Learning with permutations

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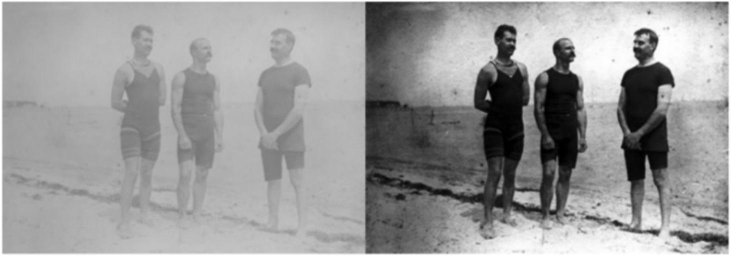
Takeuchi Laboratory, Nagoya Institute of Technology, Aug 1, 2018

Motivations

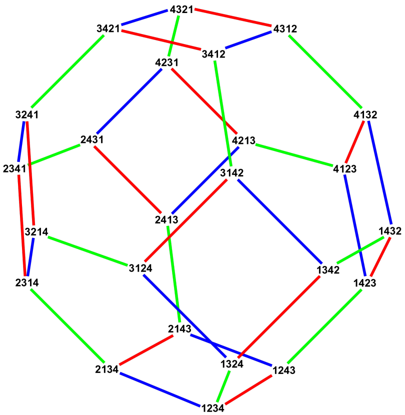
- Ranking data

- Ranks extracted from data



(histogram equalization, quantile normalization...)

Mathematically



- Permutation: a bijection

$$\sigma : [1, n] \to [1, n]$$

- $\sigma(i)$ = rank of item i
- Composition

$$(\sigma_1 \sigma_2)(i) = \sigma_1(\sigma_2(i))$$

- $\mathbb{S}_n$ the symmetric group
- $|\mathbb{S}_n| = n!$

Learning over the symmetric group

- Assume your data are permutations and you want to learn

$$f : \mathbb{S}_n \to \mathbb{R}$$

- A solutions: embed $\mathbb{S}_n$ to a Euclidean or Hilbert space

$$\Phi : \mathbb{S}_n \to \mathcal{H}$$

  and learn a function (e.g., linear):

$$f(\sigma) = \beta^\top \Phi(\sigma)$$

- The corresponding kernel is

$$K(\sigma_1, \sigma_2) = \Phi(\sigma_1)^\top \Phi(\sigma_2)$$

- A right-invariant kernel is invariant by renaming the items:

$$\forall \sigma_1, \sigma_2, \pi \in \mathbb{S}_n\,, \quad K(\sigma_1\pi, \sigma_2\pi) = K(\sigma_1, \sigma_2)$$

Outline

1. The QN embedding

2. The Kendall embedding

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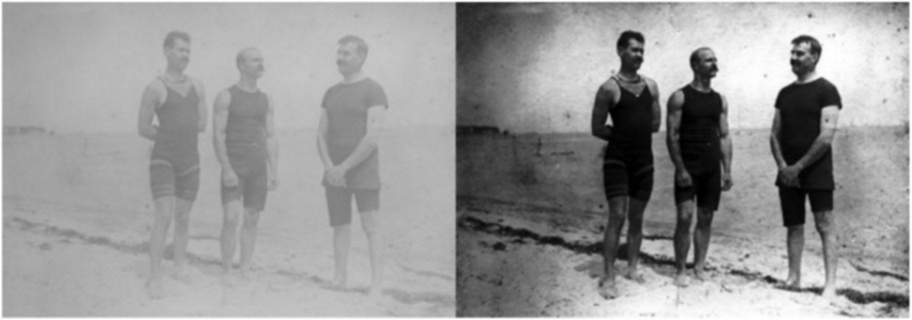
The quantile normalization (QN) embedding

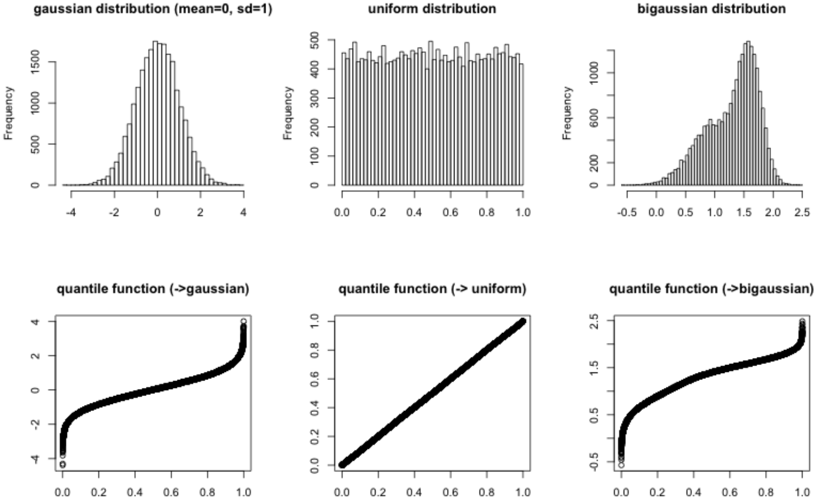


- Fix a target quantile $f \in \mathbb{R}^n$
- Define $\Phi_f : \mathbb{S}_n \to \mathbb{R}^n$ by

$$\forall \sigma \in \mathbb{S}_n , \quad [\Phi_f(\sigma)]_i = f_{\sigma(i)}$$

- "Keep the order, change the values"

How to choose a "good" target distribution?



gaussian distribution (mean=0, sd=1)

uniform distribution

bigaussian distribution

quantile function (->gaussian)

quantile function (-> uniform)

quantile function (->bigaussian)

SUQUAN (Le Morvan and Vert, 2017)

Standard QN:

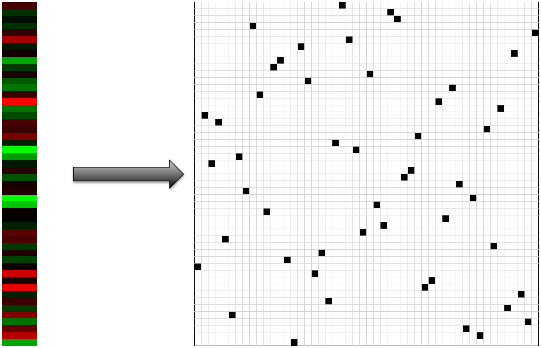
1. Fix f arbitrarily
2. QN all samples to get $\Phi_f(\sigma_1), \ldots, \Phi_f(\sigma_N)$
3. Learn a model on normalized data, e.g.:

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

Supervised QN (SUQUAN): jointly learn f and the model:

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

Computing $\Phi_f(\sigma)$



For $\sigma \in \mathbb{S}_n$ let the permutation representation (Serres, 1977):

$$[\Pi_\sigma]_{ij} = \begin{cases} 1 & \text{if } \sigma(j) = i\,, \\ 0 & \text{otherwise.} \end{cases}$$

Then

$$\Phi_f(\sigma) = \Pi_\sigma^\top f$$

Linear SUQAN as rank-1 matrix regression

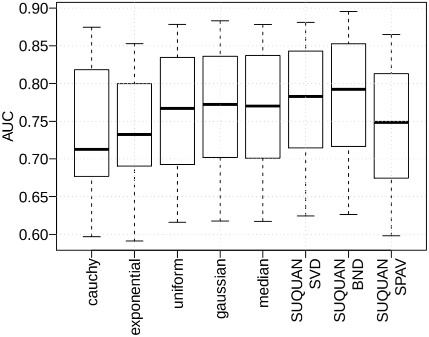
- Linear SUQAN therefore solves

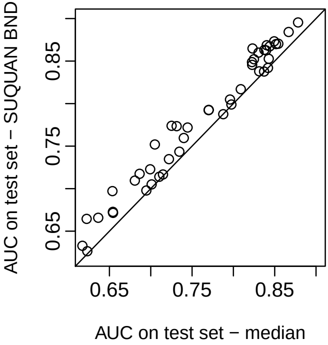
$$
\begin{aligned}
&\min_{w,b,f} \left\{ \frac{1}{N} \sum_{i=1}^{N} \ell_i \left(w^\top \Phi_f(\sigma_i) + b \right) + \lambda \Omega(w) + \gamma \Omega_2(f) \right\} \\
&= \min_{w,b,f} \left\{ \frac{1}{N} \sum_{i=1}^{N} \ell \left(w^\top \Pi_{\sigma_i}^\top f + b \right) + \lambda \Omega(w) + \gamma \Omega_2(f) \right\} \\
&= \min_{w,b,f} \left\{ \frac{1}{N} \sum_{i=1}^{N} \ell \left(< \Pi_{\sigma_i}, fw^\top >_{\text{Frobenius}} + b \right) + \lambda \Omega(w) + \gamma \Omega_2(f) \right\}
\end{aligned}
$$

- A particular linear model to estimate a rank-1 matrix $M = fw^\top$
- Each sample $\sigma \in \mathbb{S}_n$ is represented by the matrix $\Pi_\sigma \in \mathbb{R}^{n\times n}$
- Non-convex
- Alternative optimization of f and w is easy

Experiments: CIFAR-10

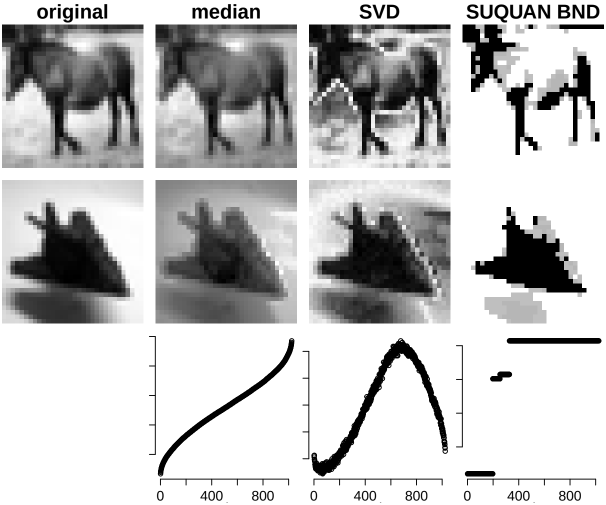
- Image classification into 10 classes (45 binary problems)
- $N = 5,000$ per class, $p = 1,024$ pixels





Experiments: CIFAR-10

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

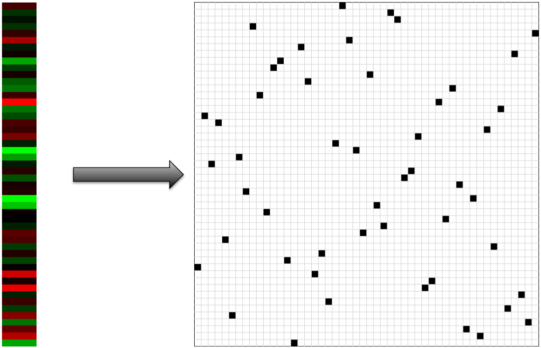


Outline

1. The QN embedding

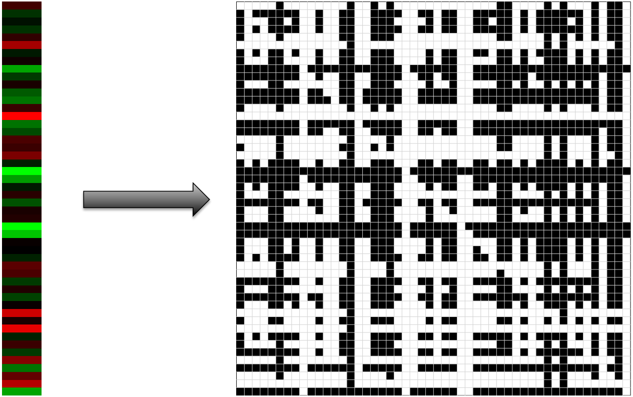
2. The Kendall embedding

Limits of the QN embedding



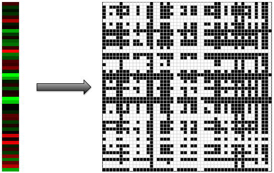
- Linear model on $\Phi(\sigma) = \Pi_\sigma \in \mathbb{R}^{n \times n}$
- Captures first-order information of the form "*i-th feature ranked at the j-th position*"
- What about higher-order information such as "*feature i larger than feature j*"?

Another representation



$$\Phi_{i,j}(\sigma) = \begin{cases} 1 & \text{if } \sigma(i) < \sigma(j)\,, \\ 0 & \text{otherwise.} \end{cases}$$

Geometry of the embedding



For any two permutations $\sigma, \sigma' \in \mathbb{S}_n$:

- Inner product

$$\Phi(\sigma)^\top \Phi(\sigma') = \sum_{1 \leq i \neq j \leq n} \mathbb{1}_{\sigma(i)<\sigma(j)} \mathbb{1}_{\sigma'(i)<\sigma'(j)} = n_c(\sigma, \sigma')$$

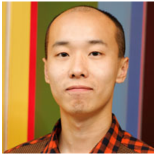
  n_c = number of concordant pairs

- Distance

$$\| \Phi(\sigma) - \Phi(\sigma') \|^2 = \sum_{1 \leq i,j \leq n} (\mathbb{1}_{\sigma(i)<\sigma(j)} - \mathbb{1}_{\sigma'(i)<\sigma'(j)})^2 = 2n_d(\sigma, \sigma')$$

  n_d = number of discordant pairs

Kendall and Mallows kernels (Jiao and Vert, 2017)



- The Kendall kernel is

$$K_\tau(\sigma, \sigma') = n_c(\sigma, \sigma')$$

- The Mallows kernel is

$$\forall \lambda \geq 0 \quad K_M^\lambda(\sigma, \sigma') = e^{-\lambda n_d(\sigma, \sigma')}$$

Theorem (Jiao and Vert, 2015, 2017)

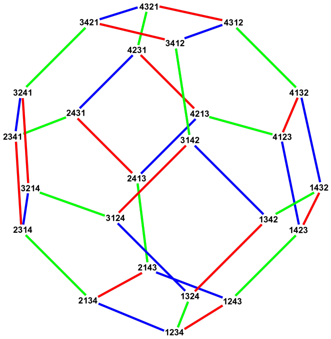
The Kendall and Mallows kernels are positive definite.

Theorem (Knight, 1966)

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

Kernel trick useful with few samples in large dimensions

Related work



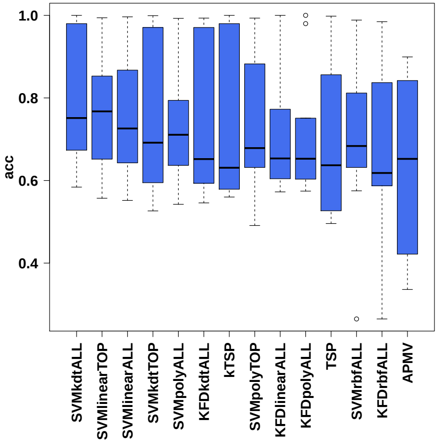
Cayley graph of $\mathbb{S}_4$

- Kondor and Barbarosa (2010) proposed the diffusion kernel on the Cayley graph of the symmetric group generated by adjacent transpositions.
- Computationally intensive ($O(n^{2n})$)
- Mallows kernel is written as

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

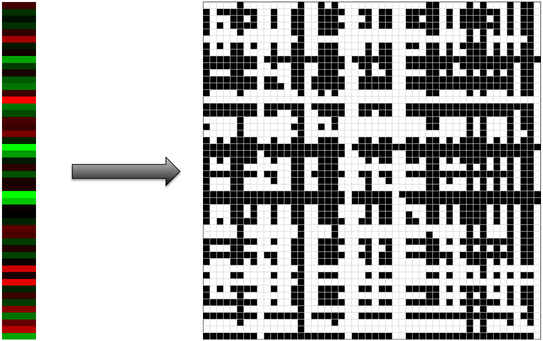
  where $n_d(\sigma, \sigma')$ is the shortest path distance on the Cayley graph.
- It can be computed in $O(n \log n)$

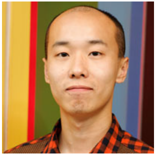
Applications



Average performance on 10 microarray classification problems (Jiao and Vert, 2017).

Extension: weighted Kendall kernel?





- Can we weight differently pairs based on their ranks?
- This would ensure a right-invariant kernel, i.e., the overall geometry does not change if we relabel the items

$$\forall \sigma_1, \sigma_2, \pi \in \mathbb{S}_n\,, \quad K(\sigma_1\pi, \sigma_2\pi) = K(\sigma_1, \sigma_2)$$

Related work

- Given a weight function $w : [1, n]^2 \to \mathbb{R}$, many weighted versions of the Kendall's τ have been proposed:

$$\sum_{1 \leq i \neq j \leq n} w(\sigma(i), \sigma(j)) \mathbb{1}_{\sigma(i) < \sigma(j)} \mathbb{1}_{\sigma'(i) < \sigma'(j)}$$

Shieh (1998)

$$\sum_{1 \leq i \neq j \leq n} w(\sigma(i), \sigma(j)) \frac{p_{\sigma(i)} - p_{\sigma'(i)}}{\sigma(i) - \sigma'(i)} \frac{p_{\sigma(j)} - p_{\sigma'(j)}}{\sigma(j) - \sigma'(j)} \mathbb{1}_{\sigma(i) < \sigma(j)} \mathbb{1}_{\sigma'(i) < \sigma'(j)}$$

Kumar and Vassilvitskii (2010)

$$\sum_{1 \leq i \neq j \leq n} w(i, j) \mathbb{1}_{\sigma(i) < \sigma(j)} \mathbb{1}_{\sigma'(i) < \sigma'(j)}$$

Vigna (2015)

- However, they are either not symmetric (1st and 2nd), or not right-invariant (3rd)

A right-invariant weighted Kendall kernel (Jiao and Vert, 2018)

Theorem

Let $W : \mathbb{N}^2 \times \mathbb{N}^2 \to \mathbb{R}$ *be a p.d. kernel on* $\mathbb{N}^2$, *then*

$$K_W(\sigma, \sigma') = \sum_{1 \leq i \neq j \leq n} W\left((\sigma(i), \sigma(j)), (\sigma'(i), \sigma'(j))\right) \mathbb{1}_{\sigma(i)<\sigma(j)} \mathbb{1}_{\sigma'(i)<\sigma'(j)}$$

is a right-invariant p.d. kernel on $\mathbb{S}_n$.

Corollary

For any matrix $U \in \mathbb{R}^{n \times n}$,

$$K_U(\sigma, \sigma') = \sum_{1 \leq i \neq j \leq n} U_{\sigma(i),\sigma(j)} U_{\sigma'(i),\sigma'(j)} \mathbb{1}_{\sigma(i)<\sigma(j)} \mathbb{1}_{\sigma'(i)<\sigma'(j)} \,,$$

is a right-invariant p.d. kernel on $\mathbb{S}_n$.

A right-invariant weighted Kendall kernel (Jiao and Vert, 2018)

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is a right-invariant p.d. kernel on $\mathbb{S}_n$.

Examples

$U_{a,b}$ corresponds to the weight of (items ranked at) positions a and b in a permutation. Interesting choices include:

- *Top-k.* For some $k \in [1, n]$,

$$U_{a,b} = \begin{cases} 1 & \text{if } a \leq k \text{ and } b \leq k\,, \\ 0 & \text{otherwise.} \end{cases}$$

- *Additive.* For some $u \in \mathbb{R}^n$, take

$$U_{ij} = u_i + u_j$$

- *Multiplicative.* For some $u \in \mathbb{R}^n$, take

$$U_{ij} = u_i u_j$$

Theorem (Kernel trick)

The weighted Kendall kernel can be computed in $O(n \ln(n))$ for the top-k, additive or multiplicative weights.

Learning the weights (1/2)

- K_U can be written as

$$K_U(\sigma, \sigma') = \Phi_U(\sigma)^\top \Phi_U(\sigma')$$

  with

$$\Phi_U(\sigma) = \left(U_{\sigma(i),\sigma(j)} \mathbb{1}_{\sigma(i)<\sigma(j)}\right)_{1 \leq i \neq j \leq n}$$

- Interesting fact: For any upper triangular matrix $U \in \mathbb{R}^{n \times n}$,

$$\Phi_U(\sigma) = \Pi_\sigma^\top U \Pi_\sigma \quad \text{with} \;\; (\Pi_\sigma)_{ij} = \mathbb{1}_{i=\sigma(j)}$$

- Hence a linear model on Φ_U can be rewritten as

$$\begin{aligned} f_{\beta,U}(\sigma) &= \langle \beta, \Phi_U(\sigma) \rangle_{\text{Frobenius}(n \times n)} \\ &= \left\langle \beta, \Pi_\sigma^\top U \Pi_\sigma \right\rangle_{\text{Frobenius}(n \times n)} \\ &= \left\langle \Pi_\sigma \otimes \Pi_\sigma, \text{vec}(U) \otimes (\text{vec}(\beta))^\top \right\rangle_{\text{Frobenius}(n^2 \times n^2)} \end{aligned}$$

Learning the weights (2/2)

$$f_{\beta,U}(\sigma) = \left\langle \Pi_\sigma \otimes \Pi_\sigma, \mathrm{vec}(U) \otimes (\mathrm{vec}(\beta))^\top \right\rangle_{\mathrm{Frobenius}(n^2 \times n^2)}$$

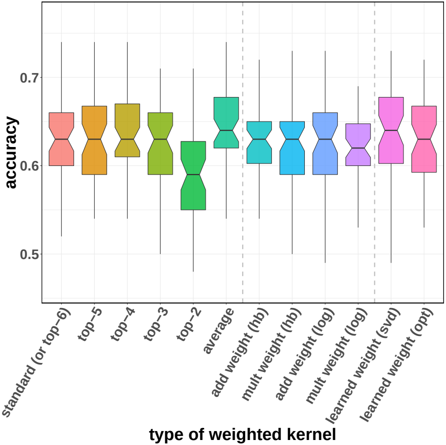
- This is symmetric in U and β
- Instead of fixing the weights U and optimizing β, we can jointly optimize β and U to learn the weights U
- Note that $\Pi_\sigma^\top = (\Pi_\sigma)^{-1} = \Pi_{\sigma^{-1}}$, hence

$$f_{\beta,U}(\sigma) = f_{U,\beta}(\sigma^{-1})$$

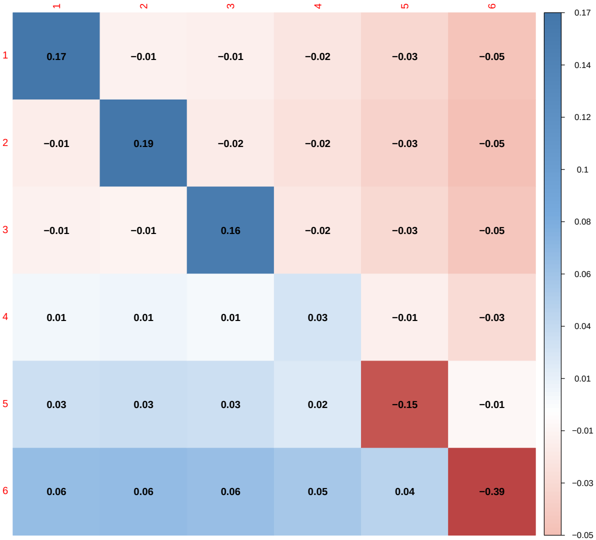
- We propose to alternate optimization in U and β
  - For U fixed, optimize β with $K_U(\sigma_1, \sigma_2)$
  - For β fixed, optimize U with $K_\beta(\sigma_1^{-1}, \sigma_2^{-1})$

Experiments

- Eurobarometer data (Christensen, 2010)
- >12k individuals rank 6 sources of information
- Binary classification problem: predict age from ranking (>40y vs <40y)



Weights learned



	1	2	3	4	5	6
1	0.17	−0.01	−0.01	−0.02	−0.03	−0.05
2	−0.01	0.19	−0.02	−0.02	−0.03	−0.05
3	−0.01	−0.01	0.16	−0.02	−0.03	−0.05
4	0.01	0.01	0.01	0.03	−0.01	−0.03
5	0.03	0.03	0.03	0.02	−0.15	−0.01
6	0.06	0.06	0.06	0.05	0.04	−0.39

Towards higher-order representations

$$f_{\beta,U}(\sigma) = \left\langle \Pi_\sigma \otimes \Pi_\sigma, \mathrm{vec}(U) \otimes (\mathrm{vec}(\beta))^\top \right\rangle_{\mathrm{Frobenius}(n^2 \times n^2)}$$

- A particular rank-1 linear model for the embedding

$$\Sigma_\sigma = \Pi_\sigma \otimes \Pi_\sigma \in (\{0,1\})^{n^2 \times n^2}$$

- Σ is the direct sum of the second-order and first-order permutation representations:

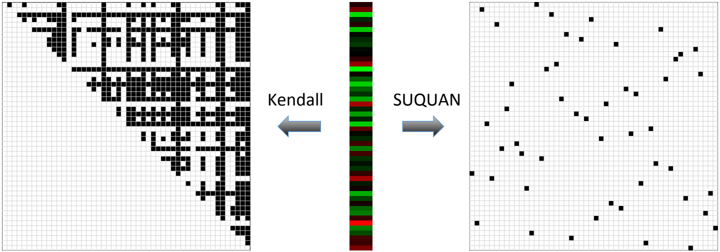
$$\Sigma \cong \tau_{(n-2,1,1)} \oplus \tau_{(n-1,1)}$$

- This generalizes SUQUAN which considers the first-order representation Π_σ only:

$$h_{\beta,w}(\sigma) = \left\langle \Pi_\sigma, w \otimes \beta^\top \right\rangle_{\mathrm{Frobenius}(n \times n)}$$

- Generalization possible to higher-order information by using higher-order linear representations of the symmetric group, which are the good basis for right-invariant kernels (Bochner theorem)...

Conclusion



- Machine learning beyond vectors, strings and graphs
- Different embeddings of the symmetric group
- Respect the group structure (right-invariance) through group representations
- Compatible with NN architectures
- Scalability? Approximate embeddings?

Thanks

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SEVENTH FRAMEWORK PROGRAMME

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Constraints on f

- Ridge

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

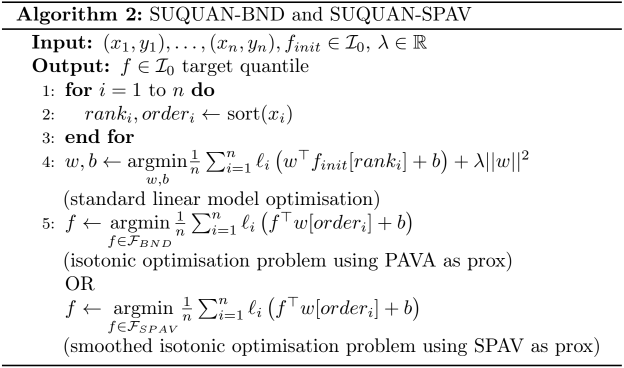
- Non-decreasing

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

- 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
for $i = 1$ to $n$ do
    $rank_i, order_i \leftarrow \mathrm{sort}(x_i)$
end for
$w, b \leftarrow \underset{w,b}{\operatorname{argmin}} \frac{1}{n} \sum_{i=1}^{n} \ell_i \left( w^\top f_{init}[rank_i] + b \right) + \lambda ||w||^2$
(standard linear model optimisation)
$f \leftarrow \underset{f \in \mathcal{F}_{BND}}{\operatorname{argmin}} \frac{1}{n} \sum_{i=1}^{n} \ell_i \left( f^\top w[order_i] + b \right)$
(isotonic optimisation problem using PAVA as prox)
OR
$f \leftarrow \underset{f \in \mathcal{F}_{SPAV}}{\operatorname{argmin}} \frac{1}{n} \sum_{i=1}^{n} \ell_i \left( f^\top w[order_i] + b \right)$
(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
$M_{LDA} \leftarrow 0 \in \mathbb{R}^{p \times p}$
$n_{+1} \leftarrow |\{i : y_i = +1\}|$
$n_{-1} \leftarrow |\{i : y_i = -1\}|$
for $i = 1$ to $n$ do
    Compute $\Pi_{x_i}$ (by sorting $x_i$)
    $M_{LDA} \leftarrow M_{LDA} + \frac{y_i}{n_{y_i}} \Pi_{x_i}$
end for
$(\sigma, w, f) \leftarrow SVD(M_{LDA}, 1)$
```

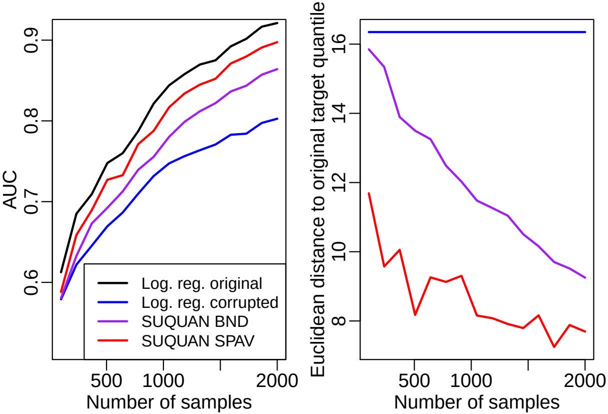
- Ridge penalty (no monotonicity constraint), equivalent to rank-1 regression problem
- SVD finds the closest rank-1 matrix to the LDA solution:

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

- 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.


AUC
Number of samples
Log. reg. original
Log. reg. corrupted
SUQUAN BND
SUQUAN SPAV
Euclidean distance to original target quantile
Number of samples