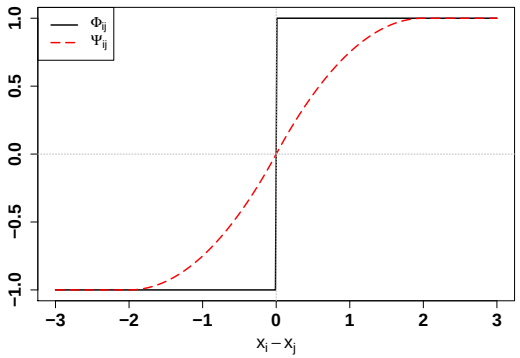
Mapping f(x)
p(p-1)/2 bits

- Instead of $\Phi : \mathbb{R}^p \to \{0,1\}^{p(p-1)/2}$, consider the continuous mapping $\Psi_a : \mathbb{R}^p \to \mathbb{R}^{p(p-1)/2}$:

$$\Psi_a(x) = \mathbb{E}\Phi(x+\epsilon) \quad \text{with} \quad \epsilon \sim (\mathcal{U}[-\frac{a}{2}, \frac{a}{2}])^n$$

- Corresponding kernel $G_a(x, x') = \Psi_a(x)^\top \Psi_a(x')$

Computation of $G(x, x')$



- $G_a(x, x')$ can be computed exactly in $O(p^2)$ by explicit computation of $\Psi_a(x)$ in $\mathbb{R}^{p(p-1)/2}$

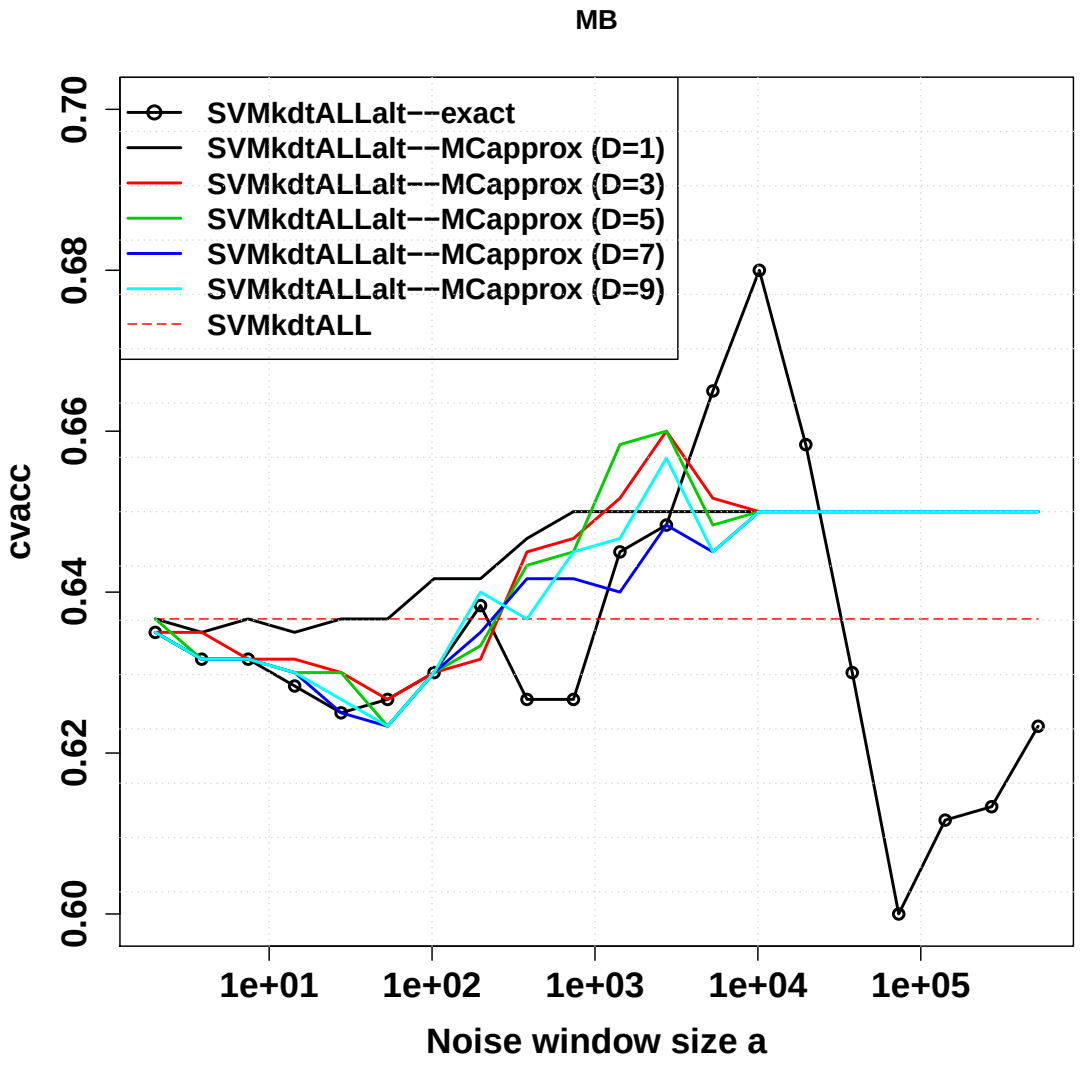
- $G_a(x, x')$ can be computed approximately in $O(D^2 p \log p)$ by Monte-Carlo approximation:

$$\tilde{G}_a(x, x') = \frac{1}{D^2} \sum_{i,j=1}^{D} K(x + \epsilon_i, x' + \epsilon'_j)$$

- Theorem: for supervised learning, Monte-Carlo approximation is better[1] than exact computation when $n = o(p^{1/3})$

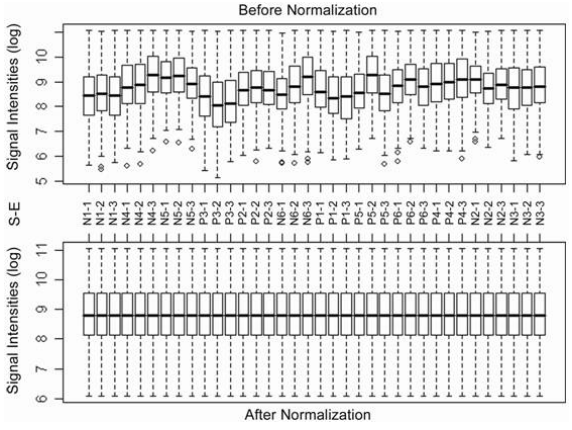
[1] faster for the same accuracy

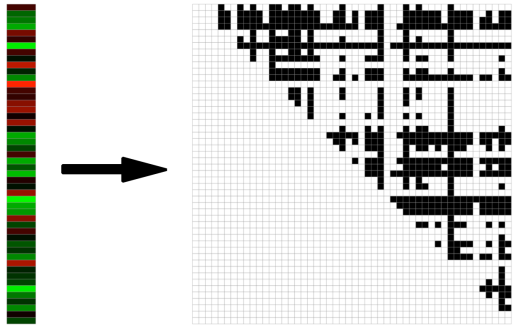
Performance of $G_a(x, x)$



Outline

Conclusion





One sample x
p features

Mapping f(x)
p(p-1)/2 bits

- Representing omics data as permutations has some potential
  - Kendall and Mallows kernel in $O(p \ln(p))$
  - SUQUAN supervised quantile normalization as matrix regression
- Understanding the benefits and cost of different representations remains very heuristic and sometimes counterintuitive
- Learning representation may help

Thanks

The Adolph C. and Mary Sprague Miller Institute for Basic Research in Science
University of California, Berkeley

References

R. E. Barlow, D. Bartholomew, J. M. Bremner, and H. D. Brunk. *Statistical inference under order restrictions; the theory and application of isotonic regression*. Wiley, New-York, 1972.

M. Le Morvan and J.-P. Vert. Supervised quantile normalisation. Technical Report 1706.00244, arXiv, 2017.

O. Sysoev and O. Burdakov. A smoothed monotonic regression via l2 regularization. Technical Report LiTH-MAT-R–2016/01–SE, Department of mathematics, Linköping University, 2016. URL `http://liu.diva-portal.org/smash/get/diva2:905380/FULLTEXT01.pdf`.

A. C. Tan, D. Q. Naiman, L. Xu, R. L. Winslow, and D. Geman. Simple decision rules for classifying human cancers from gene expression profiles. *Bioinformatics*, 21(20):3896–3904, Oct 2005. doi: 10.1093/bioinformatics/bti631. URL `http://dx.doi.org/10.1093/bioinformatics/bti631`.