Learning on the symmetric group

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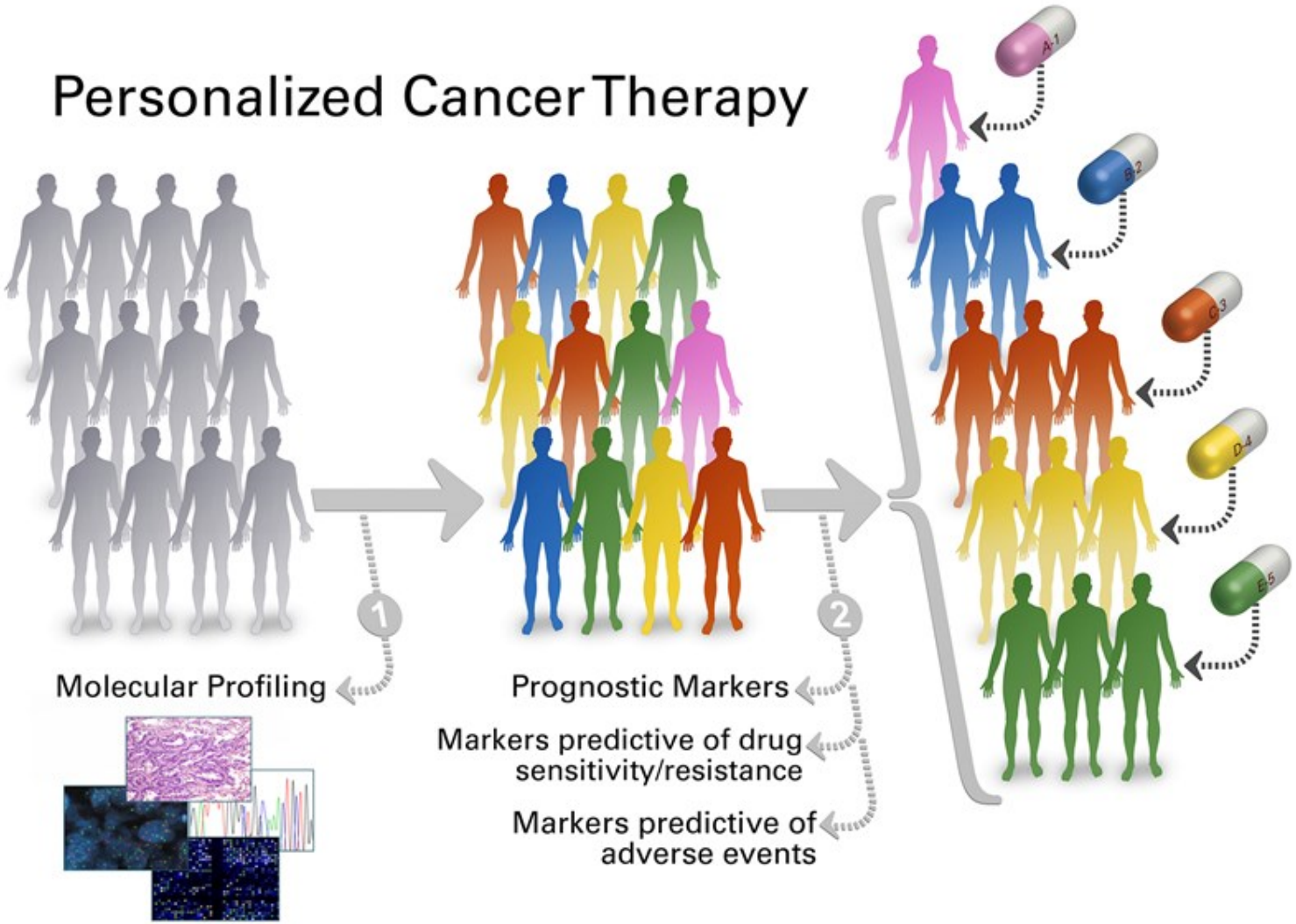
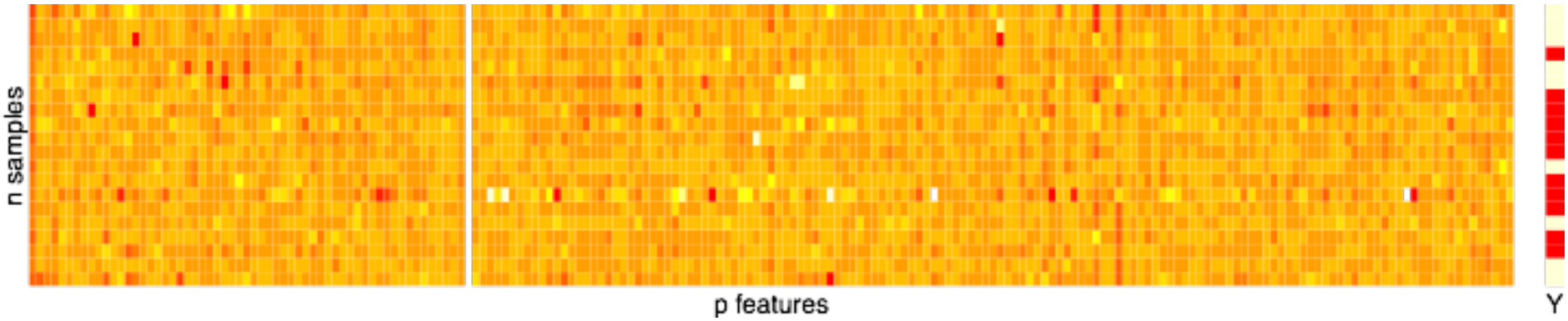
Google Zürich,
Septembre 29, 2017

Motivation



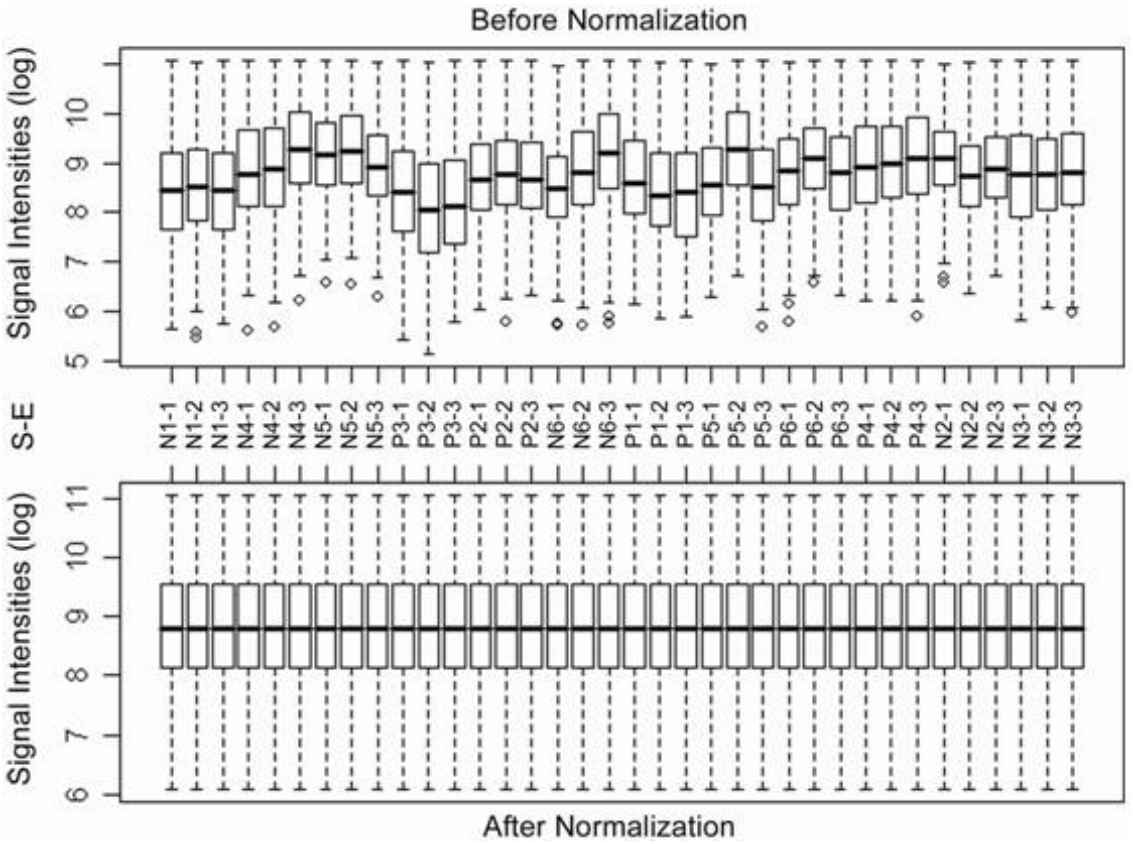
https://pct.mdanderson.org

Data



- 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?

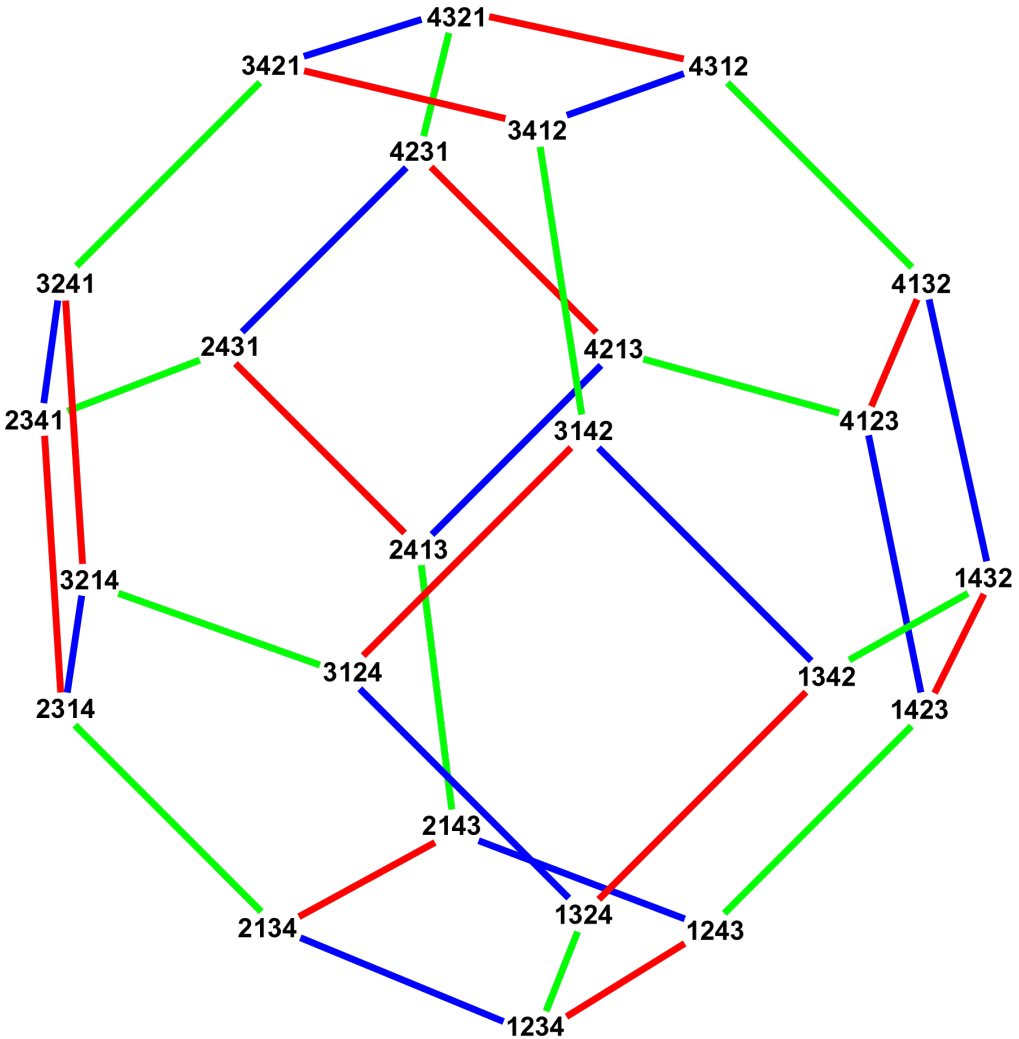
From raw data to X



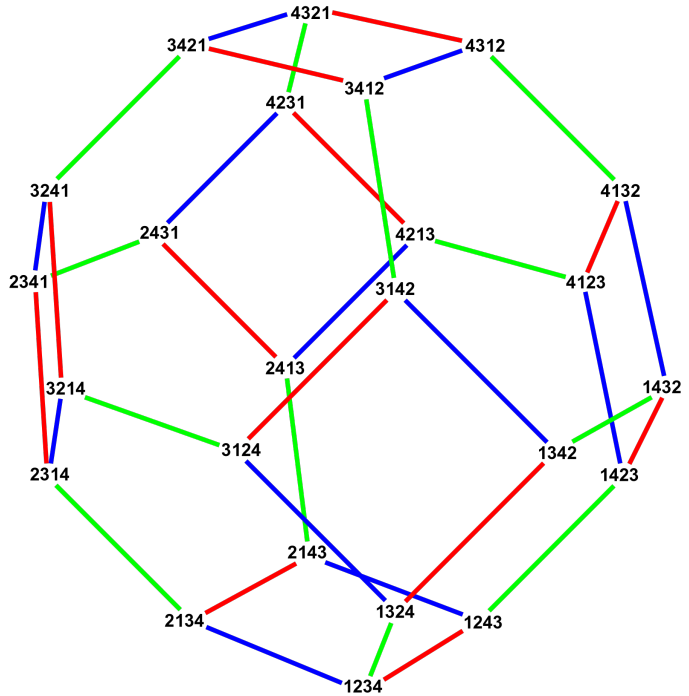
- Between-sample variability: batch effect, drift over time, ...
- Typical pre-processing: Quantile normalization per sample
- Only the relative ordering of features within each sample is used
- See also: pictures (Gonzalez and Woods, 2008), MRI scans (Shinohara et al., 2014), speech (Hilger and Ney, 2006)

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 $X \in S_p$?



Related work

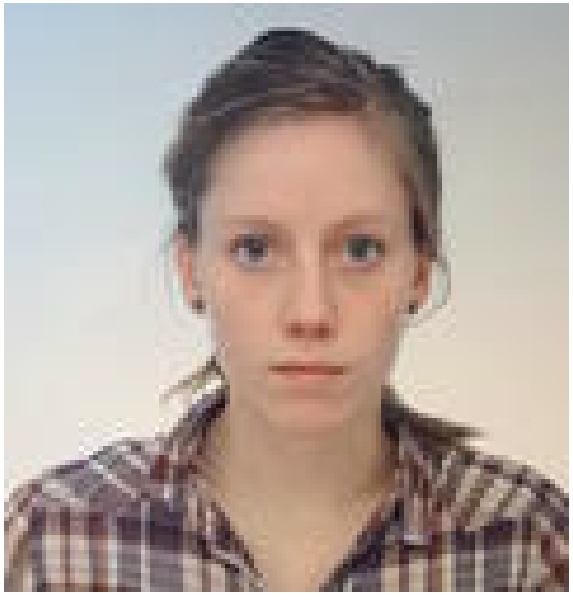


- Represent a permutation $x \in S_p$ by the vector of rank $\Phi(x) \in \mathbb{R}^p$
  - this is a particular quantile normalization
- Diffusion kernel over the Cayley's graph (Kondor and Barbosa, 2010)
  - but complexity $O(p^{2p})$
- Many other data come as permutations (votes, preferences, ...)

Outline

Outline

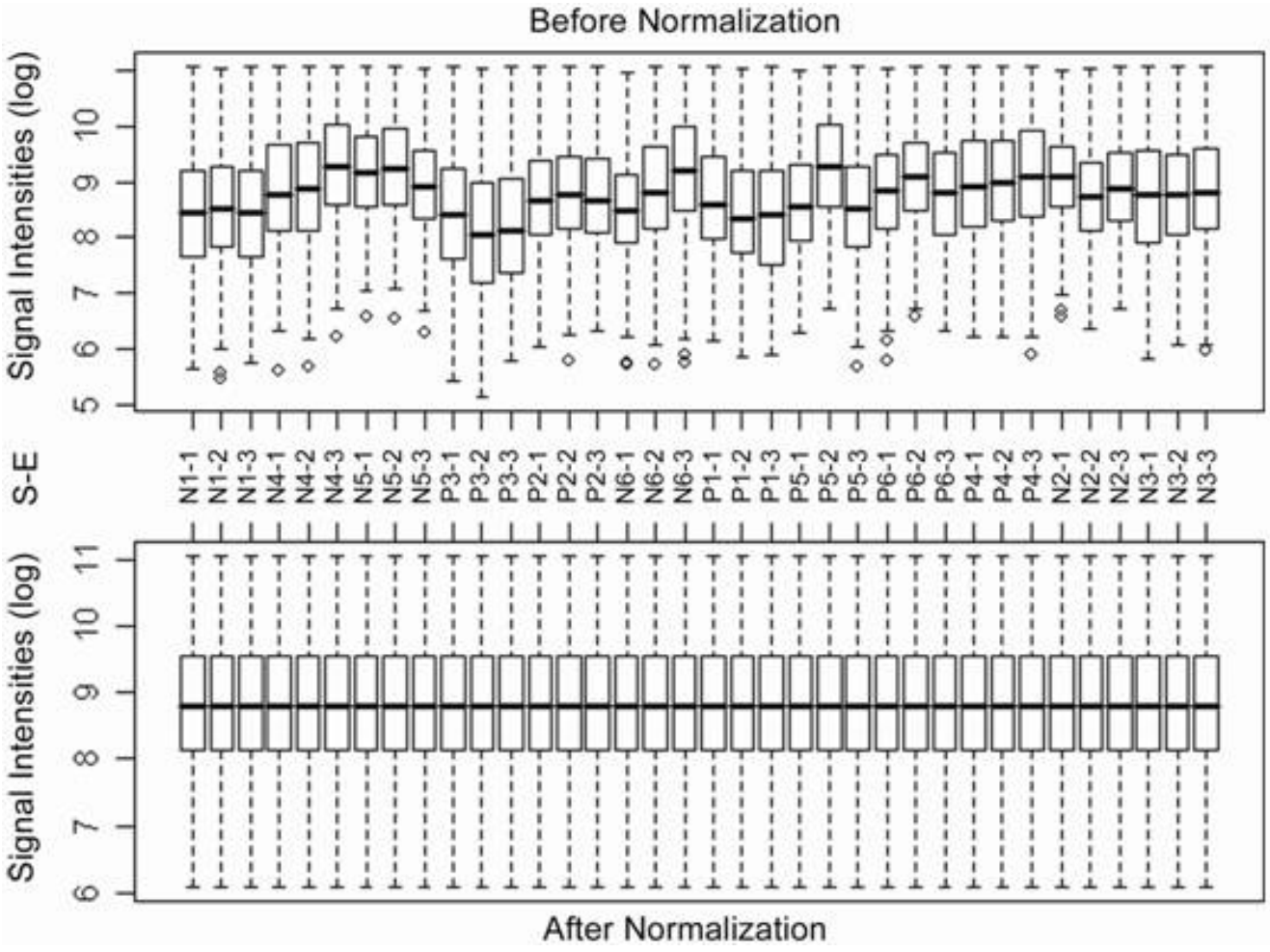
Joint work with



Marine Le Morvan

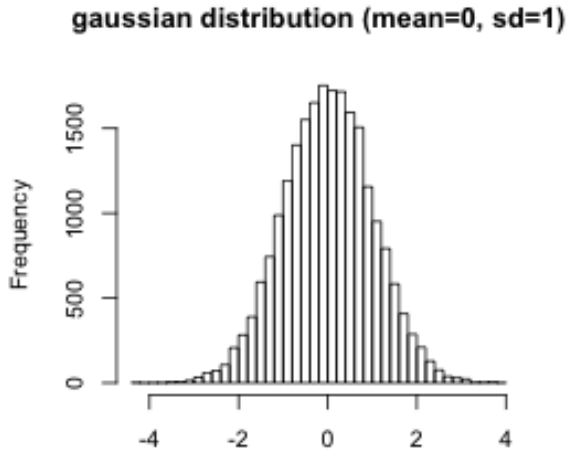
https://arxiv.org/abs/1706.00244

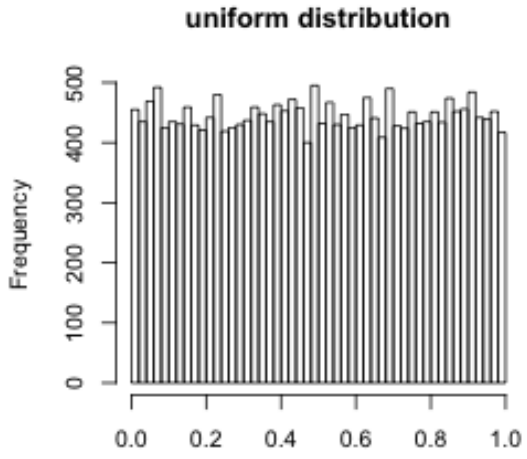
Standard full quantile normalization

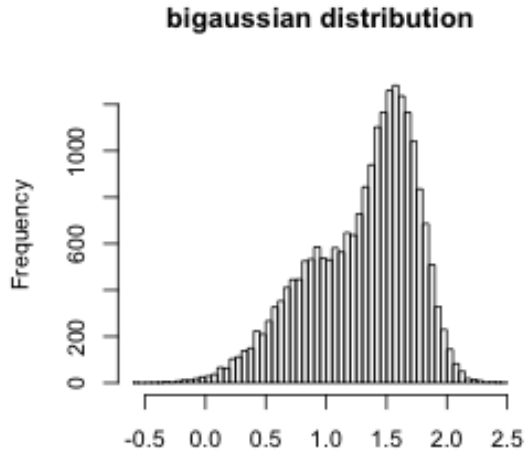


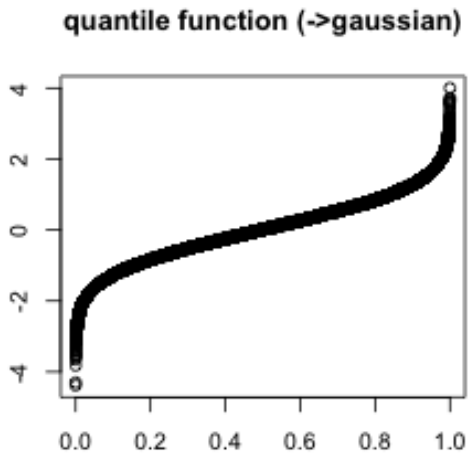
Typically followed by a predictive model $f(X)$ on the normalized data

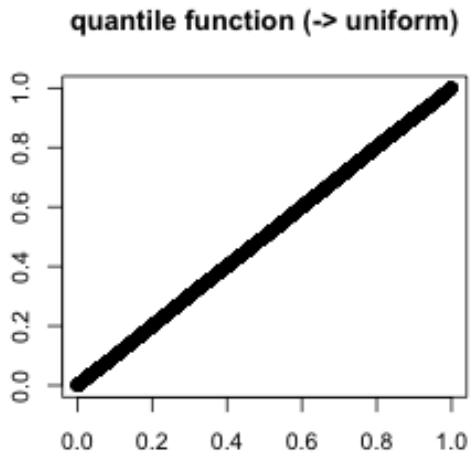
How to choose a "good" target distribution?

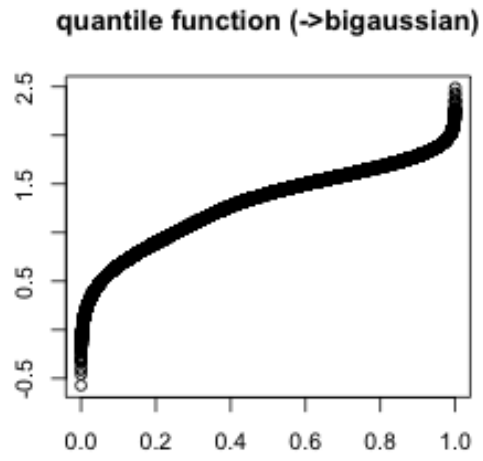






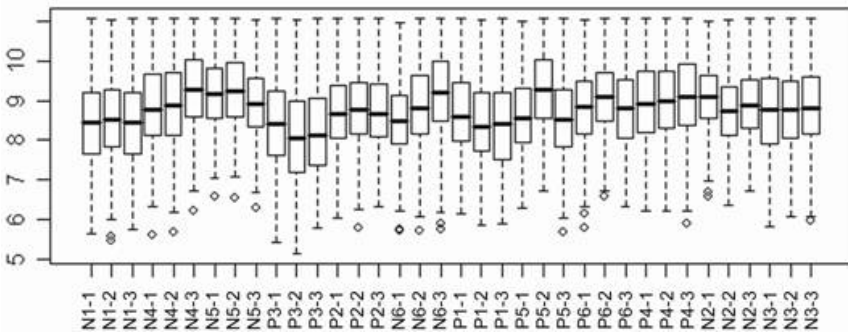




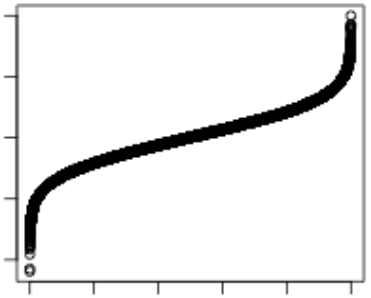


Notations

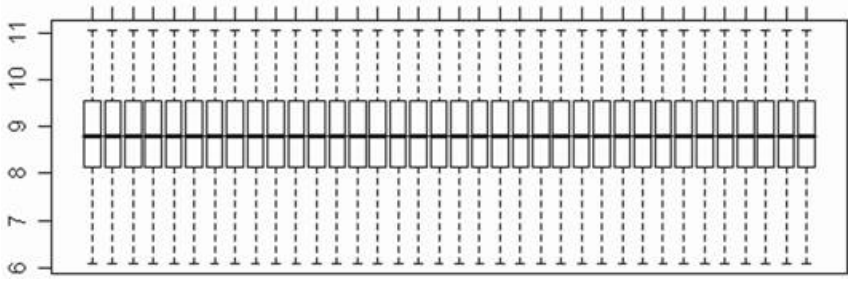
- $x_1, \ldots, x_n \in \mathbb{R}^p$ a set of p-dimensional samples



- $f \in \mathbb{R}^p$ 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, Barlow et al. (1972)) or the Smoothed Pool Adjacent Violators algorithm (SPAV, Sysoev and Burdakov (2016)) 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: $(\sigma, w, f) \leftarrow SVD(M_{LDA}, 1)$

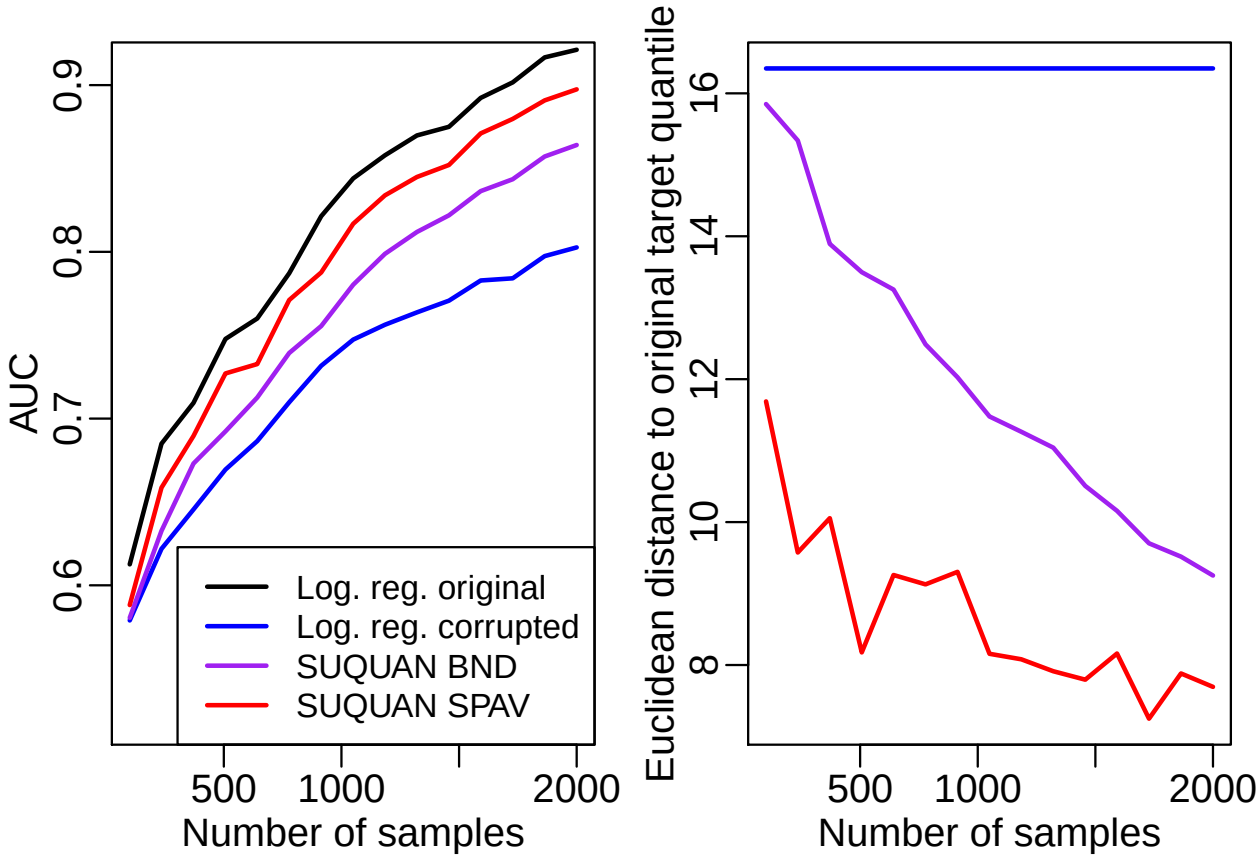
- Ridge penalty (no monotonicity constraint), equivalent to rank-1 regression problem
- SVD finds the closest rank-1 matrix to the LDA solution:

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

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

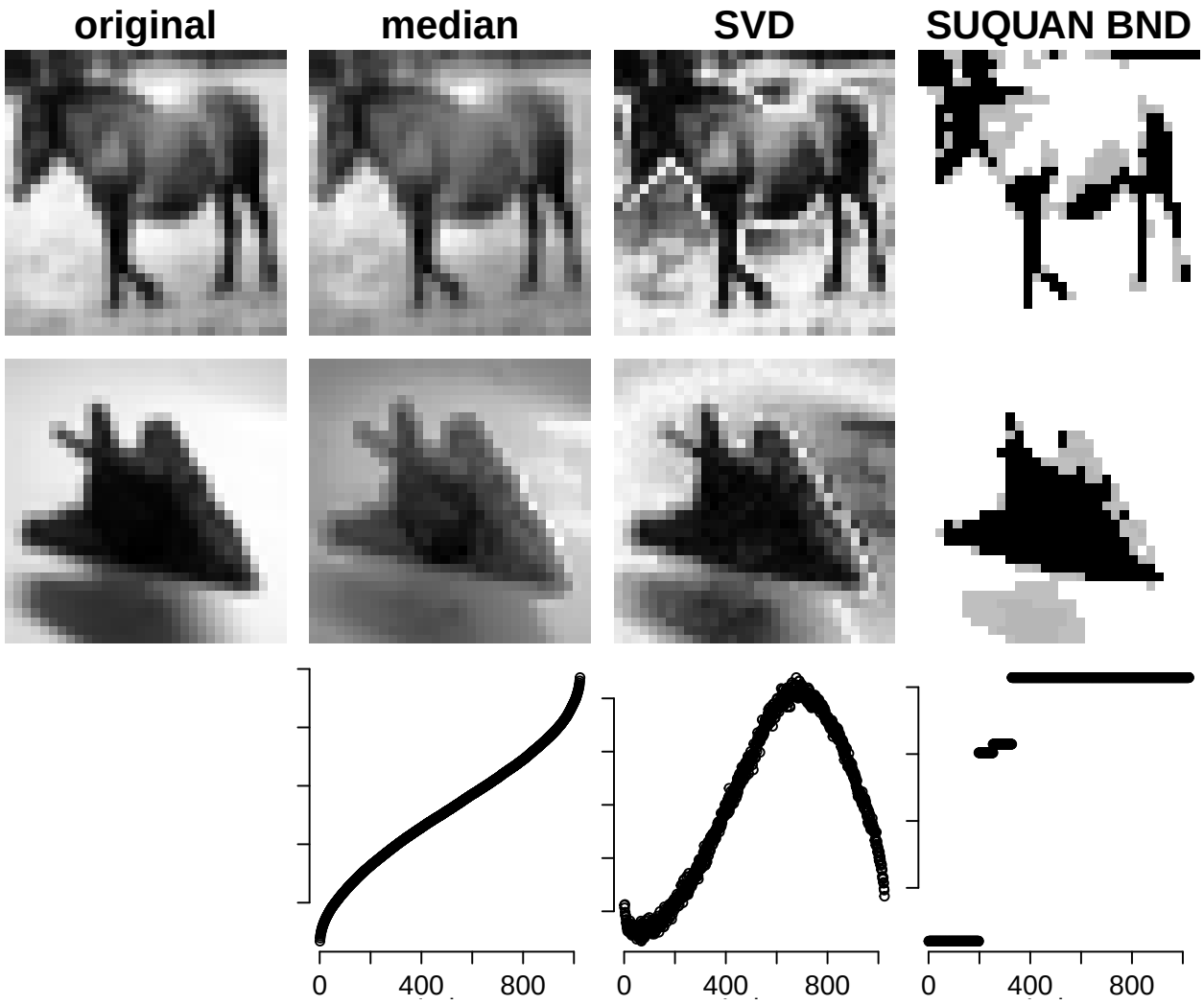
Experiments: Simulations

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



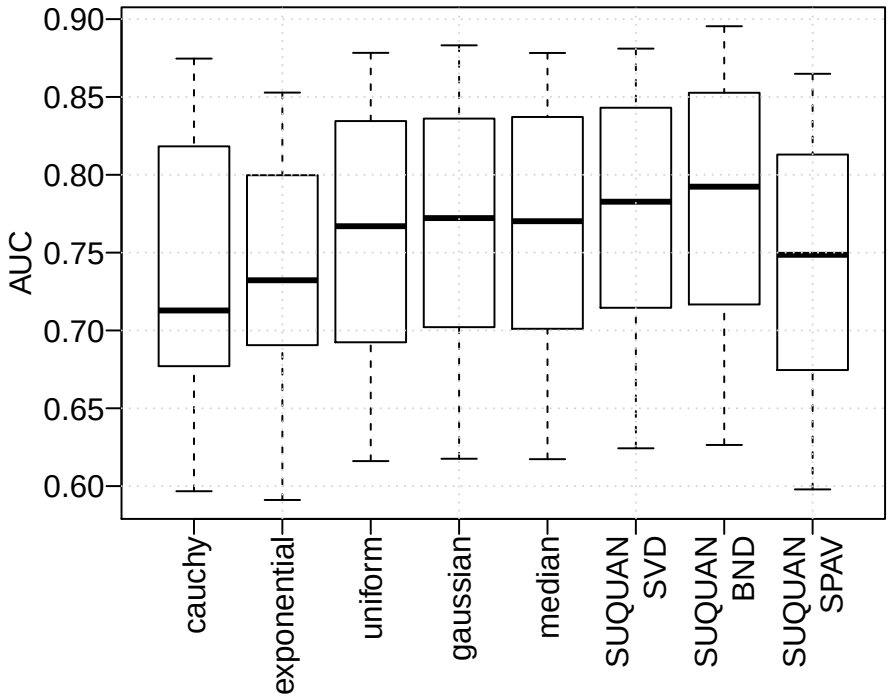
Experiments: CIFAR-10

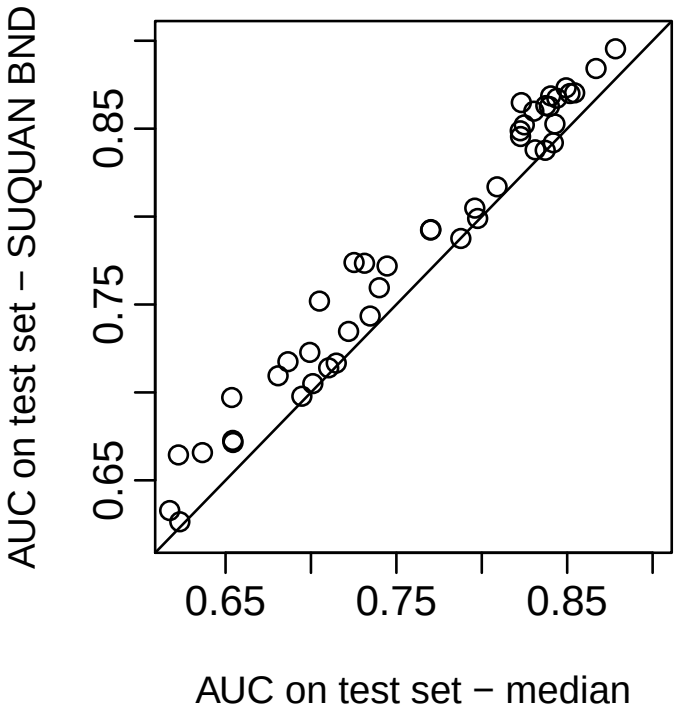
- Example: horse vs. plane
- Different methods learn different quantile distributions



Experiments: CIFAR-10

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





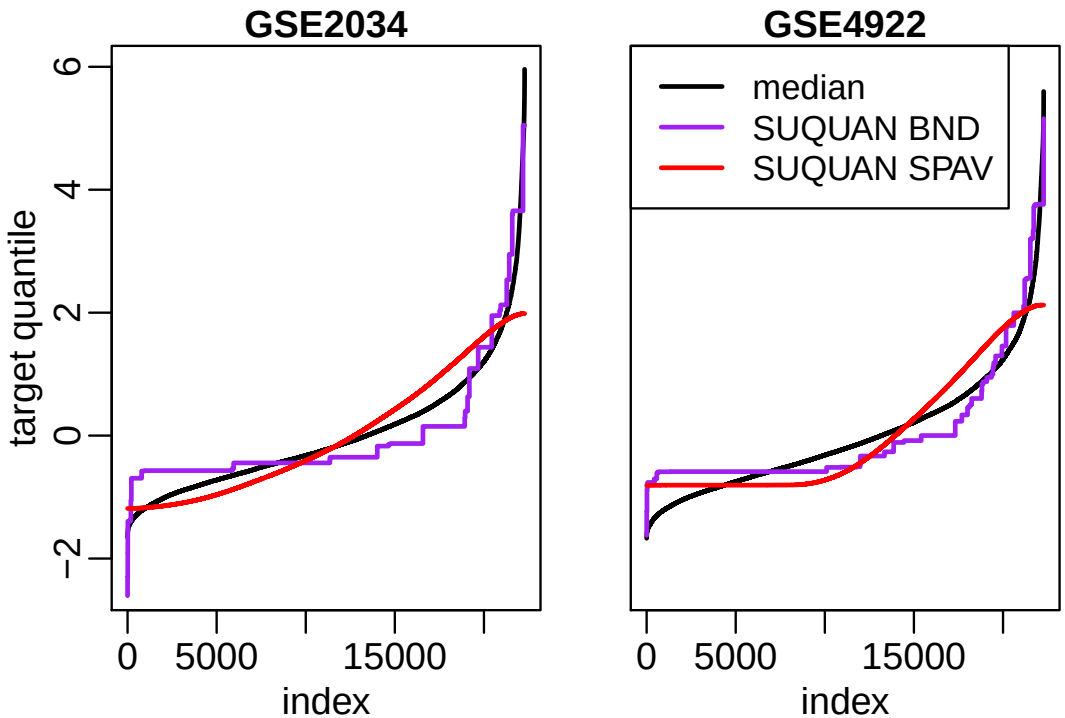
Experiments: gene expression data

- 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:

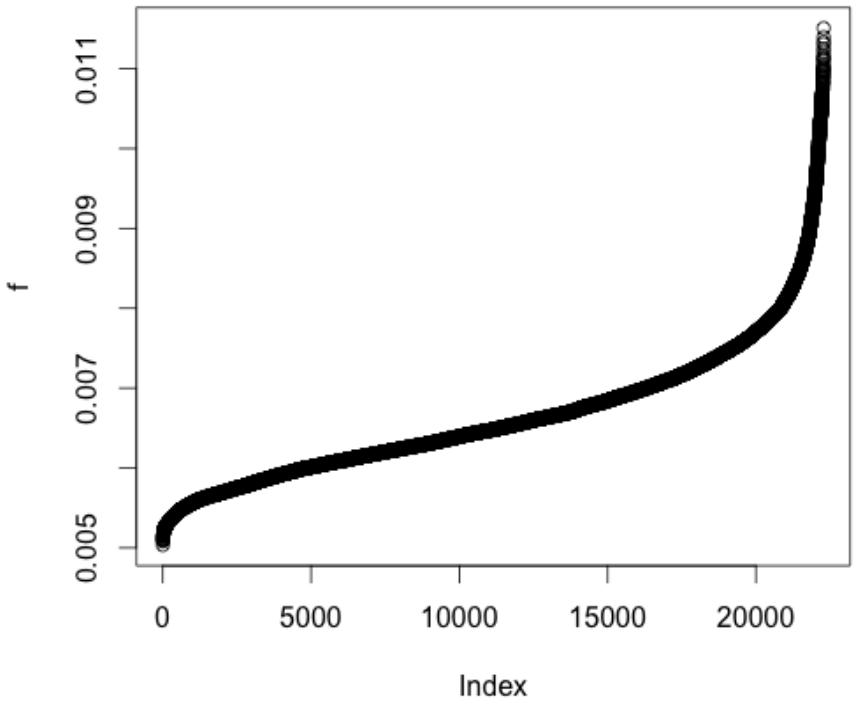
DATASET NAME	# PATIENTS	# POSITIVES	% POSITIVES
GSE1456	141	37	0.26
GSE2034	271	104	0.38
GSE2990	106	32	0.30
GSE4922	225	73	0.32

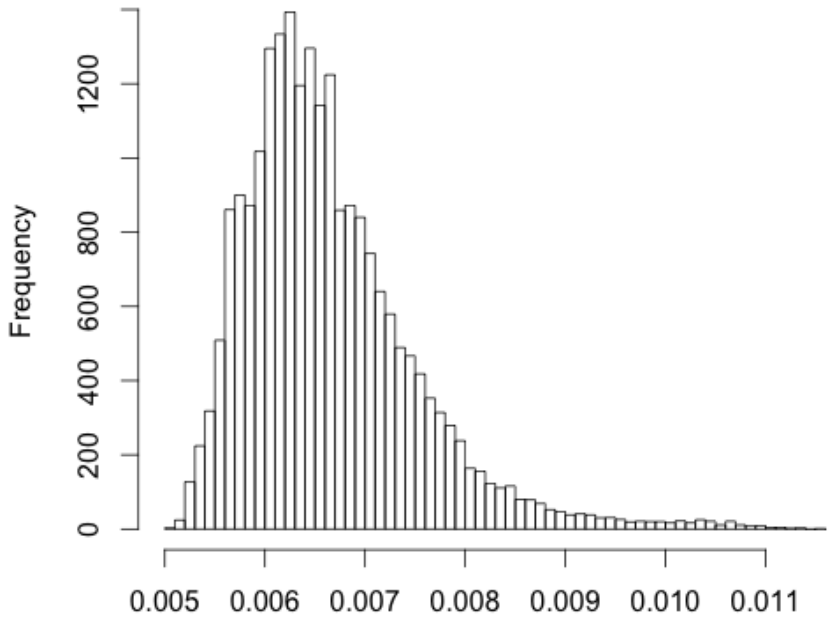
Results: gene expression data

	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**

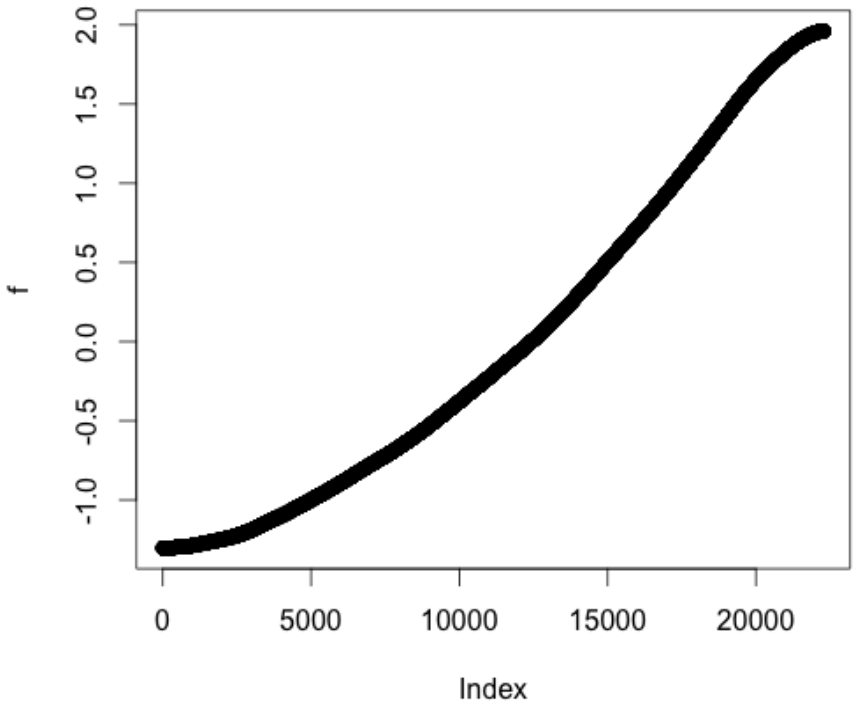


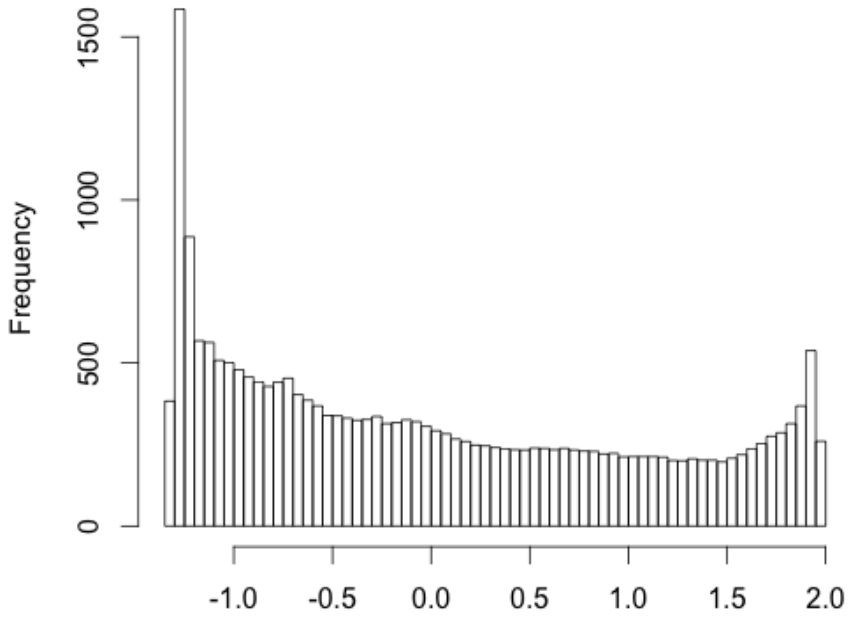
Estimated distribution: iteration=0



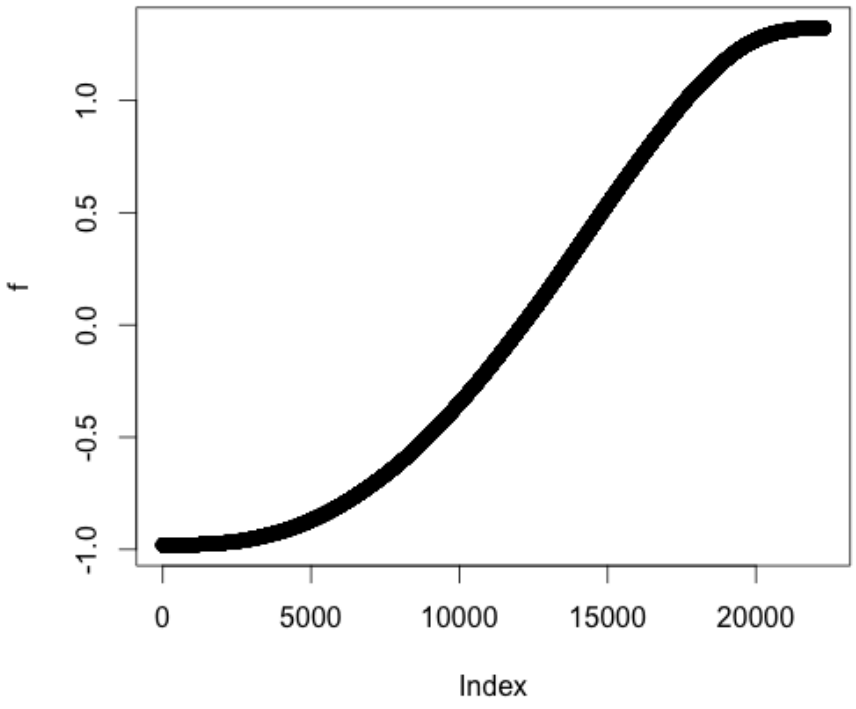


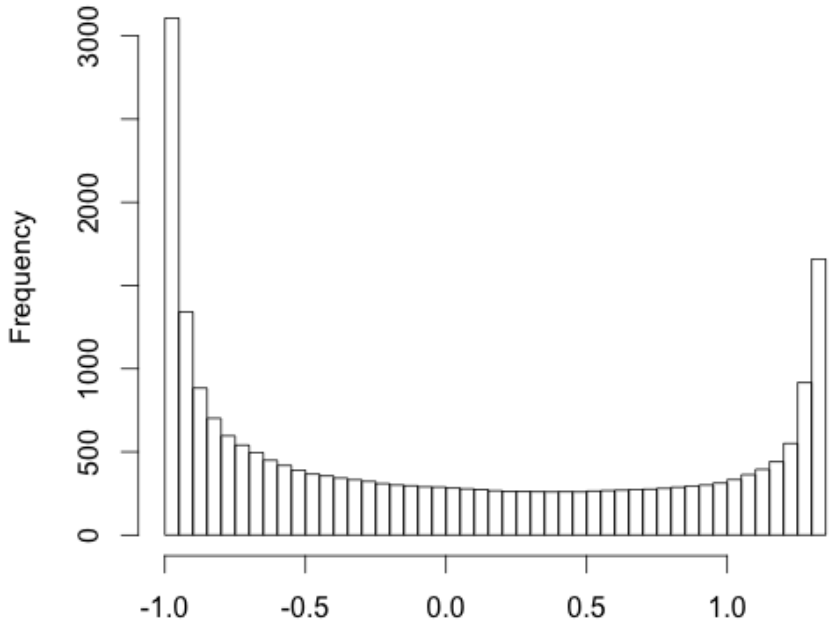
Estimated distribution: iteration=1





Estimated distribution: iteration=2





Outline

Joint work with

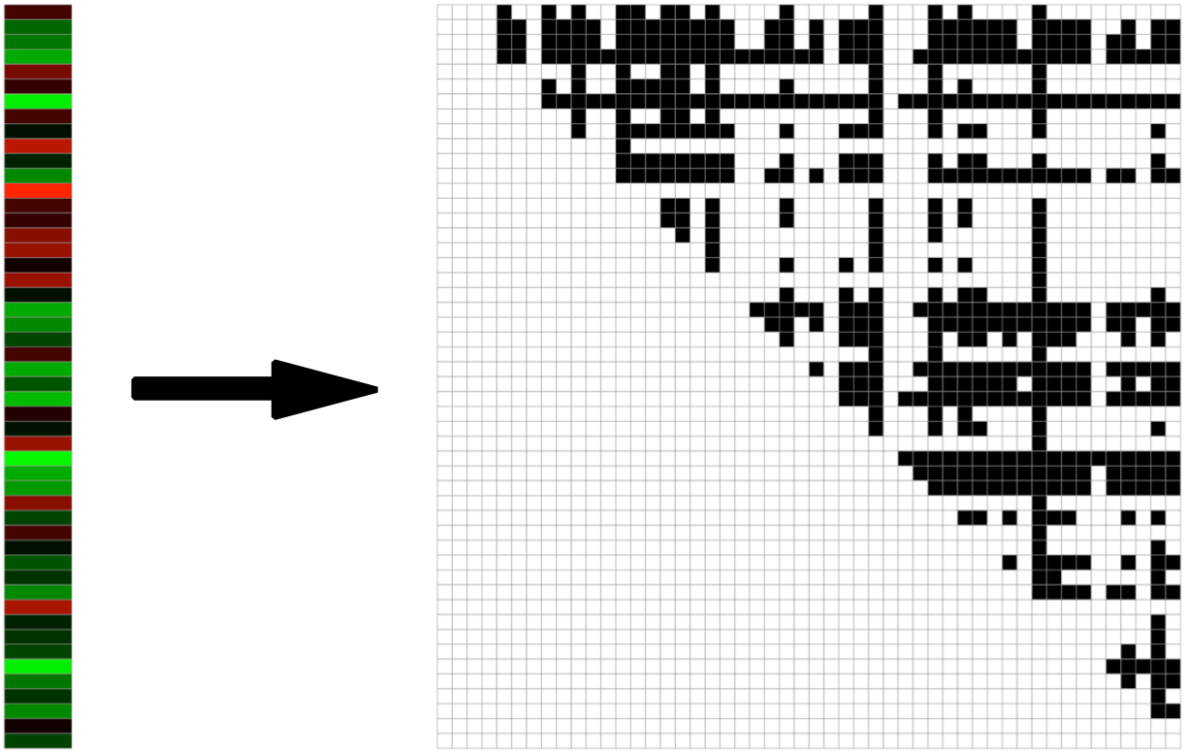
Yunlong Jiao

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

An idea: all pairwise comparisons

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

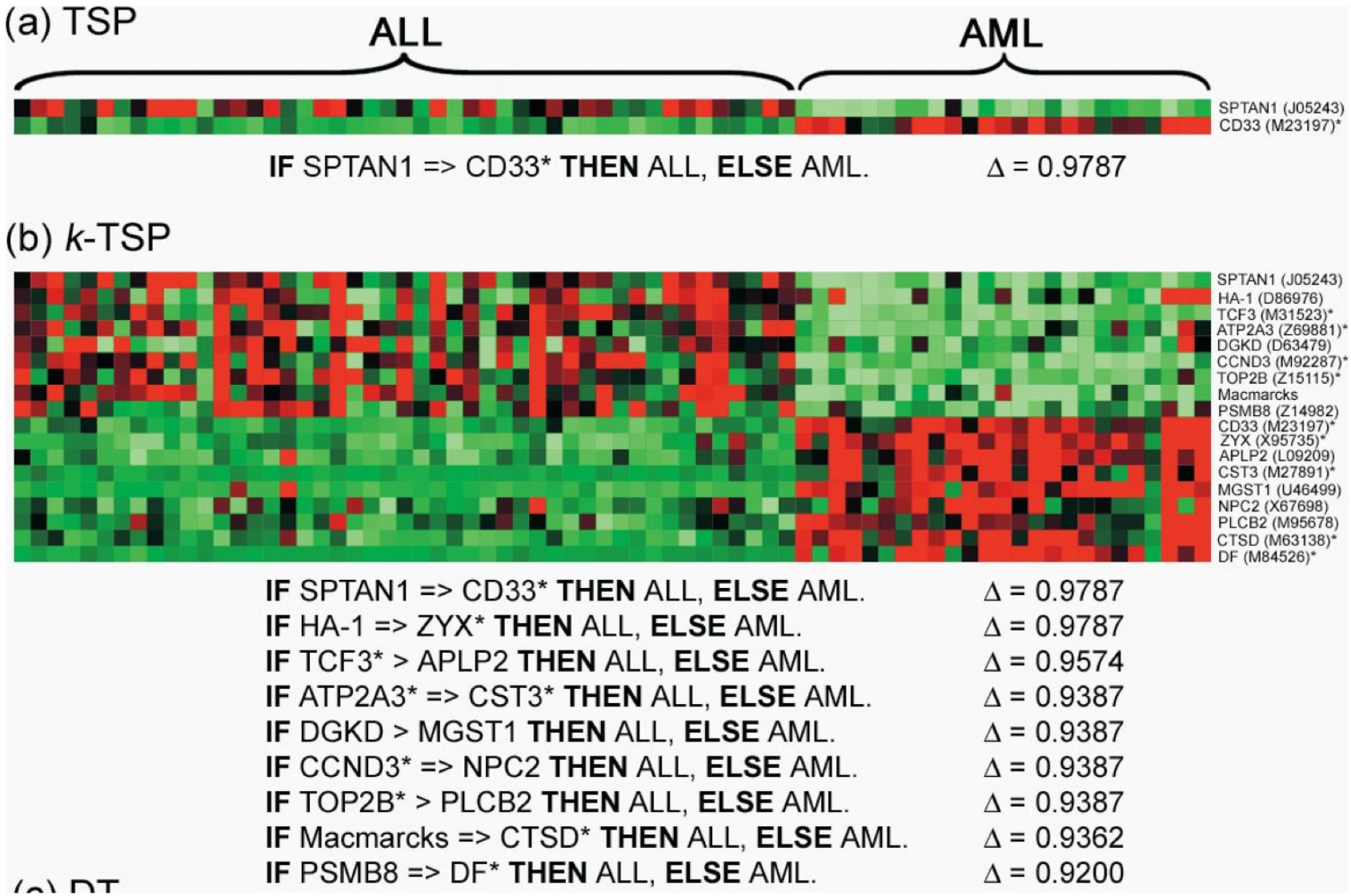
$$\Phi_{i,j}(x) = \begin{cases} 1 & \text{if } x_i \leq x_j\,, \\ 0 & \text{otherwise.} \end{cases}$$



One sample x
p features

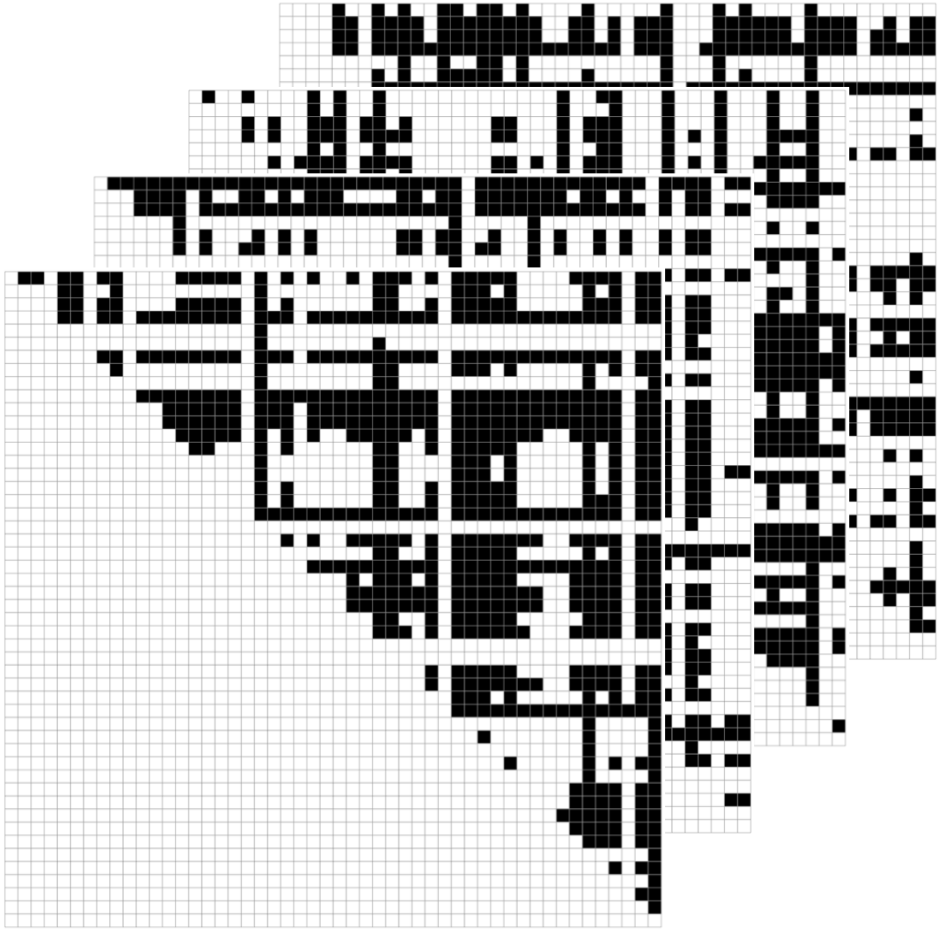
Mapping f(x)
p(p-1)/2 bits

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

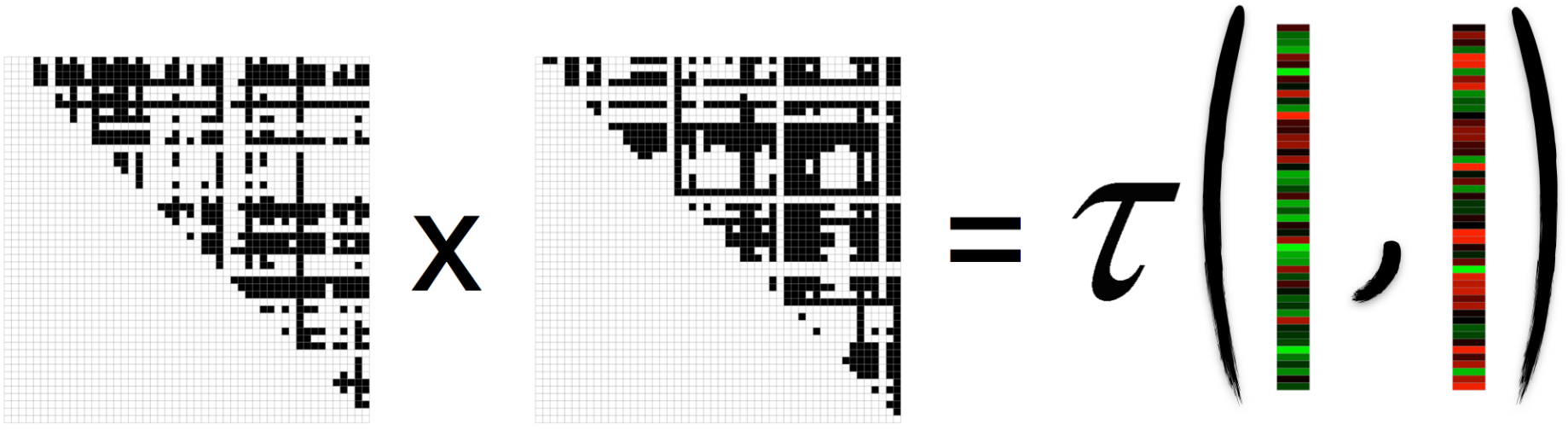
$$K(x, x') = \Phi(x)^\top \Phi(x')$$

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

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

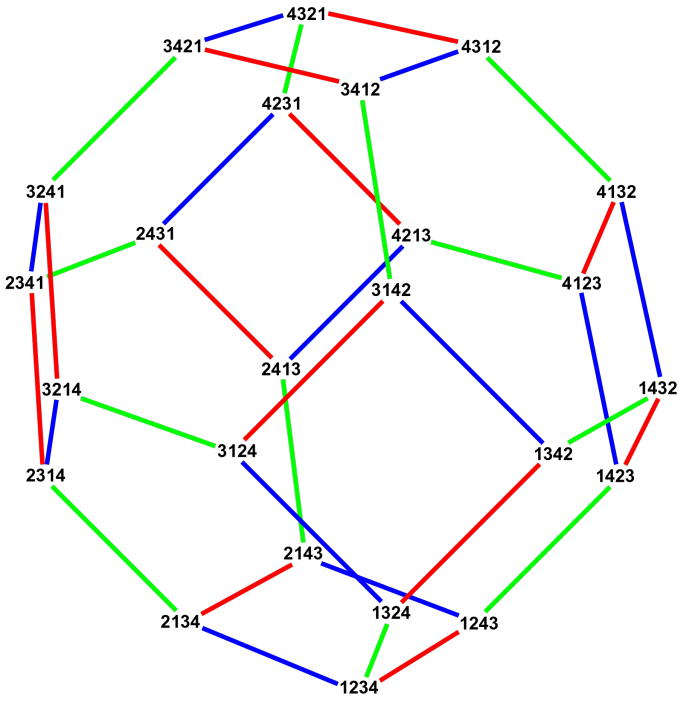
Theorem (Jiao and V., 2015)

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 ($O(p^{2p})$)
- 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

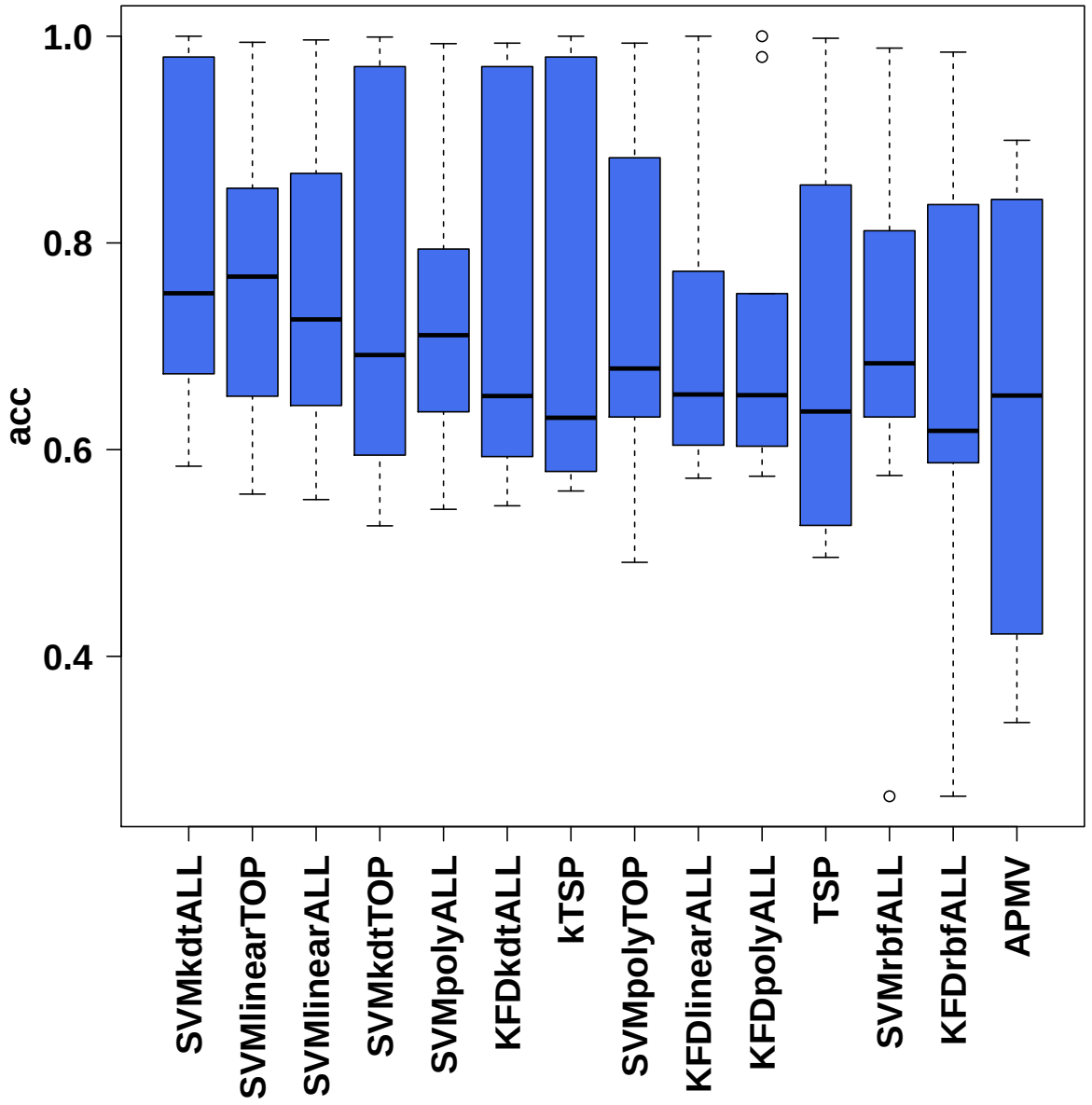
Datasets

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 Tan et al. (2005).
- Hybrid scheme of SVM + TSP feature selection algorithm.

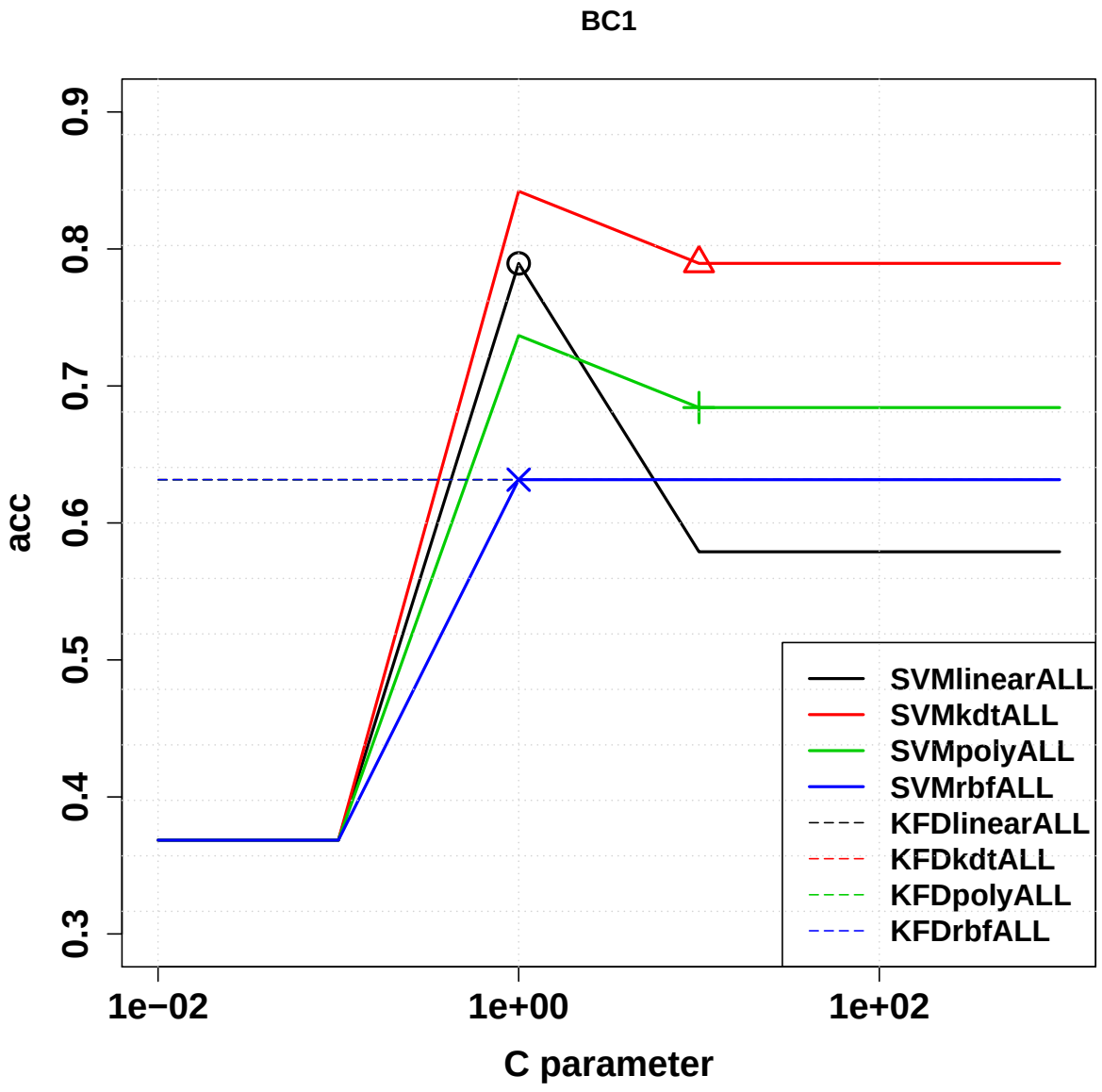
Results



Kendall kernel SVM

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

Results



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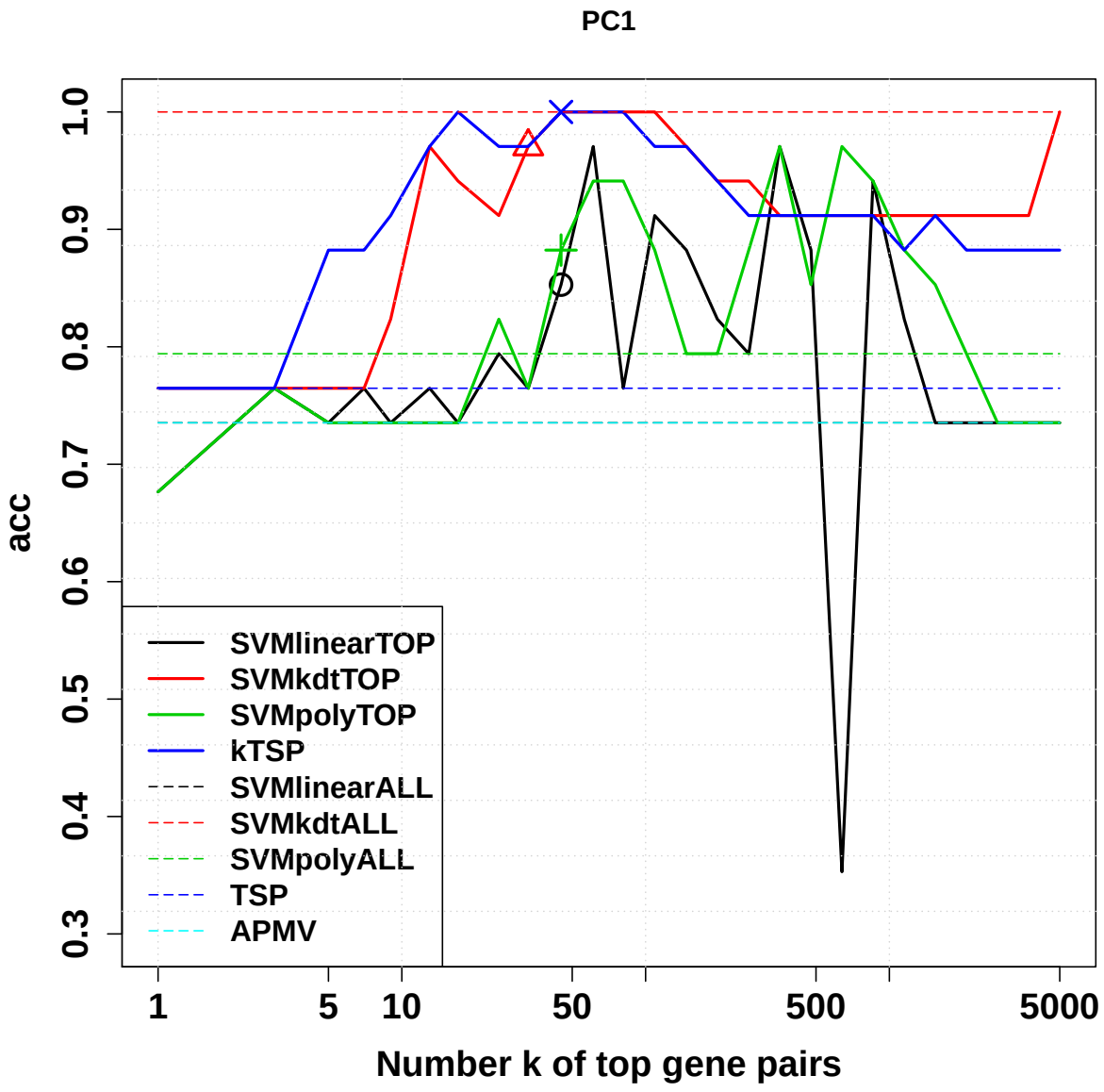

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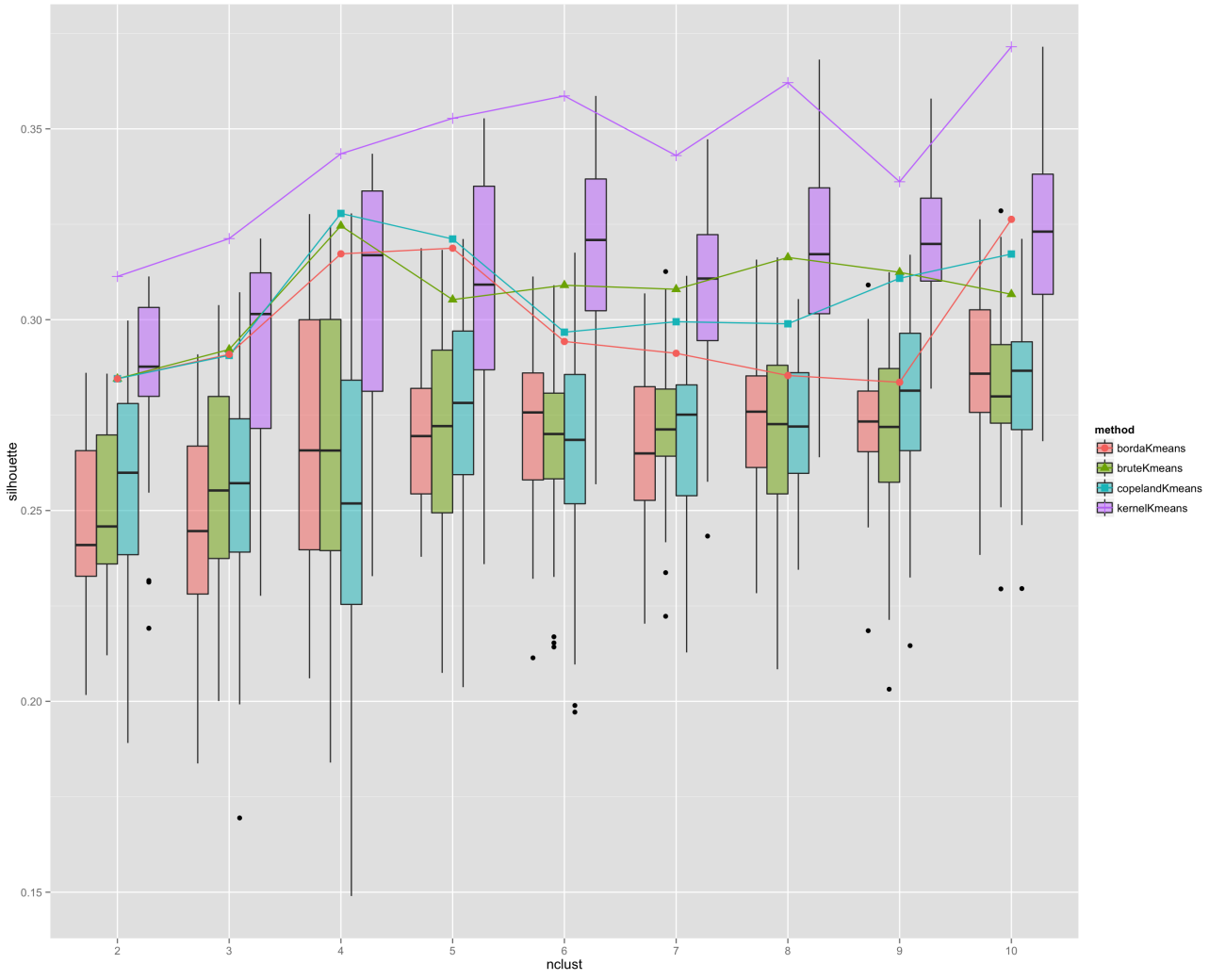
Application: clustering



- 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.

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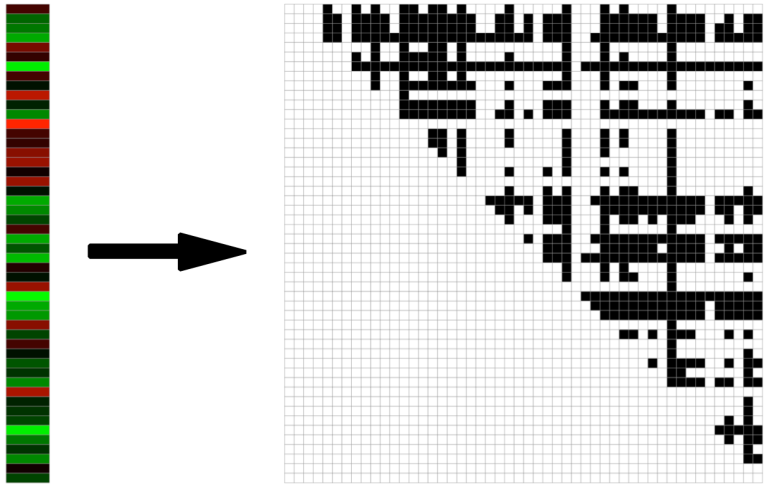
Extension to smoother, continuous representations



One sample x
p features

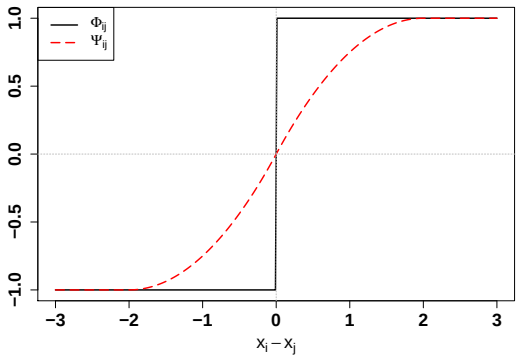
Mapping f(x)
p(p-1)/2 bits

- 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 $\mathbb{R}^{p(p-1)/2}$

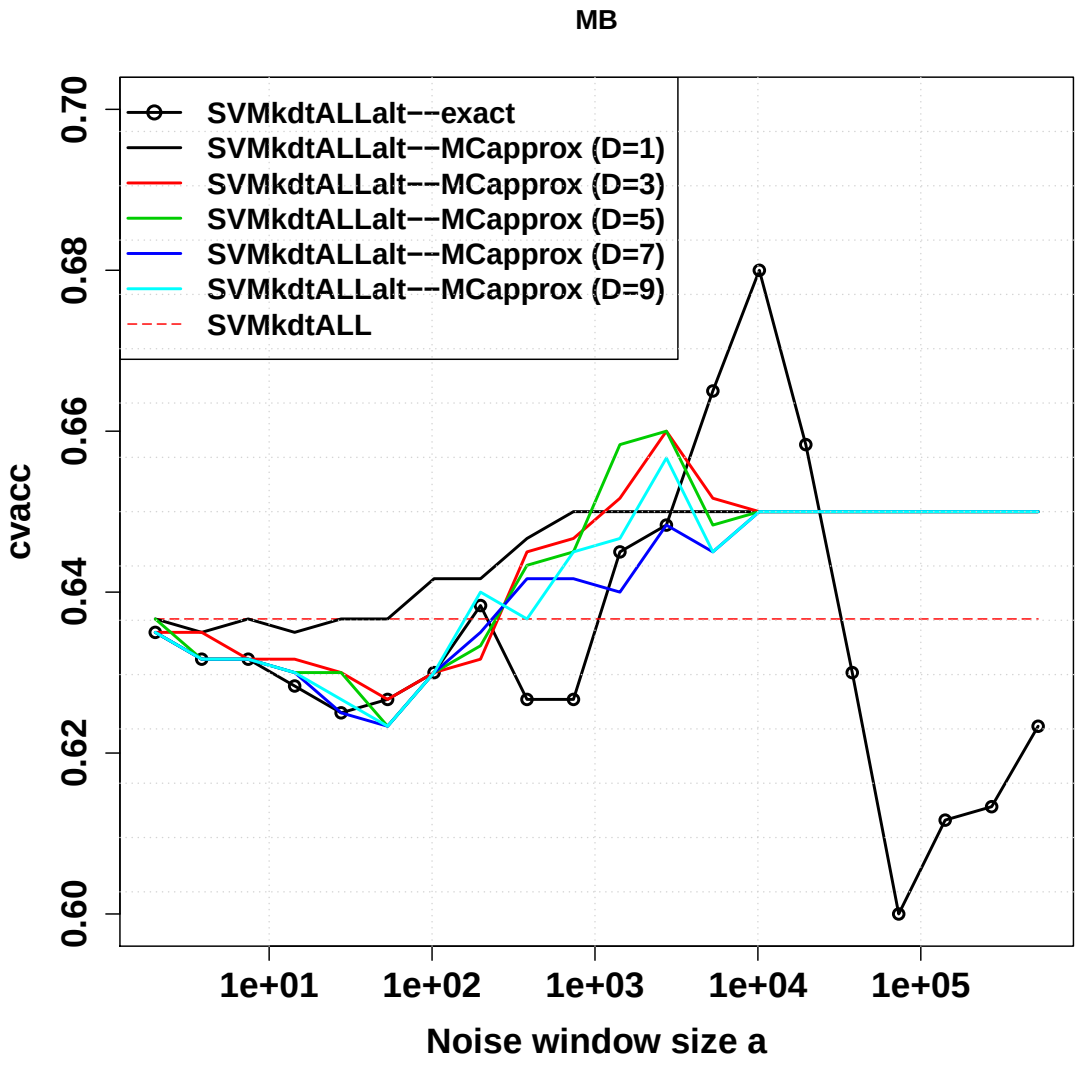
- $G_a(x, x')$ can be computed approximately in $O(D^2 p \log p)$ by Monte-Carlo approximation:

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

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

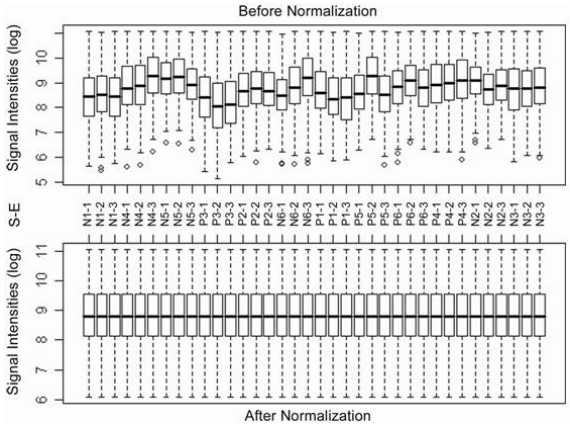
[1] faster for the same accuracy

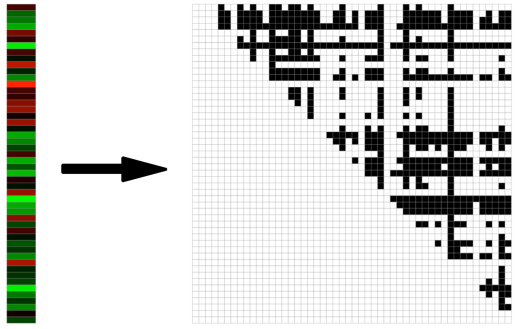
Performance of $G_a(x, x)$



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
- Ongoing work:
  - Extension of SUQUAN to nonlinear models (neural nets..)
  - Extention of SUQUAN to Kendall representation (weighted Kendall correlation...)

Thanks

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

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