Differentiable ranking and sorting

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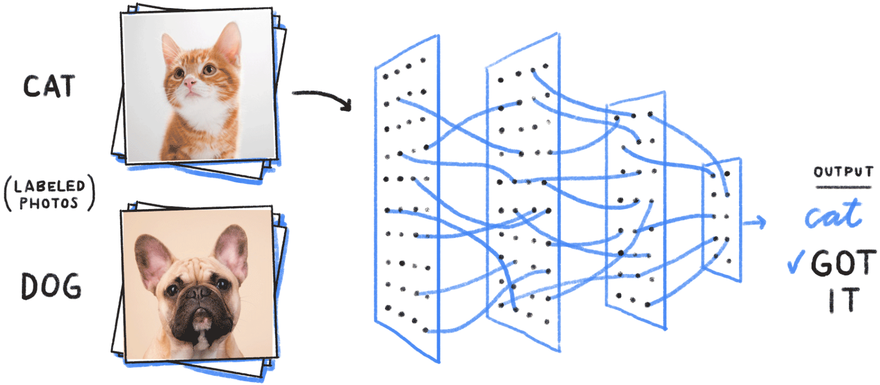
Outline

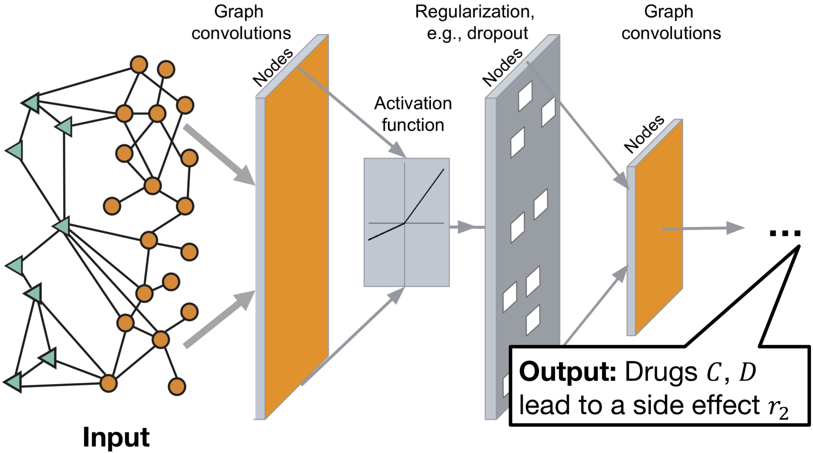
Outline

Differentiable programming



https://codeburst.io/machine-learning-243cc92247a1

Going beyond vectors (strings, graphs...)



http://snap.stanford.edu/decagon

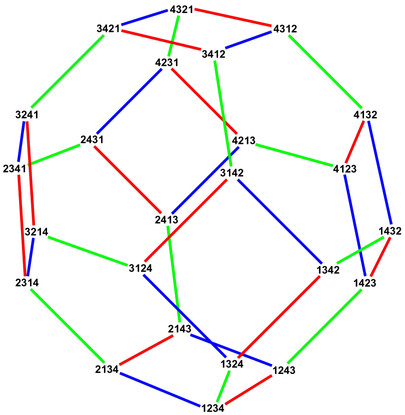
What about rankings / permutations?

- Some data are permutations (input, output)

- Some operations may involve ranking

(histogram equalization, quantile normalization...)

More formally



- 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
- $|\mathbb{S}_N| = N!$

Goal

$$\begin{tikzcd} \mathbb{R}^N \arrow[r, "\texttt{argsort}"] \arrow[rr, bend right, "\texttt{differentiate}"'] & \mathbb{S}_N \arrow[r, "\texttt{embed}"] & \mathbb{R}^p \end{tikzcd}$$

1. Embed
   - To define / optimize $f_\theta(\sigma) = g_\theta(\text{embed}(\sigma))$ for $\sigma \in \mathbb{S}_N$
   - E.g., σ given as input, or output
2. Differentiate
   - To define / optimize $h_\theta(x) = f_\theta(\text{argsort}(x))$ for $x \in \mathbb{R}^n$
   - E.g., normalization layer or rank-based loss

Outline

Argmax

$$\operatorname{argmax} \begin{pmatrix} 2.1 \\ -0.4 \\ 5.7 \end{pmatrix} = 3$$

is not differentiable because:

- As a function $\mathbb{R}^n \to [1, n]$, the output space is not continuous
- It is piecewise constant (ie, gradient=0 almost everywhere even if the output space was continuous, eg, $(1, n) \subset \mathbb{R}$)

Softmax

$$\text{softmax}_1 \begin{pmatrix} 2.1 \\ -0.4 \\ 5.7 \end{pmatrix} = \begin{pmatrix} 0.027 \\ 0.002 \\ 0.971 \end{pmatrix}$$

is a differentiable function $\mathbb{R}^n \to \mathbb{R}^n$, where

$$\text{softmax}_\epsilon(x)_i = \frac{e^{x_i/\epsilon}}{\sum_{j=1}^n e^{x_j/\epsilon}}$$

From Softmax to Argmax

$$\lim_{\epsilon \to 0} \text{softmax}_\epsilon \begin{pmatrix} 2.1 \\ -0.4 \\ 5.7 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \Psi\,(3)\ ,$$

where $\Psi : [1, n] \to \mathbb{R}^n$ is the one-hot encoding. More generally,

$$\forall x \in \mathbb{R}^n, \quad \lim_{\epsilon \to 0} \text{softmax}_\epsilon(x) = \Psi(\operatorname{argmax}(x))$$

$$\begin{tikzcd}
\mathbb{R}^n \arrow[r, "\texttt{argmax}"] \arrow[rr, bend right, "\texttt{softmax}"'] & {[1, n]} \arrow[r, "\texttt{one-hot}"] & \mathbb{R}^n
\end{tikzcd}$$

From Argmax to Softmax (1): embedding

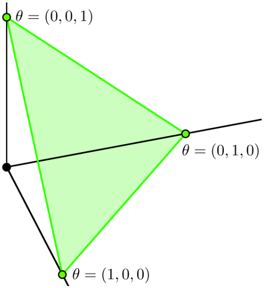
$$\mathbb{R}^n \xrightarrow{\texttt{argmax}} [1, n] \xrightarrow{\texttt{one-hot}} \mathbb{R}^n$$

Let the simplex

$$\Delta_{n-1} = \mathrm{conv}\left(\{\Psi(y) \,:\, y \in [1, n]\}\right)$$

Then we have a variational characterization (*exercice*):

$$\Psi(\mathrm{argmax}\,(x)) = \underset{z \in \Delta_{n-1}}{\mathrm{argmax}}\,(x^\top z)$$

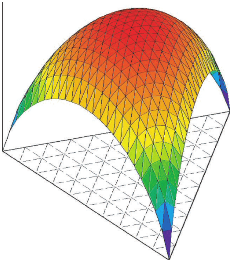


From Argmax to Softmax (2a): regularization

$$\begin{tikzcd} \mathbb{R}^n \arrow[r, "\texttt{argmax}"] \arrow[rr, bend right, "\texttt{softmax}"'] & {[1, n]} \arrow[r, "\texttt{one-hot}"] & \mathbb{R}^n \end{tikzcd}$$

Let the entropy $H(z) = -\sum_{i=1}^{n} z_i \ln(z_i)$ for $z_i \in \Delta_{n-1}$.
Then we have (*exercice*):

$$\mathrm{softmax}_{\epsilon}(x) = \underset{z \in \Delta_{n-1}}{\mathrm{argmax}} \left[x^{\top} z + \epsilon H(z) \right]$$

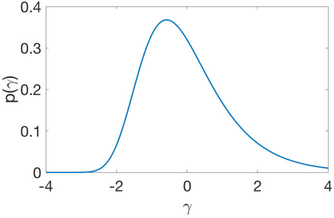


From Argmax to Softmax (2b): perturbation

$$\begin{tikzcd} \mathbb{R}^n \arrow[r, "\texttt{argmax}"] \arrow[rr, bend right, "\texttt{softmax}"'] & {[1,n]} \arrow[r, "\texttt{one-hot}"] & \mathbb{R}^n \end{tikzcd}$$

Let $G = (G_1, \ldots, G_n)$ be i.i.d. Gumbel(0,1) random variables[1] Then we have (*exercice*):

$$\mathrm{softmax}_\epsilon(x) = E \operatorname*{argmax}_{z \in \Delta_{n-1}} \left[(x + \epsilon G)^\top z \right]$$



[1] $G_i = -\ln(-ln(U_i))$ where $U_i \sim \mathrm{unif}(0, 1)$

From Argmax to Softmax: summary

$$\begin{tikzcd}
\mathbb{R}^n \arrow[r, "\texttt{argmax}"] \arrow[rr, bend right, "\texttt{softmax}"'] & {[1, n]} \arrow[r, "\texttt{one-hot}"] & \mathbb{R}^n
\end{tikzcd}$$

1. Embed, such that

$$\Psi(\operatorname{argmax}(x)) = \operatorname*{argmax}_{z \in \Delta_{n-1}} (x^\top z)$$

2. Regularize or perturb:

$$\text{softmax}_\epsilon(x) = \operatorname*{argmax}_{z \in \Delta_{n-1}} \left[x^\top z + \epsilon H(z) \right] = E \operatorname*{argmax}_{z \in \Delta_{n-1}} \left[x^\top (z + \epsilon G) \right]$$

Both lead to efficient (stochastic) Jacobian estimates.
Can we generalize this to other discrete operations, such as ranking?

Outline

How to define an embedding $\Phi : \mathbb{S}_N \to \mathbb{R}^p$?

$$\begin{tikzcd}
\mathbb{R}^N \arrow[r, "\texttt{argsort}"] \arrow[rr, bend right, "\texttt{differentiate}"'] & \mathbb{S}_N \arrow[r, "\texttt{embed}"] & \mathbb{R}^p
\end{tikzcd}$$

- Should encode interesting features
- Should lead to efficient algorithms

- Geometry should not change by arbitrary renaming of items, i.e.,

$$\forall \sigma_1, \sigma_2, \pi \in \mathbb{S}_N\,, \quad \| \Phi(\sigma_1 \pi) - \Phi(\sigma_2 \pi) \| = \| \Phi(\sigma_1) - \Phi(\sigma_2) \|$$

- Equivalently, the kernel should be translation-invariant

$$\forall \sigma_1, \sigma_2 \in \mathbb{S}_N\,, \quad K(\sigma_1, \sigma_2) = < \Phi(\sigma_1), \Phi(\sigma_2) > = \kappa(\sigma_1 \sigma_2^{-1})$$

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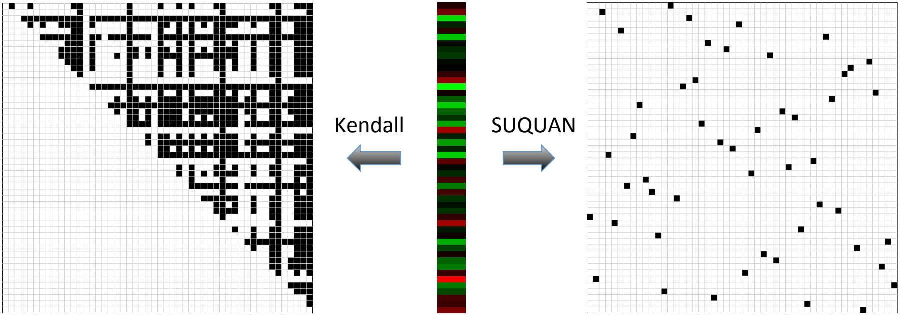
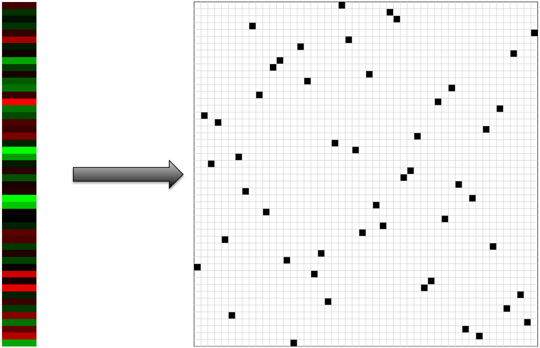
Some attempts



(Jiao and Vert, 2015, 2017, 2018; Le Morvan and Vert, 2017)

Outline

SUQUAN embedding (Le Morvan and Vert, 2017)



- Let $\Phi(\sigma) = \Pi_\sigma$ the permutation representation (Serres, 1977):

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

- Right invariant:

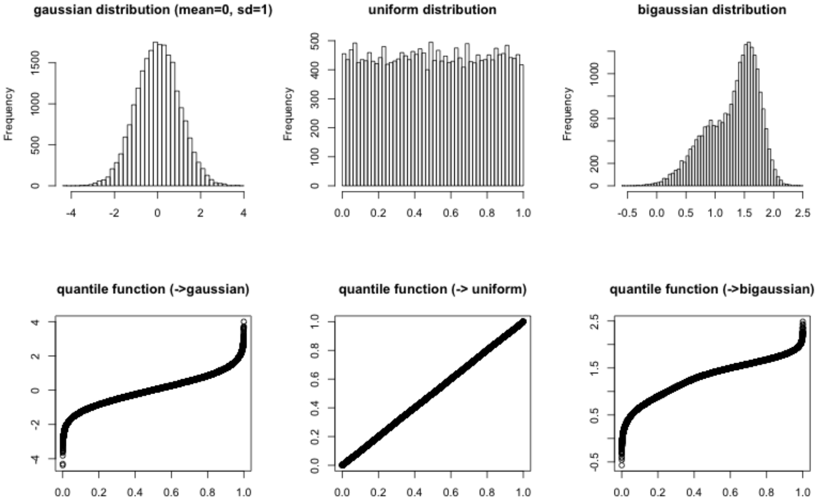
$$< \Phi(\sigma), \Phi(\sigma') >= \mathrm{Tr}\left(\Pi_\sigma \Pi_{\sigma'}^\top\right) = \mathrm{Tr}\left(\Pi_\sigma \Pi_{\sigma'}^{-1}\right) = \mathrm{Tr}\left(\Pi_\sigma \Pi_{\sigma'^{-1}}\right) = \mathrm{Tr}\left(\Pi_{\sigma\sigma'^{-1}}\right)$$

Link with quantile normalization (QN)

- Take $\sigma(x) = \mathtt{rank}(x)$ with $x \in \mathbb{R}^N$
- Fix a target quantile $f \in \mathbb{R}^n$
- "Keep the order of x, change the values to f"

$$[\Psi_f(x)]_i = f_{\sigma(x)(i)} \quad \Leftrightarrow \quad \Psi_f(x) = \Pi_{\sigma(x)}^\top f$$

How to choose a "good" target distribution?



Supervised QN (SUQUAN)

Standard QN:

1. Fix f arbitrarily
2. QN all samples to get $\Psi_f(x_1), \ldots, \Psi_f(x_N)$
3. Learn a model on normalized data, e.g.:

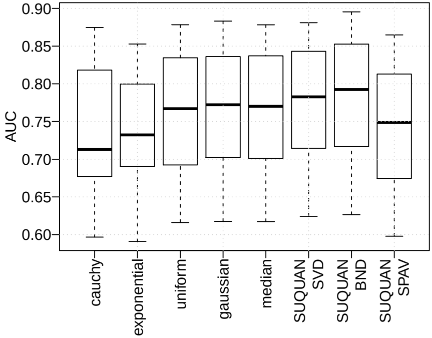
$$\min_{\theta} \left\{ \frac{1}{N} \sum_{i=1}^{N} \ell_i \left(f_\theta(\Psi_f(x_i)) \right) \right\}$$

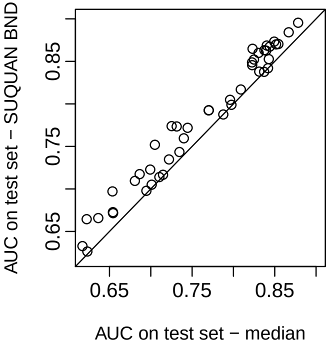
SUQUAN: jointly learn f and the model:

$$\min_{\theta, f} \left\{ \frac{1}{N} \sum_{i=1}^{N} \ell_i \left(f_\theta(\Psi_f(x_i)) \right) \right\} = \min_{\theta, f} \left\{ \frac{1}{N} \sum_{i=1}^{N} \ell_i \left(f_\theta(\Pi_{\sigma(x_i)}^\top f) \right) \right\}$$

Experiments: CIFAR-10

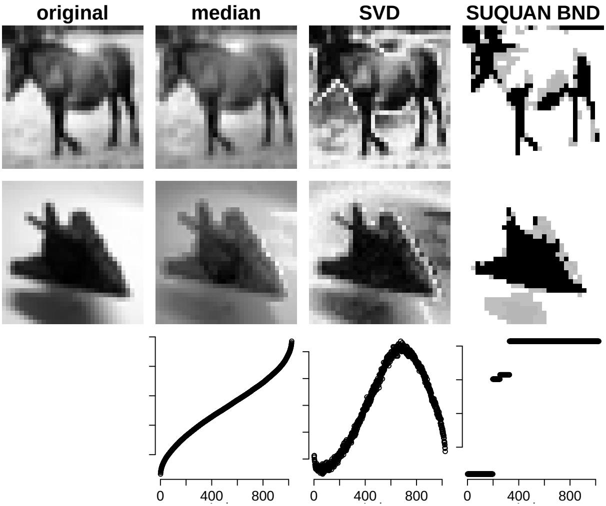
- Image classification into 10 classes (45 binary problems)
- $N = 5,000$ per class, $p = 1,024$ pixels
- Linear logistic regression on raw pixels



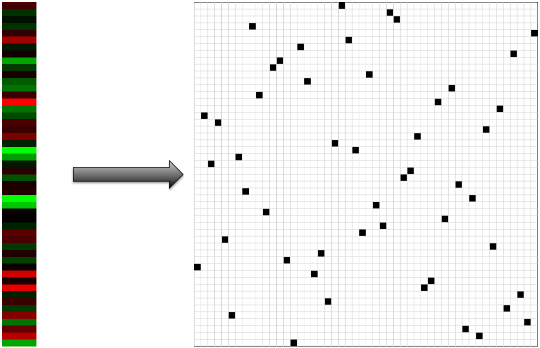


Experiments: CIFAR-10

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



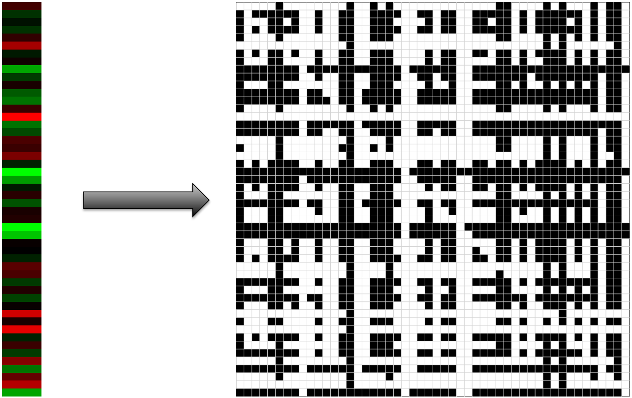
Limits of the SUQUAN embedding



- 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*"?

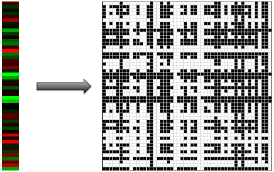
Outline

The Kendall embedding (Jiao and Vert, 2015, 2017)



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

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

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

  n_d = number of discordant pairs

Kendall and Mallows kernels

- The Kendall kernel is

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

- The Mallows kernel is

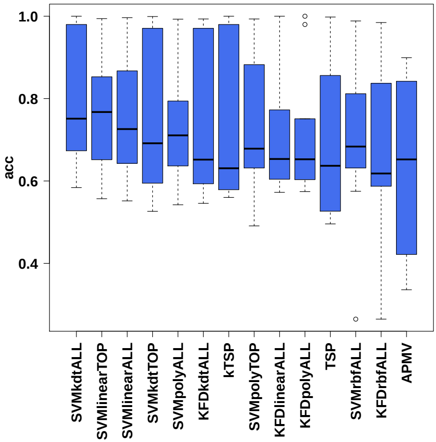
$$\forall \lambda \geq 0 \quad K_M^\lambda(\sigma, \sigma') = e^{-\lambda n_d(\sigma, \sigma')}$$

Theorem (Jiao and Vert, 2015, 2017)

The Kendall and Mallows kernels are positive definite right-invariant kernels and can be evaluated in $O(N \log N)$ time

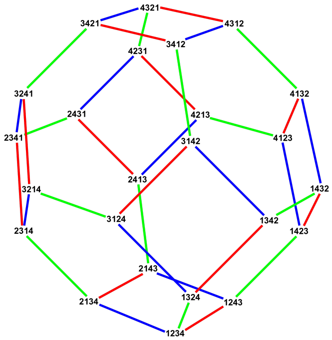
Kernel trick useful with few samples in large dimensions

Applications



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

Remark



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 $O(N \log N)$
- Extension to weighted Kendall kernel (Jiao and Vert, 2018)

Remark

The SUQUAN and Kendall representations are two particular cases of the more general

Bochner's theorem

An embedding $\Phi : \mathbb{S}_N \to \mathbb{R}^p$ defines a right-invariant kernel $K(\sigma_1, \sigma_2) = \Phi(\sigma_1)^\top \Phi(\sigma_2)$ if and only there exists $\phi : \mathbb{S}_N \to \mathbb{R}$ such that

$$\forall \sigma_1, \sigma_2 \in \mathbb{S}_N \,, \quad K(\sigma_1, \sigma_2) = \phi(\sigma_2^{-1}\sigma_1)$$

and

$$\forall \lambda \in \Lambda \,, \quad \hat{\phi}(\rho_\lambda) \succeq 0$$

where for any $f : \mathbb{S}_N \to \mathbb{R}$, the Fourier transform of f is

$$\forall \lambda \in \Lambda \,, \quad \hat{f}(\rho_\lambda) = \sum_{\sigma \in \mathbb{S}_N} f(\sigma) \rho_\lambda(\sigma)$$

with $\{\rho_\lambda \ : \ \lambda \in \Lambda\}$ the irreductible representations of the symmetric group.

Outline

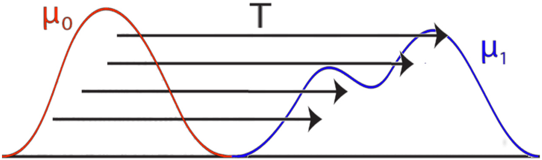
The problem

$$
\begin{tikzcd}
\mathbb{R}^N \arrow[r, "\texttt{argsort}"] \arrow[rr, bend right, "\texttt{differentiate}"'] & \mathbb{S}_N \arrow[r, "\texttt{embed}"] & \mathbb{R}^p
\end{tikzcd}
$$

- $x \in \mathbb{R}^N \mapsto \texttt{argsort}(x) \in \mathbb{S}_N$ is piecewise constant
- Derivative a.e. equal to zero
- Same for $x \mapsto \Phi(\texttt{argsort}(x))$, for any embedding Φ

How to create a differentiable approximation to $\Phi(\texttt{argsort}(x))$?

Optimal transport (OT)

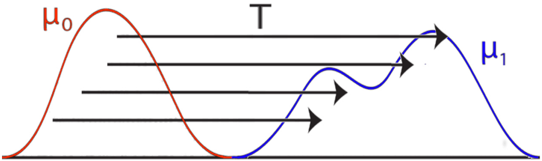


Given a cost matrix $C \in \mathbb{R}^{n \times n}$ (where C_{ij} is the cost of moving the i-th point to the j-th location), OT solves

$$\min_{P \in B_n} \langle P, C \rangle$$

where $B_n = \left\{ P \in \mathbb{R}_+^{n \times n} \,|\, P\mathbf{1}_n = P^\top \mathbf{1}_n = \mathbf{1}_n \right\}$ is the Birkhoff polytope.

Variational formulation of SUQUAN embedding



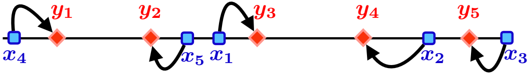
Lemma

Take

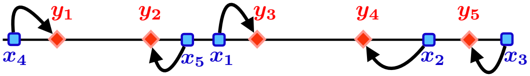
- $y \in \mathbb{R}^n$ *with* $y_1 < \ldots < y_n$,
- $h \in C^2(\mathbb{R}^2)$ *and* $\partial^2 h / \partial x \partial y > 0$ *(eg,* $h(a,b) = (b-a)^2$*).*

For any $x \in \mathbb{R}^n$*, let* $C(x) \in \mathbb{R}^{n \times n}$ *given by* $C(x)_{ij} = h(y_i, x_j)$*. Then*

$$\operatorname*{argmin}_{P \in B_n} \langle P, C(x) \rangle = \Pi_{\sigma(x)} \,.$$



Entropic regularization (Cuturi et al., 2019)



$$P_\epsilon(x) = \underset{P \in B_n}{\operatorname{argmin}} \langle P, C(x) \rangle - \epsilon H(P)$$

Algorithm 1: Sinkhorn

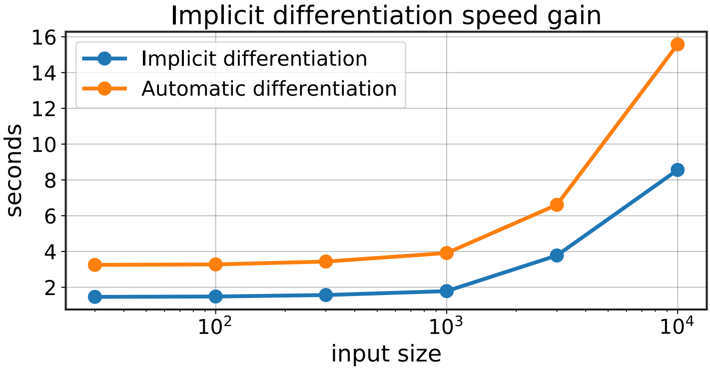
Inputs: $\mathbf{a}, \mathbf{b}, \mathbf{x}, \mathbf{y}, \varepsilon, \ell$
$K \leftarrow e^{-C_{\mathbf{xy}}/\varepsilon}, \mathbf{u}_0 = \mathbf{1}_n;$
for $t \leftarrow 0$ **to** $\ell - 1$ **do**
  $\mathbf{v}_{t+1} \leftarrow \mathbf{b}/K^T \mathbf{u}_t$
  $\mathbf{u}_{t+1} \leftarrow \mathbf{a}/K \mathbf{v}_{t+1}$
end
Result: $\mathbf{u}_\ell, K, \mathbf{v}_\ell$

- $P = \mathrm{diag}(u_\ell) K \mathrm{diag}(v_\ell)$ is the differentiable approximate permutation matrix of the input vector x
- Complexity $O(nm\ell)$, GPU-friendly

Derivatives

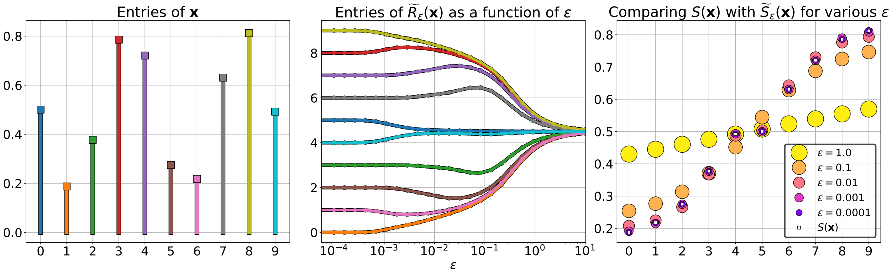
$\nabla P_\epsilon(x)$ can be computed by

- Automatic differentiation of Sinkhorn iterations (Cuturi et al., 2019)
- Implicit differentiation (Cuturi et al., 2020)



Differentiable `sort`, `argsort` and `rank`

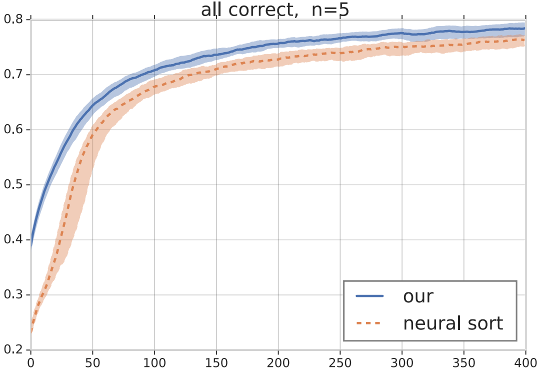
$$S_\epsilon(x) = P_\epsilon(x)x \qquad R_\epsilon(x) = P_\epsilon(x)^\top(1, 2, \ldots, n)^\top$$



https://github.com/google-research/google-research/tree/master/soft_sort

Application: learning to rank

Task: Sort 5 numbers between 0000 and 9999 (concatenation of MNIST digits) (Grover et al, 2019)



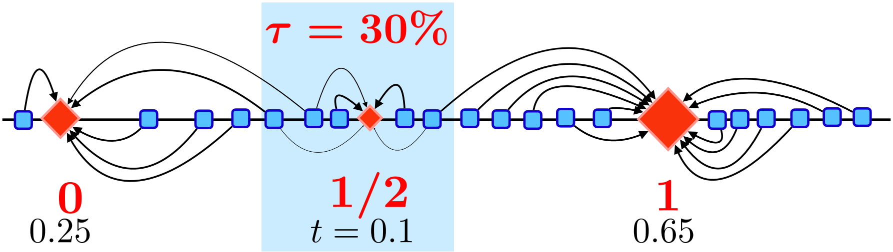
Outline

1. Motivation
2. Warm-up: from argmax to softmax
3. Embed
   - SUQUAN embedding
   - Kendall embedding
4. Differentiate
5. Extensions
   - Differentiable quantiles
   - Matrix factorization with quantile normalization
   - Smoothing by regularization
   - Smoothing by perturbation
   - Extensions to other discrete problems
6. Conclusion

Outline

Soft quantization and soft quantiles

- Take $C(x) \in \mathbb{R}^{m\times n}$ with $m < n$ and
  $B_n = \left\{P \in \mathbb{R}_+^{m\times n} \,|\, P\mathbf{1}_n = \mathbf{b}\,, P^\top \mathbf{1}_m = \mathbf{1}_n\right\}$
- E.g., $m = 3$, $\mathbf{y} = (0, 0.5, 1)$, $\mathbf{b} = (\tau - t/2, t, \tau + t/2)$
- Overall complexity $O(nm\ell)$



Application: soft top-k loss

$$\text{S-top-}k\text{-loss}(f_\theta(\omega_0), l_0) = J_k\left(1 - \left(\widetilde{F}^\ell\left(\frac{\mathbf{1}_L}{L}, f_\theta(\omega); \frac{\mathbf{1}_m}{m}, \mathbf{y}\right)\right)_{l_0}\right)$$

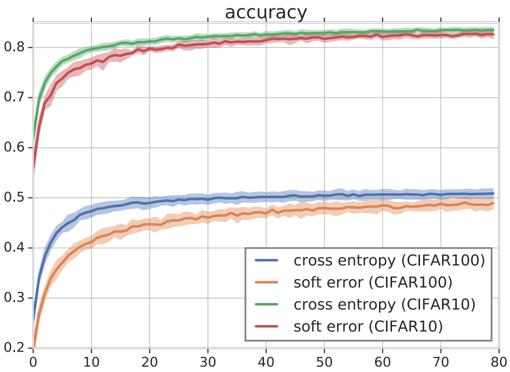
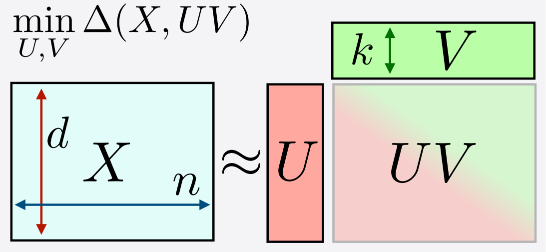


Figure 4: Error bars for test accuracy curves on CIFAR-100 and CIFAR-10 using the same network (averages over 12 runs).

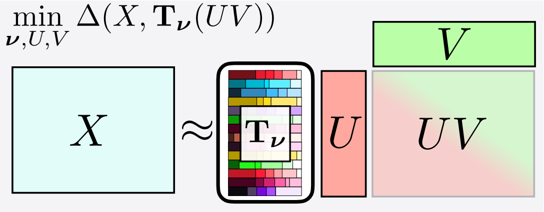
Outline

Nonnegative Matrix Factorization (NMF)

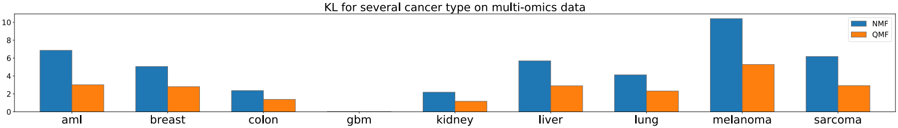


- Useful to decompose a signal as a superposition of basic elements
  - e.g., images, text, genomics...
- But one usually pre-process X so that it resembles a low-rank matrix
  - e.g., tf-idf, log-transform, quantile normalization etc...
- Can we jointly learn U, V and the pre-processing of X?

NMF with quantile normalization (Cuturi et al., 2020)



- T_ν is a *soft-quantile normalization* operator, applied row-wise, differentiable w.r.t. the input row and the target quantiles (generalization of SUQUAN)
- T_ν is optimized jointly with the low-rank matrix *UV*
- Application: multiomics data integration for cancer stratification



Outline

What we have done

$$\begin{tikzcd} \mathbb{R}^N \arrow[r, "\texttt{argsort}"] \arrow[rr, bend right, "\texttt{differentiate}"'] & \mathbb{S}_N \arrow[r, "\texttt{embed}"] & \mathbb{R}^p \end{tikzcd}$$

1. Variational formulation through OT:

$$\Phi(\texttt{argsort}(x)) = \arg\min_{z \in B_n} < z, C(x) >$$

   with $\Phi : \mathbb{S}_N \to \mathbb{R}^{n \times n}$ the SUQUAN embedding

2. Smooth by entropy regularization

$$P_\epsilon(x) = \arg\min_{z \in B_n} [< z, C(x) > -\epsilon H(z)]$$

More general differentiable `argsort`

$$\begin{tikzcd} \mathbb{R}^N \arrow[r, "\texttt{argsort}"] \arrow[rr, bend right, "\texttt{differentiate}"'] & \mathbb{S}_N \arrow[r, "\texttt{embed}"] & \mathbb{R}^p \end{tikzcd}$$

1. Variational formulation: For a given embedding $\Phi : \mathbb{S}_N \to \mathbb{R}^p$, find $\mathcal{Z} \subset \mathbb{R}^p$ and $\Psi : \mathbb{R}^N \to \mathbb{R}^p$ such that

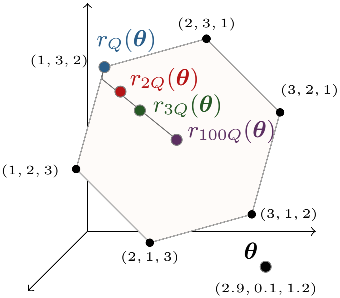
$$\Phi(\texttt{argsort}(x)) = \arg\min_{z \in \mathcal{Z}} < z, \Psi(x) >$$

2. Smooth by regularization

$$h_\epsilon(x) = \arg\min_{z \in \mathcal{Z}} [< z, \Psi(x) > + \epsilon\Omega(z)]$$

with $\Omega : \mathcal{Z} \to \mathbb{R}$ a regularization that makes h_ϵ differentiable

Example: FastSoftSort (Blondel et al., 2020)



- Embed to the permutahedron ($\mathcal{P}_N = B_N \times (1, 2, \ldots, N)^\top$)
- Ranking: $h(x) = \arg\min_{z \in \mathcal{P}_N} < x, z >$
- Regularization by negative entropy or Euclidean norm
- Fast $O(n \log(n))$ algorithm using isotonic regression to project onto the permutahedron and compute $h_\epsilon(x)$ and $\nabla h_\epsilon(x)$

`https://github.com/google-research/fast-soft-sort`

Outline

Reminder: the "Gumbel trick" for soft-max

- For $x \in \mathbb{R}^N$, the one-hot encoded argmax of x is

$$\arg\min_{z \in \Delta^{N-1}} < z, -x >$$

- The soft-max of x is

$$\mathrm{softmax}(x) = e^x / (\sum_i e^{x_i})$$

- It is obtained from the argmax by entropic regularization

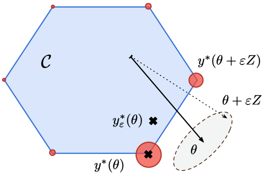
$$\mathrm{softmax}(x) = \arg\min_{z \in \Delta^{N-1}} [< z, -x > -H(z)]$$

- It is also equal to (Gumbel, 1954):

$$\mathrm{softmax}(x) = E\left[\arg\min_{z \in \Delta^{N-1}} < z, -(x + U) >\right]$$

where U is a random variable following the Gumbel distribution.

Smoothing by perturbation (Berthet et al., 2020)

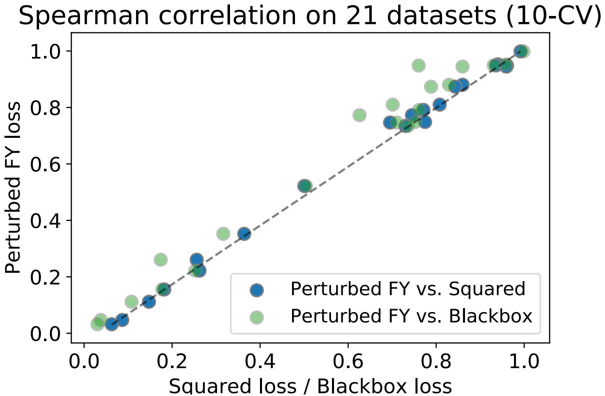


$$h(x) = \arg\min_{z \in \mathcal{Z}} < z, \Psi(x) >$$

$$h_\epsilon(x) = E\left[\arg\min_{z \in \mathcal{Z}} < z, \Psi(x + \epsilon U) >\right]$$

- Generalization of the “Gumbel trick” for soft-max (Gumbel, 1954)
- h_ϵ is differentiable if the density of U is smooth (e.g. normal)
- Stochastic gradient of h_ϵ can be computed efficiently
- Fast gradient for Fenchel-Young losses (Blondel et al., 2019)
- Sometimes equivalent to smoothing by regularization

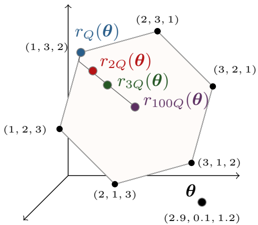
Experiments

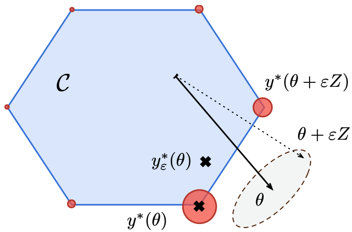


- 21 datasets (simulations and biology) of ranking prediction
- Compare perturbed FY loss on the permutahedron, with squared loss and Blackbox loss of Vlastelica et al. (2020)

Outline

General setting





Given a non-smooth (discrete) mapping $h : \mathbb{R}^n \to \mathbb{R}^p$ with a variational form:

$$h(x) = \left[\arg\min_{z \in \mathcal{Z}} < z, \Psi(x) >\right]$$

create differentiable versions:

$$h_\epsilon^{\text{Regularization}}(x) = \arg\min_{z \in \mathcal{Z}} [< z, \Psi(x) > -\epsilon\Omega(z)]$$

$$h_\epsilon^{\text{Perturbation}}(x) = E\left[\arg\min_{z \in \mathcal{Z}} < z, \Psi(x + \epsilon U) >\right]$$

Example: shortest path (Berthet et al., 2020)

- Take a graph $G = (V, E)$, positive edge costs $c \in \mathbb{R}_+^E$, polytope

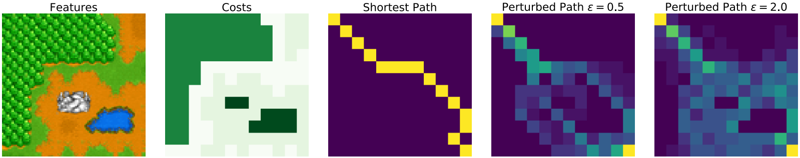
$$\mathcal{C} = \left\{ y \in \mathbb{R}_+^E \;:\; \forall i \in V \,, (\mathbf{1}_{\to i} - \mathbf{1}_{i \to})^\top y = \delta_{i=s} - \delta_{i=t} \right\}$$

- Shortest path (computable in $O(|E|)$ by DP) solves

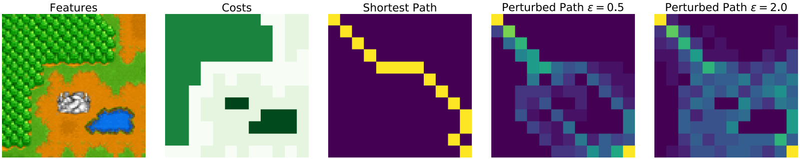
$$y^* = \arg\min_{y \in \mathcal{C}} < c, y >$$

- Differentiable shortest path (w.r.t c):

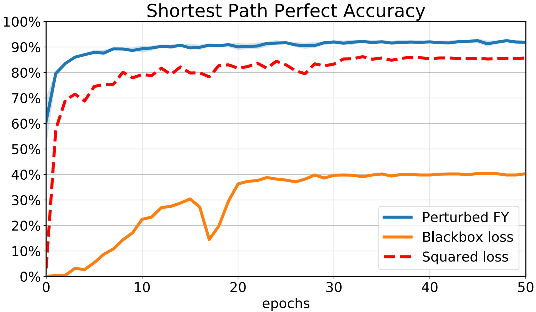
$$y^*_\epsilon = E \left[\arg\min_{y \in \mathcal{C}} < c + \epsilon U, y > \right]$$



(Toy) application



- Given 10k images of Warcraft terrains with 12x12 patches, and a shortest-path from upper-left to lower-right..
- Learn the cost of a patch (with a ResNet18 deep CNN)



Outline

Conclusion

$$\begin{tikzcd} \mathbb{R}^N \arrow[r, "\texttt{argsort}"] \arrow[rr, bend right, "\texttt{differentiate}"'] & \mathbb{S}_N \arrow[r, "\texttt{embed}"] & \mathbb{R}^p \end{tikzcd}$$

- Machine learning beyond vectors, strings and graphs
- Different embeddings of the symmetric group
- Differentiable sorting and ranking through regularization and perturbation
- Can be generalized to other discrete operations

THANK YOU!

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Harmonic analysis on $\mathbb{S}_N$

- A representation of $\mathbb{S}_N$ is a matrix-valued function $\rho : \mathbb{S}_N \to \mathbb{C}^{d_\rho \times d_\rho}$ such that

$$\forall \sigma_1, \sigma_2 \in \mathbb{S}_N\,, \quad \rho(\sigma_1\sigma_2) = \rho(\sigma_1)\rho(\sigma_2)$$

- A representation is irreductible (irrep) if it is not equivalent to the direct sum of two other representations
- $\mathbb{S}_N$ has a finite number of irreps $\{\rho_\lambda \,:\, \lambda \in \Lambda\}$ where $\Lambda = \{\lambda \vdash N\}$[2] is the set of partitions of N
- For any $f : \mathbb{S}_N \to \mathbb{R}$, the Fourier transform of f is

$$\forall \lambda \in \Lambda\,, \quad \hat{f}(\rho_\lambda) = \sum_{\sigma \in \mathbb{S}_N} f(\sigma)\rho_\lambda(\sigma)$$

[2] $\lambda \vdash N$ iff $\lambda = (\lambda_1, \ldots, \lambda_r)$ with $\lambda_1 \geq \ldots \geq \lambda_r$ and $\sum_{i=1}^{r} \lambda_i = N$

Right-invariant kernels

Bochner's theorem

An embedding $\Phi : \mathbb{S}_N \to \mathbb{R}^p$ defines a right-invariant kernel $K(\sigma_1, \sigma_2) = \Phi(\sigma_1)^\top \Phi(\sigma_2)$ if and only there exists $\phi : \mathbb{S}_N \to \mathbb{R}$ such that

$$\forall \sigma_1, \sigma_2 \in \mathbb{S}_N \,, \quad K(\sigma_1, \sigma_2) = \phi(\sigma_2^{-1}\sigma_1)$$

and

$$\forall \lambda \in \Lambda \,, \quad \hat{\phi}(\rho_\lambda) \succeq 0$$