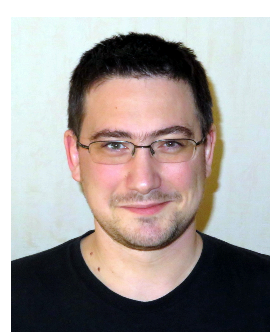
Distributional Reduction: Unifying Dimensionality Reduction and Clustering with Gromov-Wasserstein Projection



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Motivation

Baran *et al. Genome Biology* (2019) 20:206
https://doi.org/10.1186/s13059-019-1812-2

Genome Biology

METHOD Open Access

MetaCell: analysis of single-cell RNA-seq data using *K*-nn graph partitions

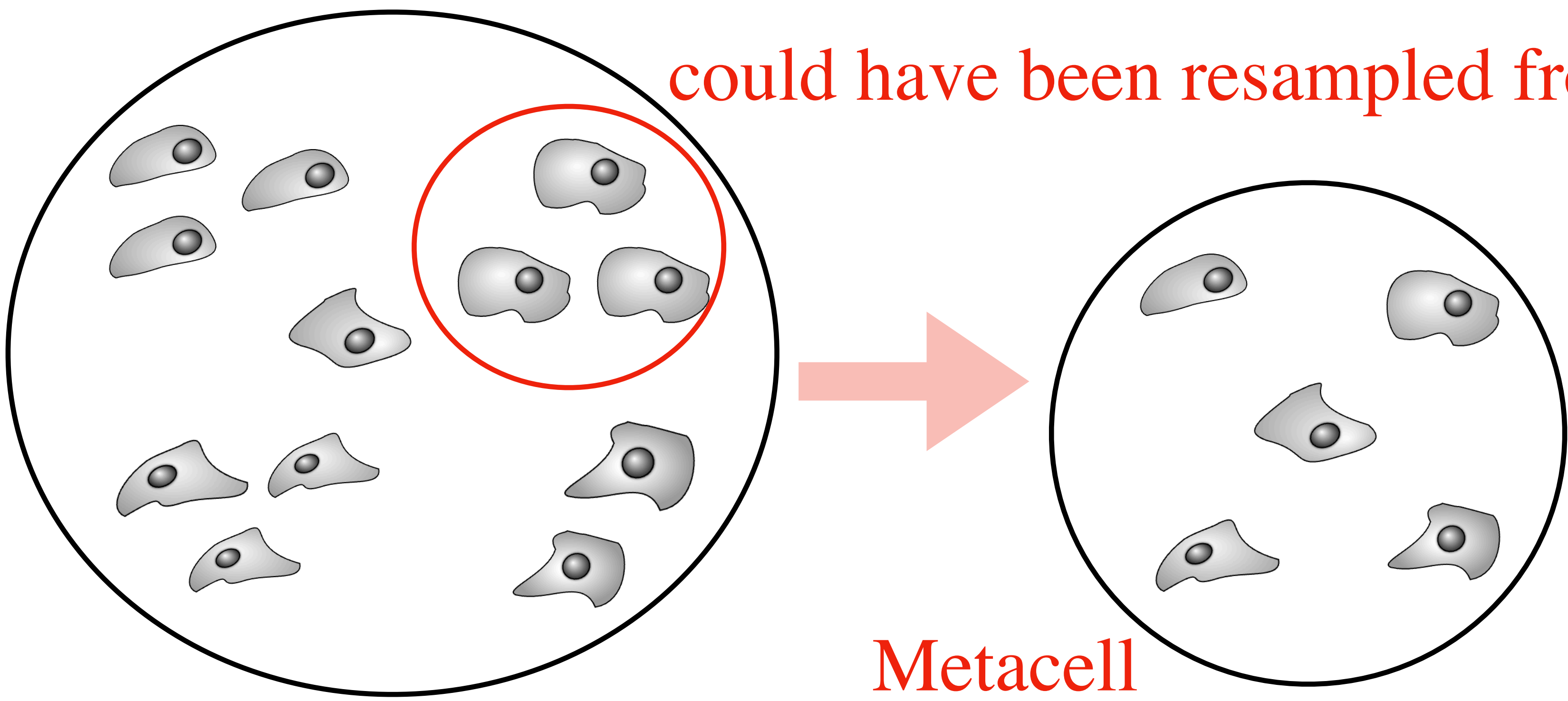
Yael Baran[1], Akhiad Bercovich[1], Arnau Sebe-Pedros[1], Yaniv Lubling[1], Amir Giladi[2], Elad Chomsky[1], Zohar Meir[1], Michael Hoichman[1], Aviezer Lifshitz[1] and Amos Tanay[1*]

✦ **Single-cell RNA-seq**

Technical noise due to partial sampling of RNA molecules within cells.

Problem : **impossible to resample** a cell

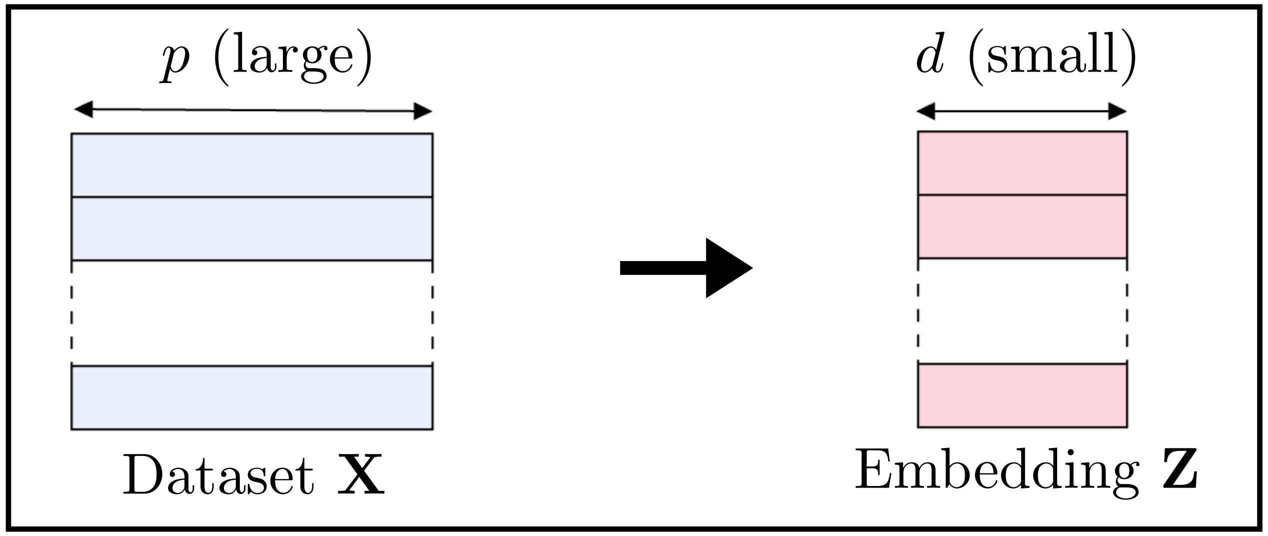
- integration of data from different cells
- need to **separate the sampling effect from biological variance**



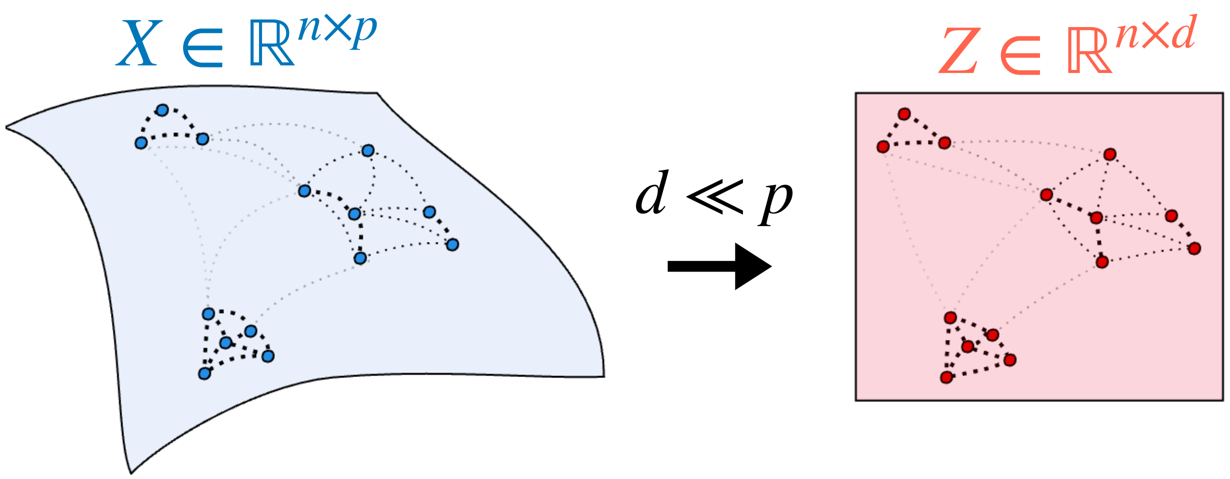
✦ **We would like to choose the granularity of the output data**

Dimension reduction

Dimension reduction



✦ **Preserving geometric properties**



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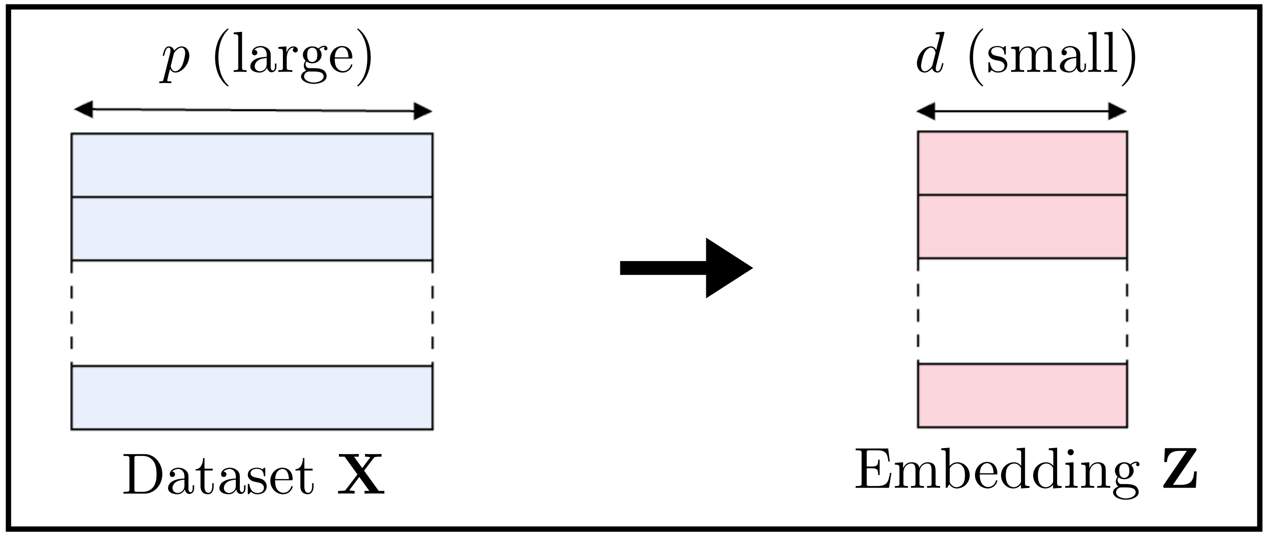

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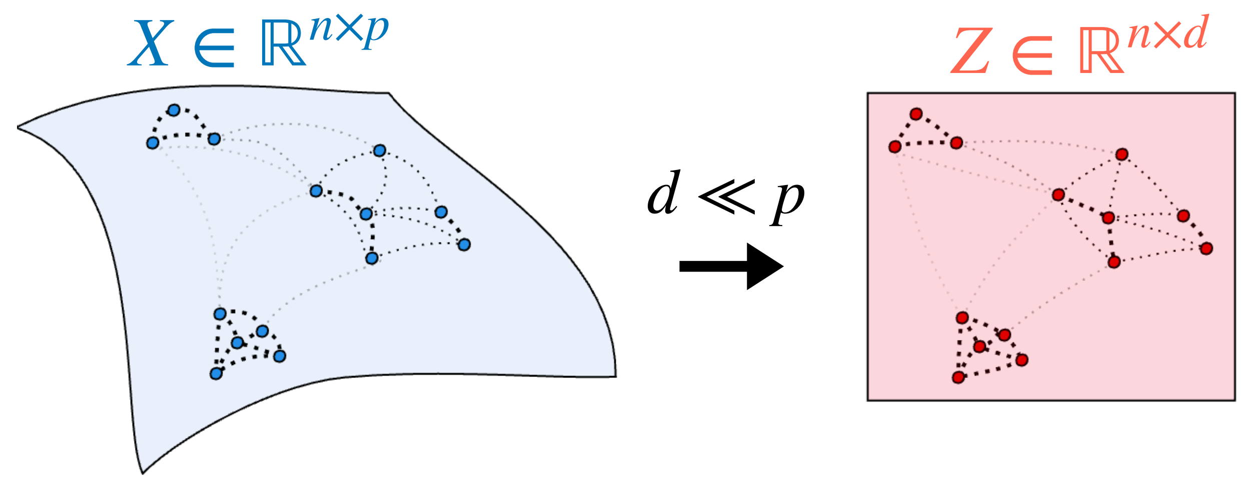
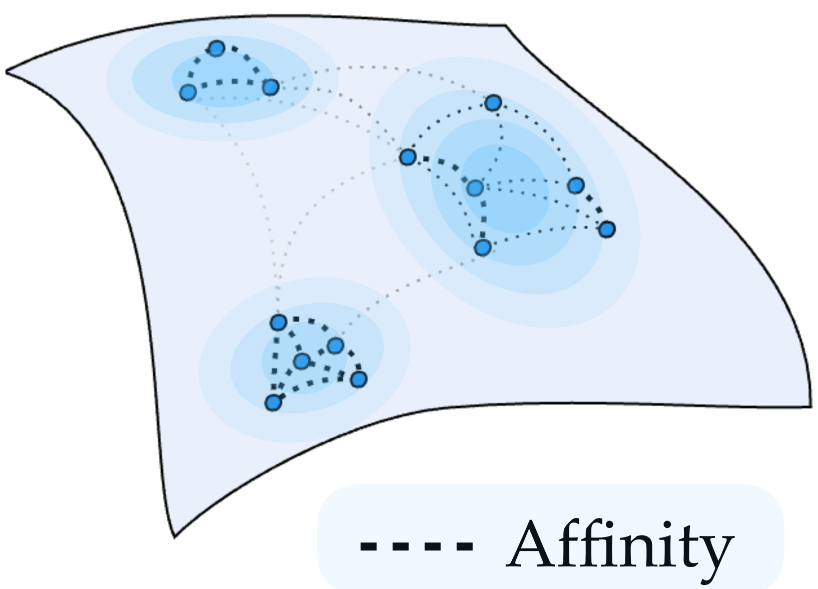
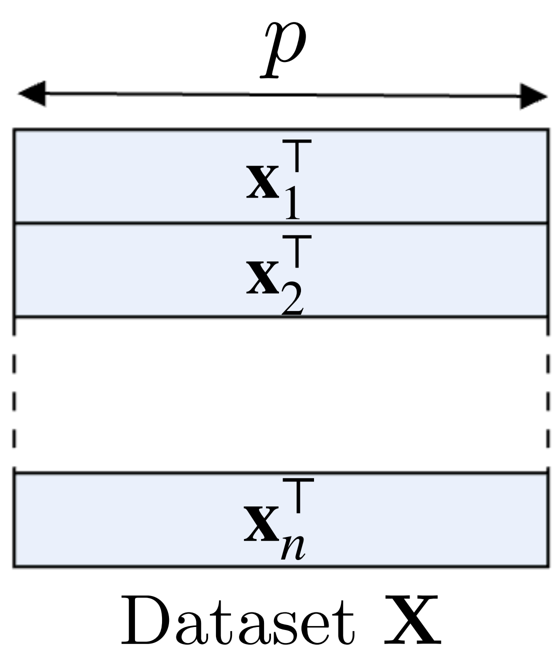


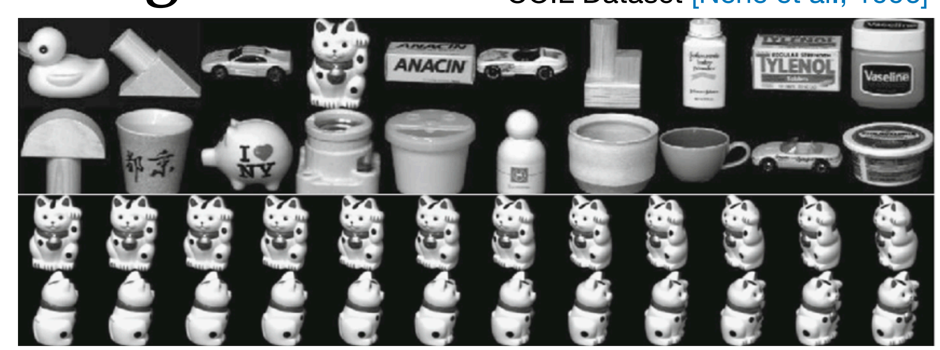
✦ Affinity Matrices



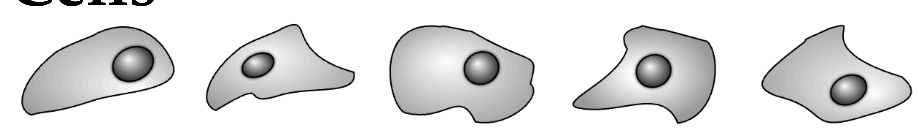


Images

COIL Dataset [Nene et al., 1996]



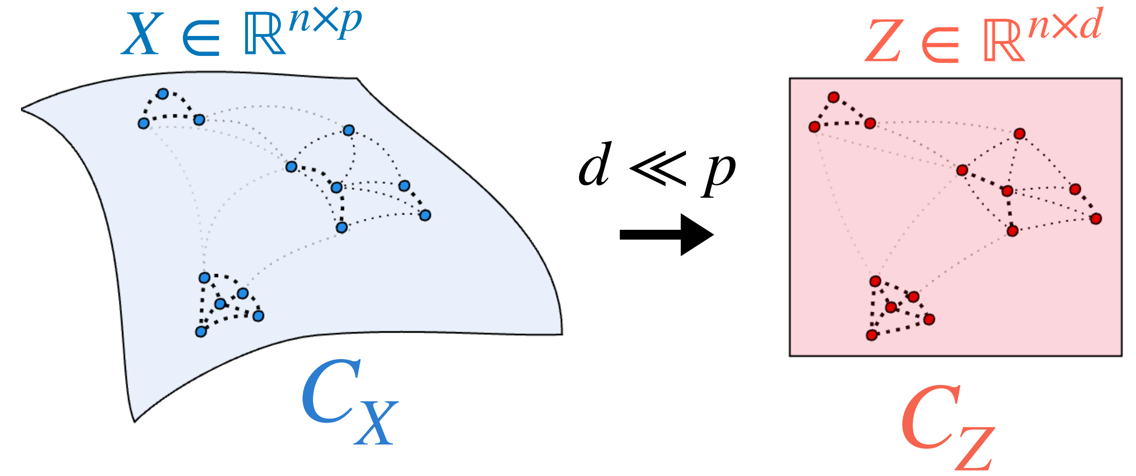
Cells



Symmetric matrix with **non-negative coefficients**.

Coefficient (i, j) = similarity between $\boldsymbol{x}_i$ and $\boldsymbol{x}_j$.

Dimension reduction



✦ A general optimization problem

$$\min_{Z \in \mathbb{R}^{n \times d}} \sum_{i,j=1}^{n} L\Big([C_X]_{ij} \, , \, [C_Z]_{ij}\Big) \quad \text{for some loss} \quad L : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$$

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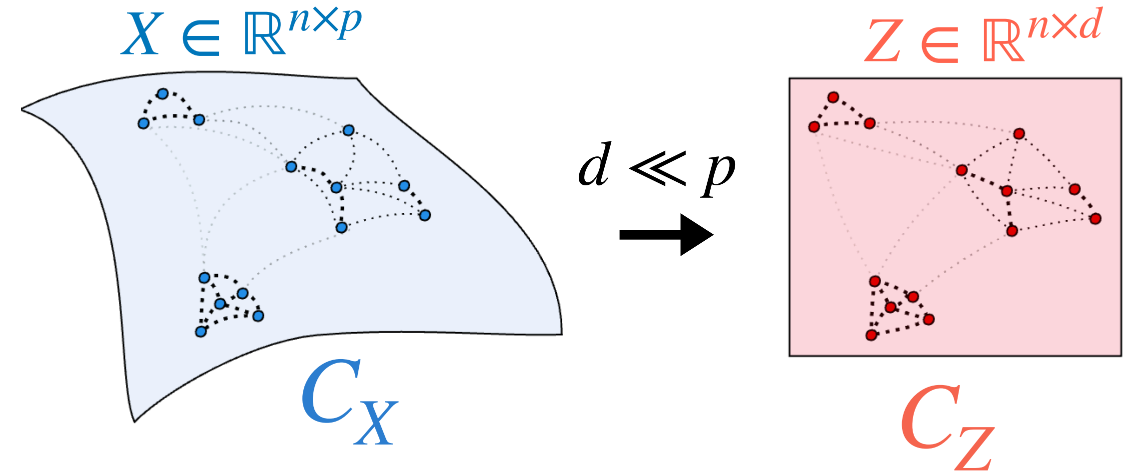

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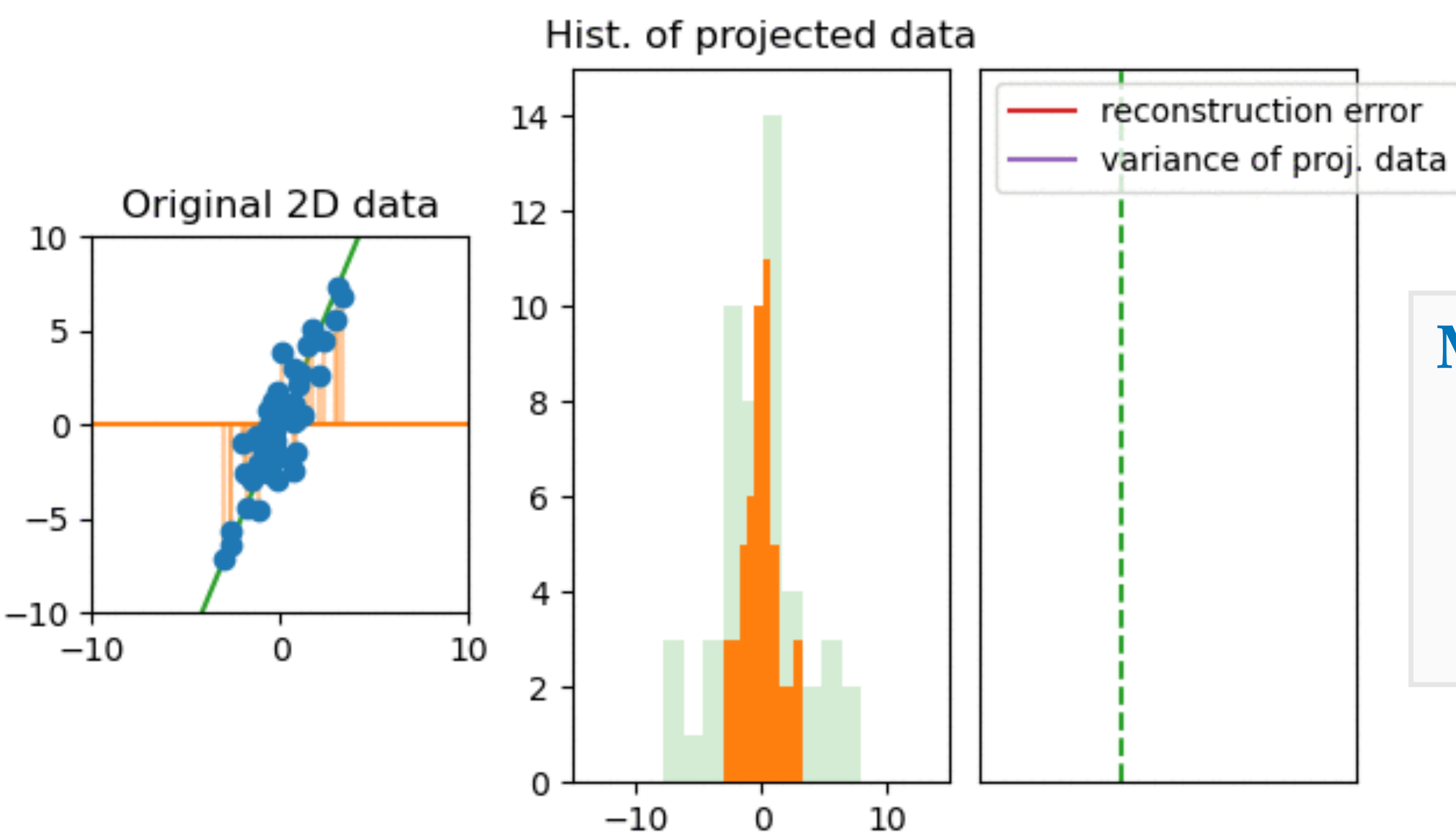
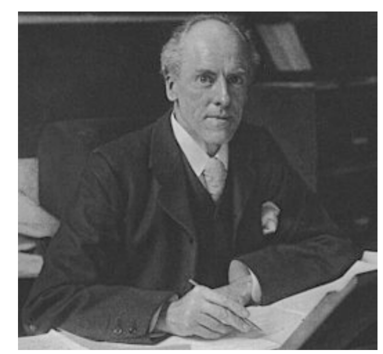
✦ Principal components analysis



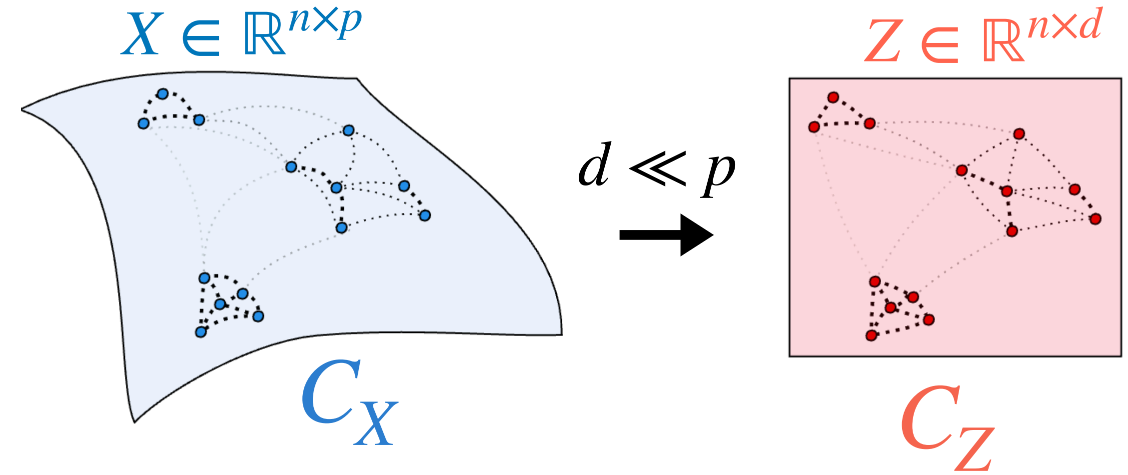


(Pearson, 1901)

Minimizing the reconstruction error

$$\min_{H:\dim(H)=d} \frac{1}{n}\sum_{i=1}^{n} \|\mathbf{x}_i - P_H(\mathbf{x_i})\|_2^2$$

Dimension reduction



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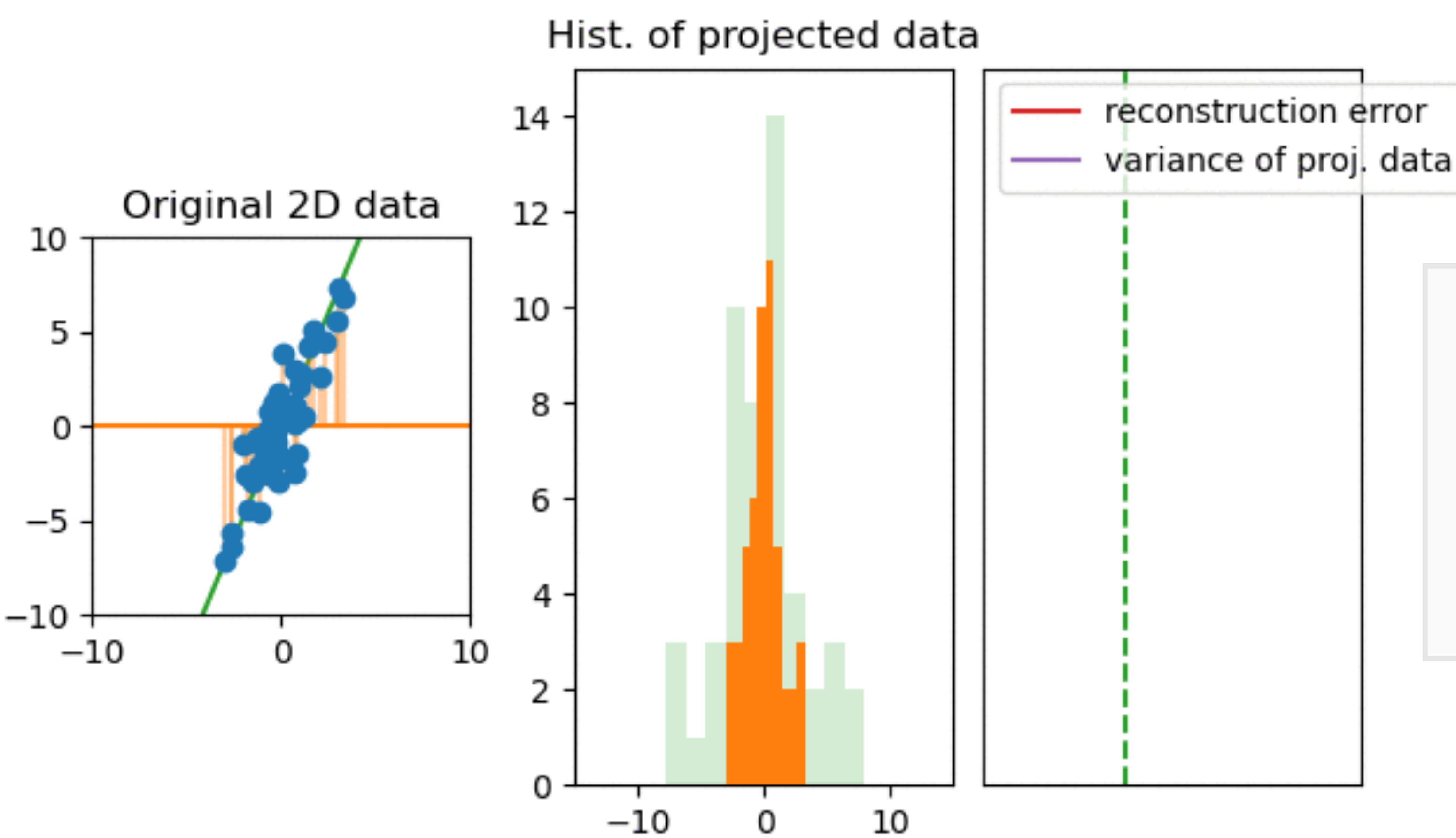

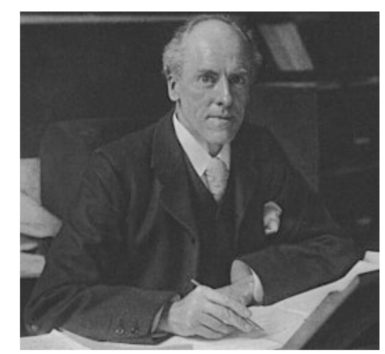

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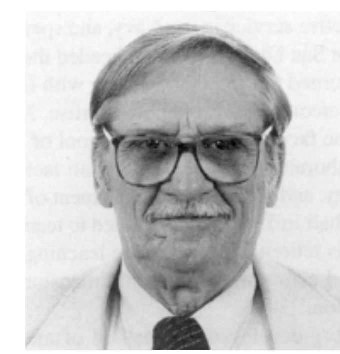

(Torgerson, 1958)

Preserving the inner products

$$\min_{Z\in\mathbb{R}^{n\times d}} \sum_{i=1}^{n} \Big(\langle \mathbf{x}_i, \mathbf{x}_j\rangle - \langle \mathbf{z}_i, \mathbf{z}_j\rangle\Big)^2$$

$$Z \leftarrow \mathrm{EVD}\left(\frac{1}{n}XX^\top\right)$$

Dimension reduction

- **Spectral methods**

$$\min_{Z \in \mathbb{R}^{n \times d}} \sum_{i=1}^{n} \Big([C_X]_{ij} - \langle \mathbf{z}_i, \mathbf{z}_j \rangle \Big)^2$$

Dimension reduction

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$C_X \succeq 0$

solution →

(Eckart & Young, 1936)

$$Z^\star = (\sqrt{\lambda_1}\mathbf{v}_1, \cdots, \sqrt{\lambda_d}\mathbf{v}_d)^\top$$

λ_i i-th **largest** eigenvalue of C_X with eigenvector $\mathbf{v}_i$

$$[C_X]_{ij} = \langle \phi(X_i), \phi(X_j) \rangle_{\mathcal{H}}$$

Dimension reduction

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✦ **Kernel PCA** $C_X \succeq 0$ $[C_X]_{ij} = \langle \phi(X_i), \phi(X_j) \rangle_{\mathscr{H}}$

(Schölkopf, 1997)

PCA: $C_X = XX^\top$ $(Z \leftarrow \mathrm{SVD}(X))$

Dimension reduction

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→ (classical) Multidimensional scaling: $C_X = -\frac{1}{2} H D_X H$

Dimension reduction

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$C_X \succeq 0$ **solution** →

(Eckart & Young, 1936)

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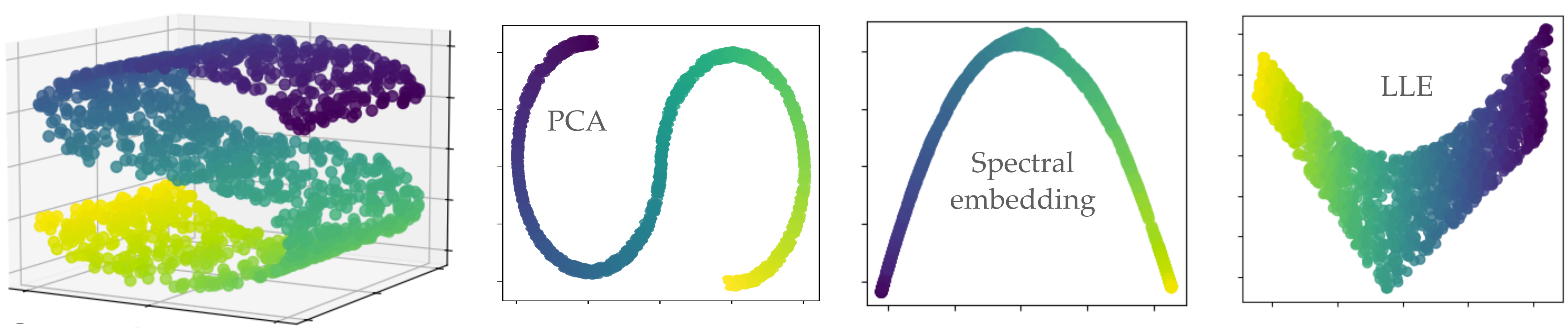
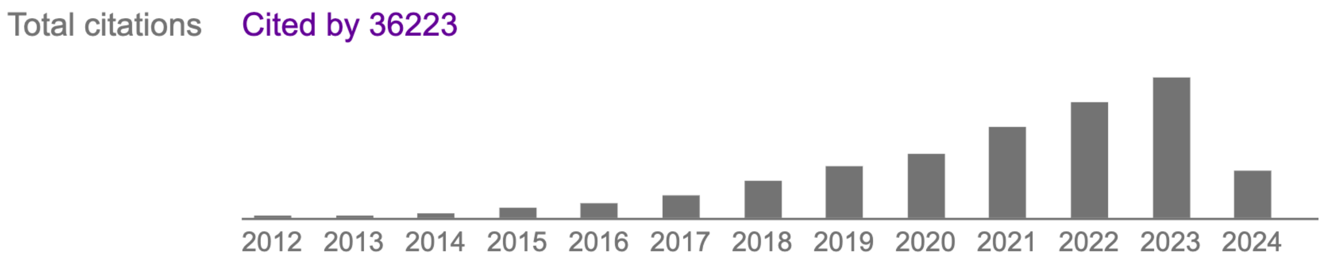
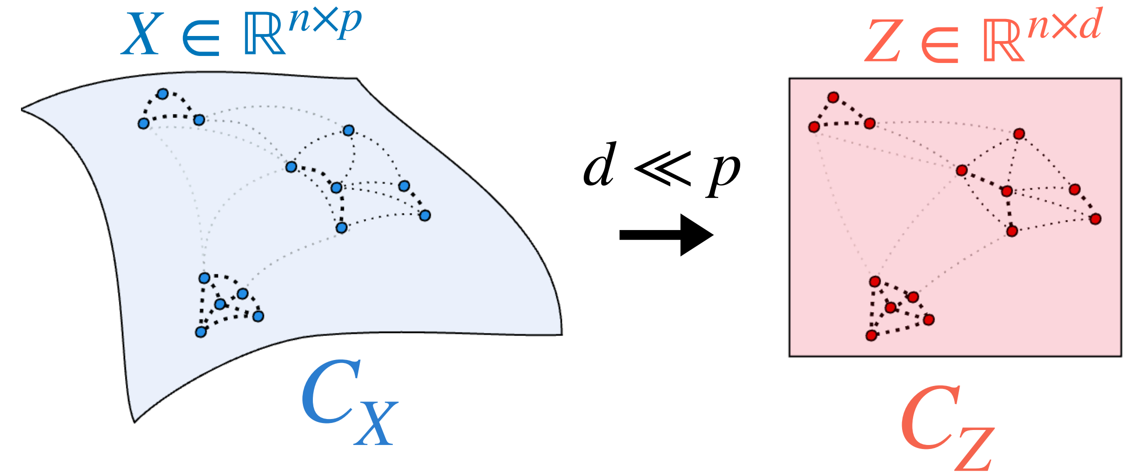
- PCA: $C_X = XX^\top$ $(Z \leftarrow \mathrm{SVD}(X))$
- (classical) Multidimensional scaling: $C_X = -\frac{1}{2} H D_X H$
- Laplacian Eigenmap (spectral embedding): $C_X = L_X^\dagger$
  (Belkin & Niyogi, 2003)
- Locally Linear Embedding, Diffusion Map …
  (Roweis & Saul, 2000) (Coifman & Lafon, 2006)



Dimension reduction





✦ Neighbor embedding methods

$$\min_{Z \in \mathbb{R}^{n \times d}} \sum_{i,j=1}^{n} \mathrm{KL}\left([C_X]_{ij} \, , \, [C_Z]_{ij} \right)$$

Dimension reduction

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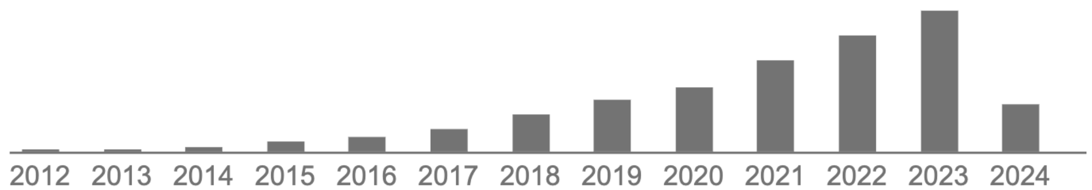

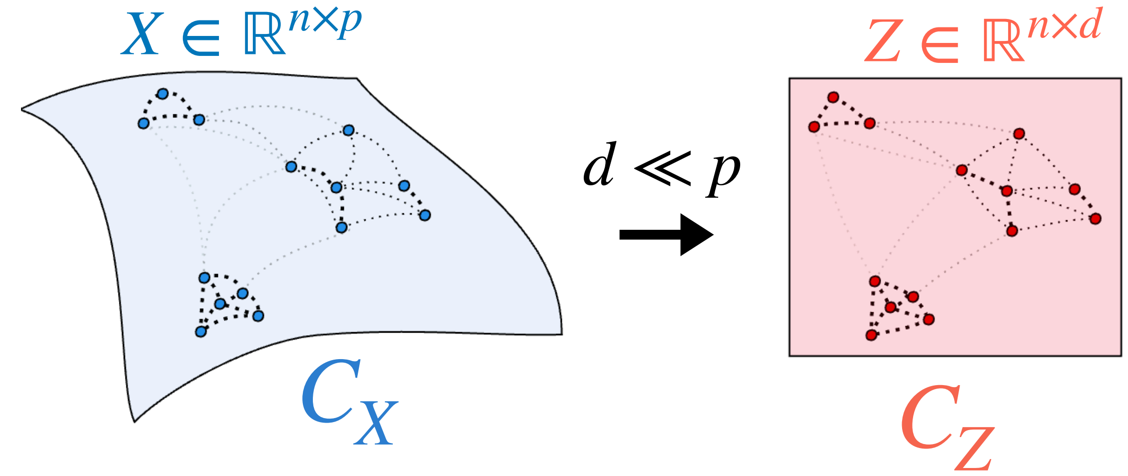

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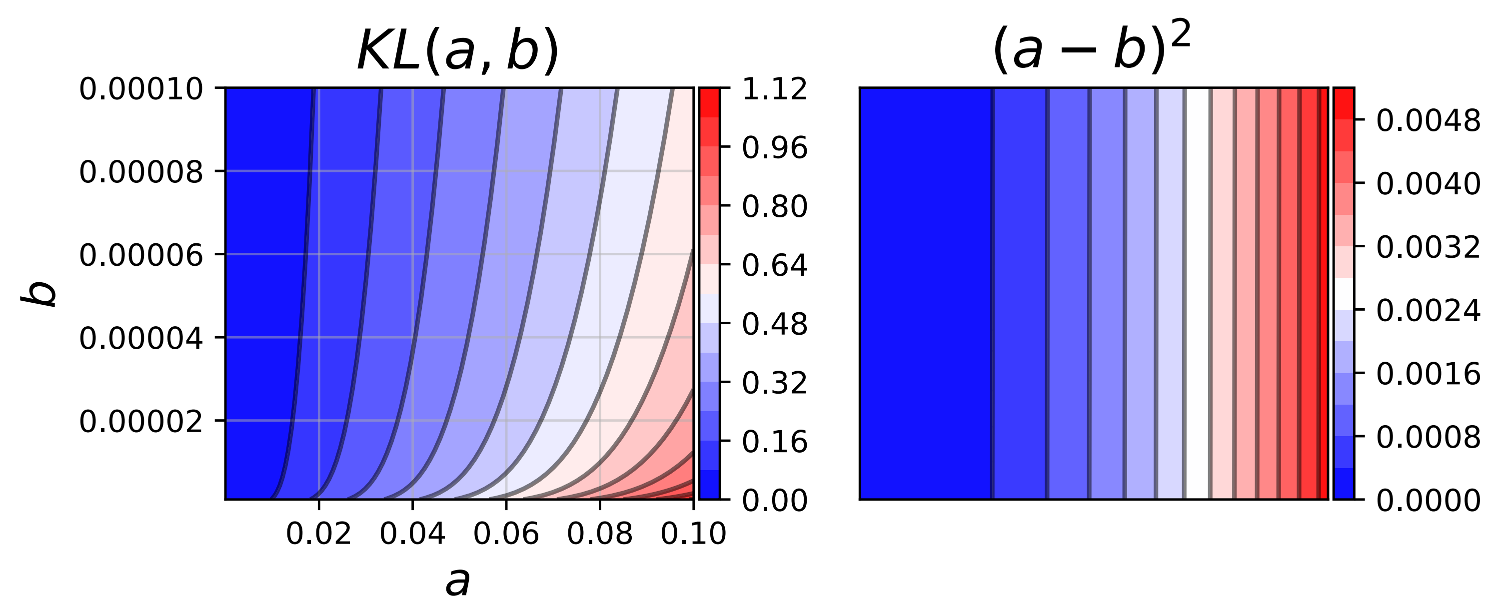
✦ Kullback-Leiber divergence

$$\mathrm{KL}(a,b) = a \log(a/b) - a + b = D_\phi(a,b)$$

Shannon–Boltzman entropy $\phi(x) = x \log(x) - x + 1$



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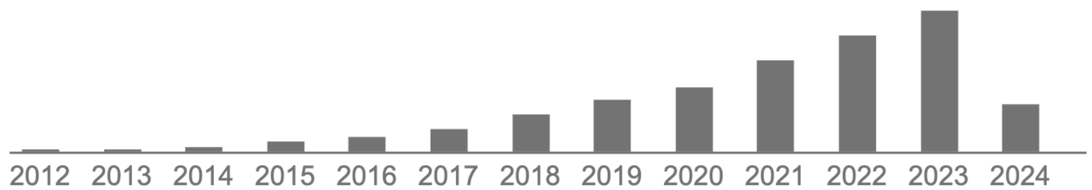

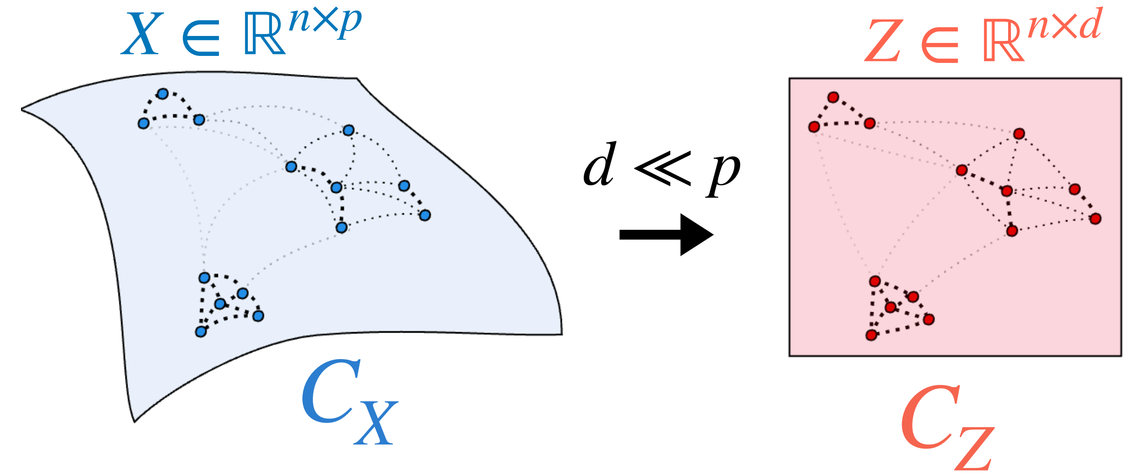

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$$\sim \min_{Z\in\mathbb{R}^{n\times d}} \underbrace{\sum_{i,j=1}^{n} [C_X]_{ij} \log\left(\frac{[C_X]_{ij}}{[C_Z]_{ij}}\right)}_{\mathbf{KL}}$$

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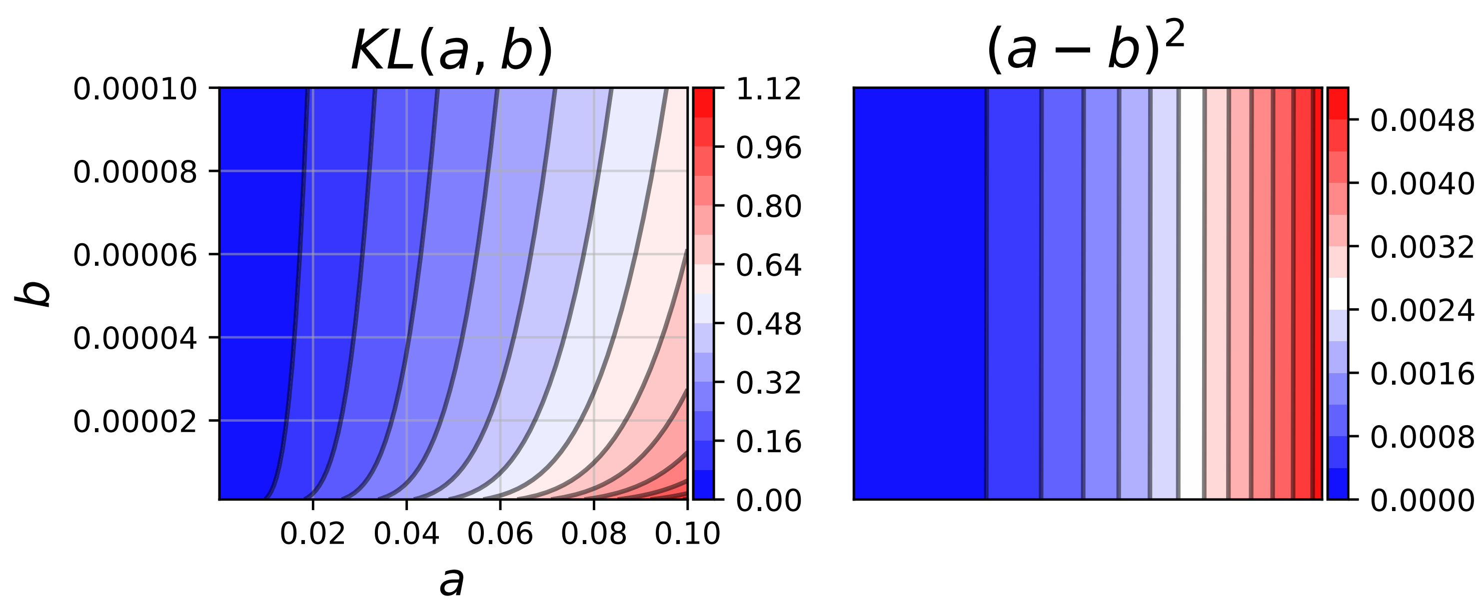

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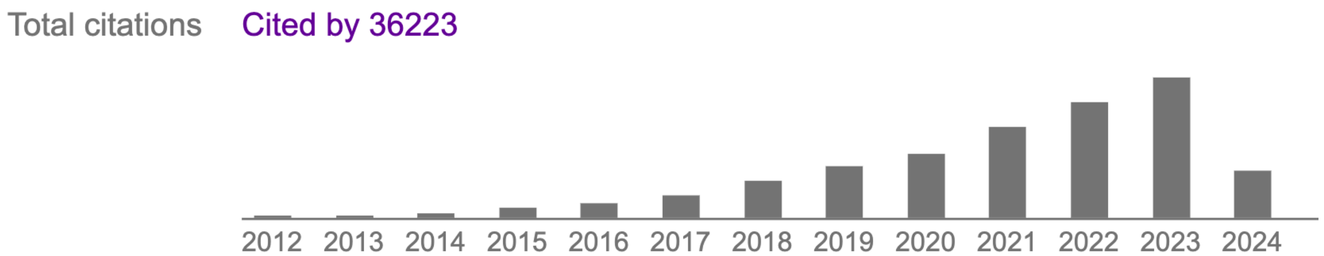

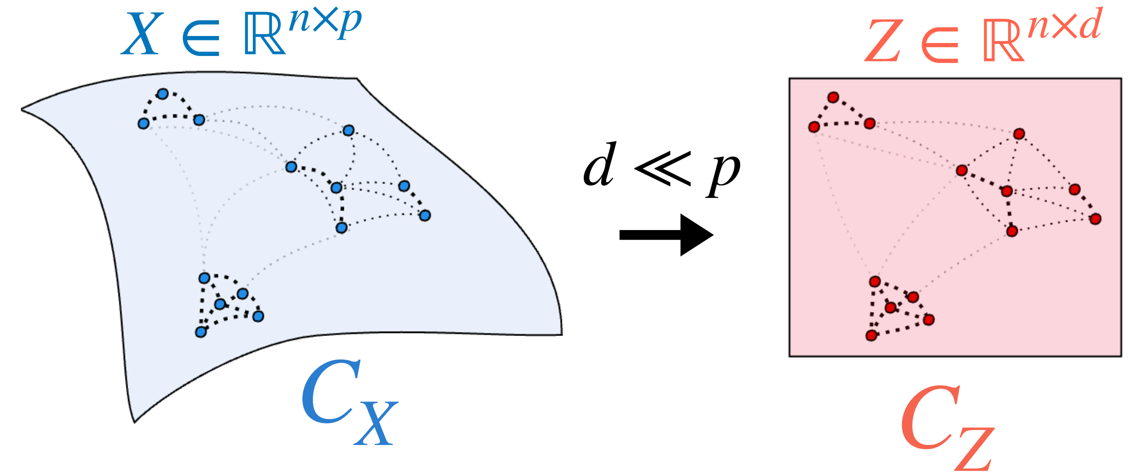

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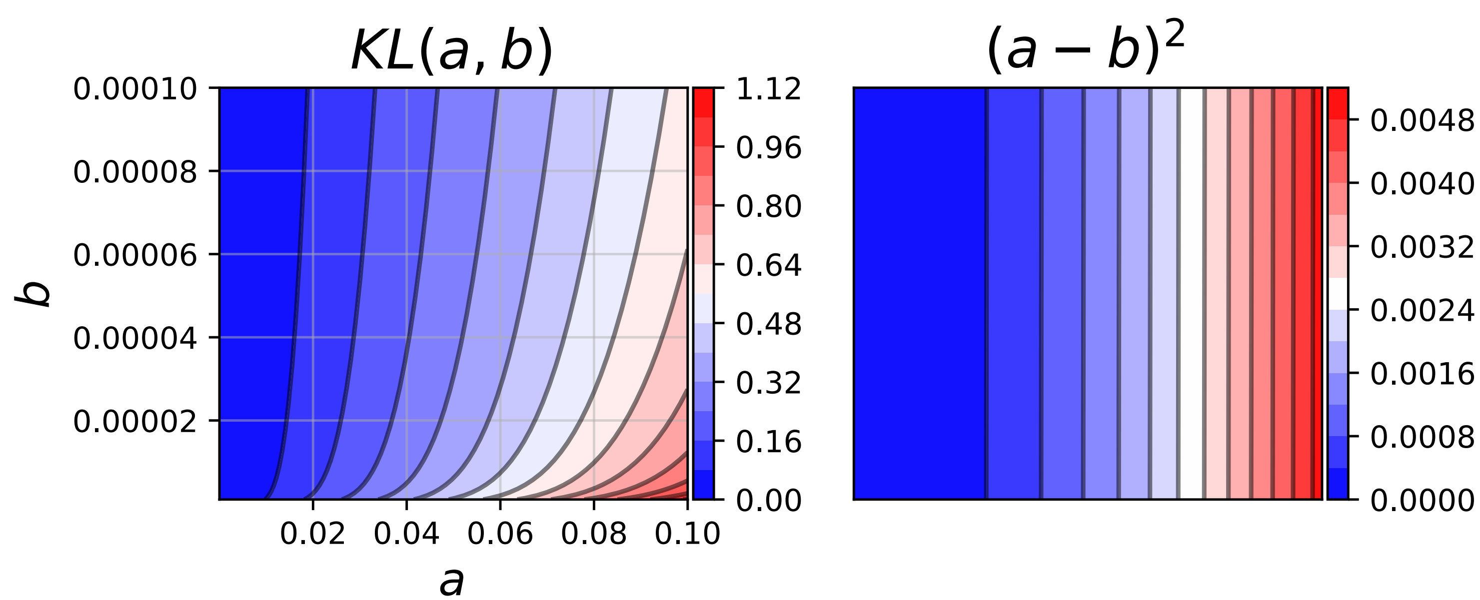
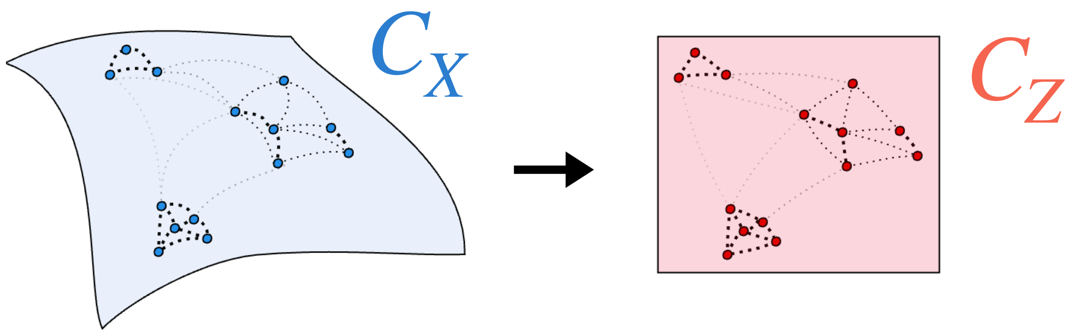


✦ What choices for C_X, C_Z?

- ✦ Encode the non-linear geometry
- ✦ Some kind of normalization
- ✦ Robustness to noise, varying density
- ✦ Similar for both high and low dim

Dimension reduction



- ✦ **SNE** (Hinton & Roweis, 2002)

Embedding space

$$[C_Z]_{ij} = \frac{\exp(-\|\mathbf{z}_i - \mathbf{z}_j\|_2^2)}{\sum_k \exp(-\|\mathbf{z}_i - \mathbf{z}_k\|_2^2)} (= \mathbb{P}(j \mid i))$$

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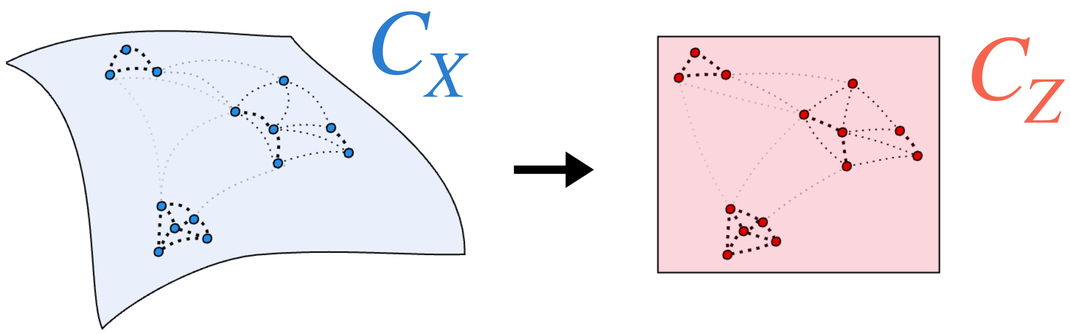

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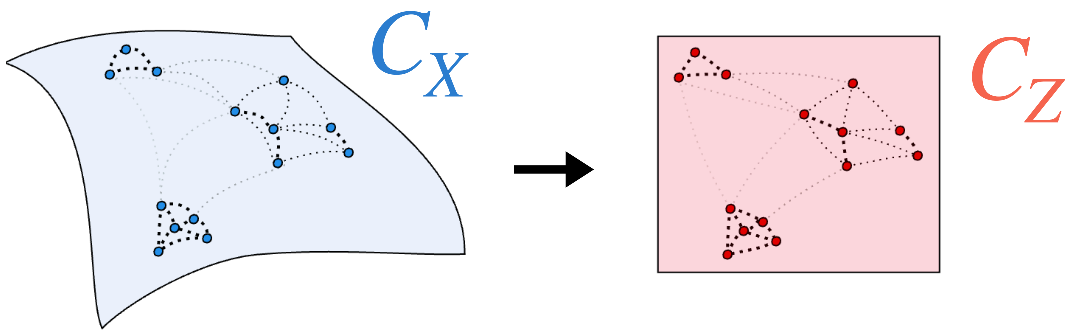

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- Local bandwidths **optimized** s.t.

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- Perplexity = effective number of **neighbors**
- Account for **varying density**

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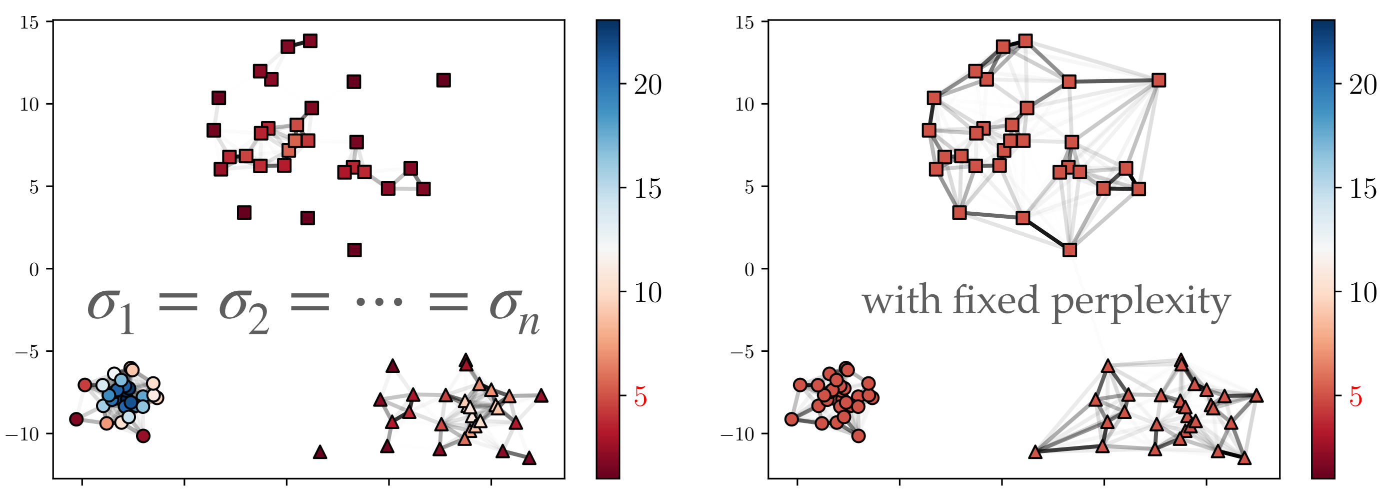

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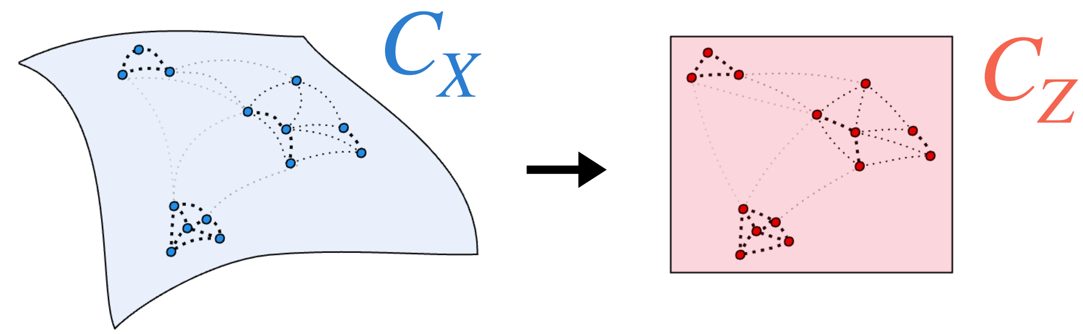

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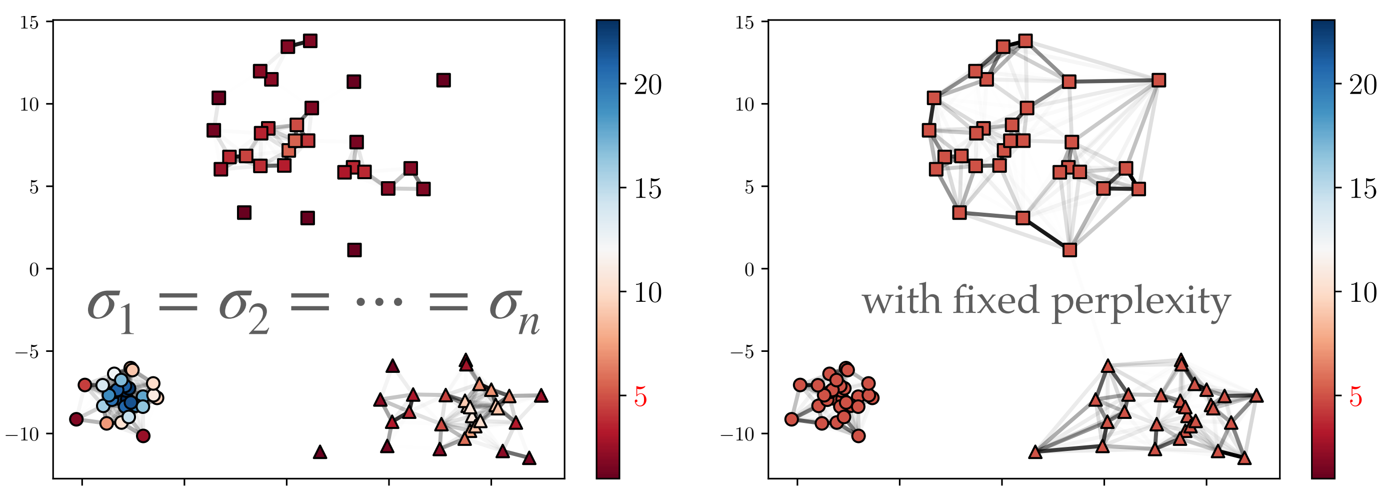

✦ (t)-SNE (Van der Maaten & Hinton, 2008)

- Joint distributions:

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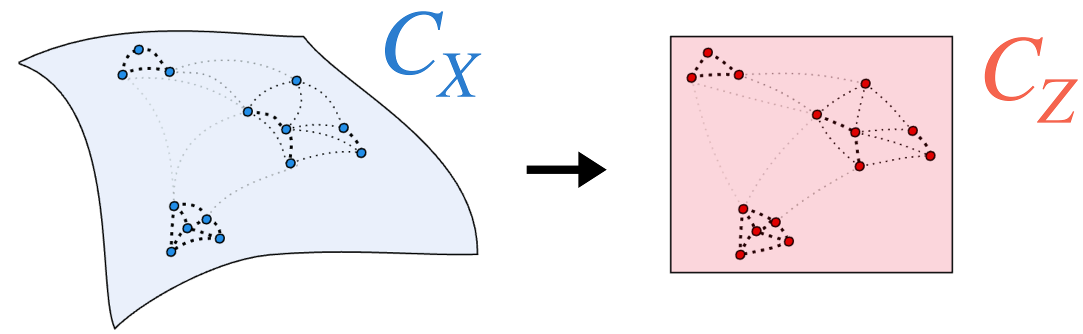
$$[C_X]_{ij} \leftarrow \frac{[C_X]_{ij} + [C_X]_{ji}}{2n}$$

- Crowding effect: Student t-distribution instead of Gaussian in Z

Dimension reduction



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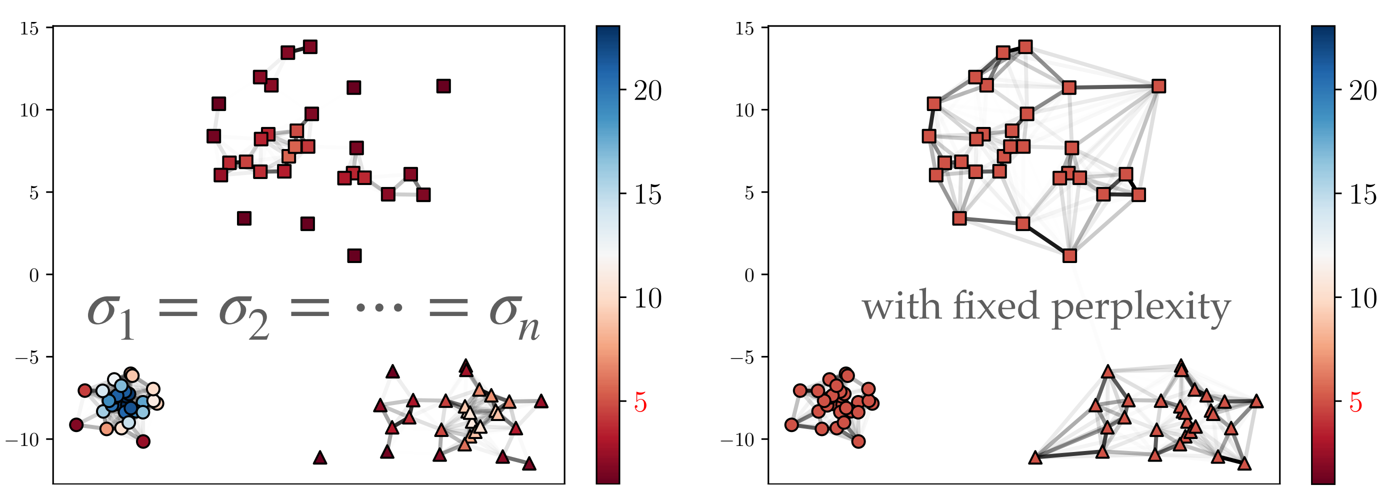
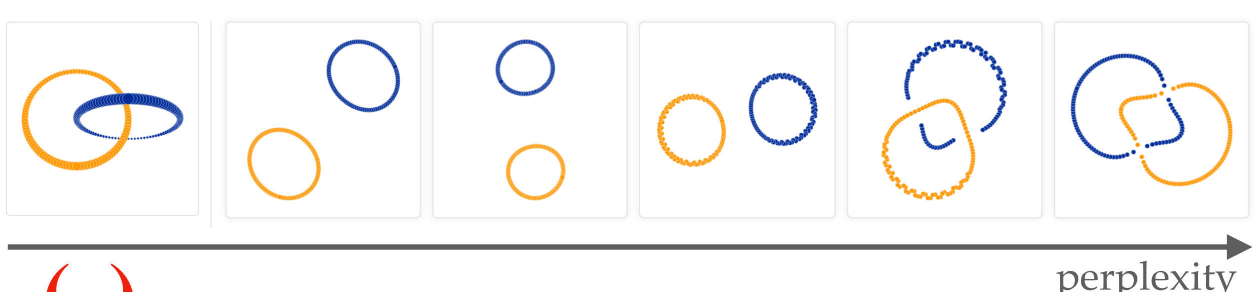
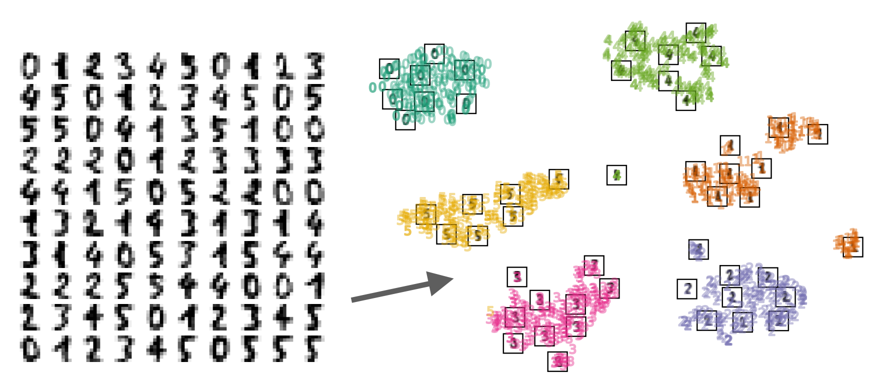
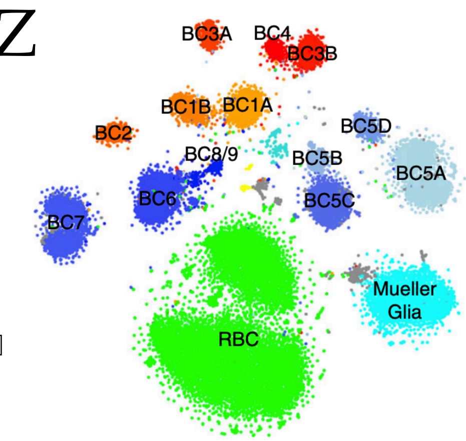


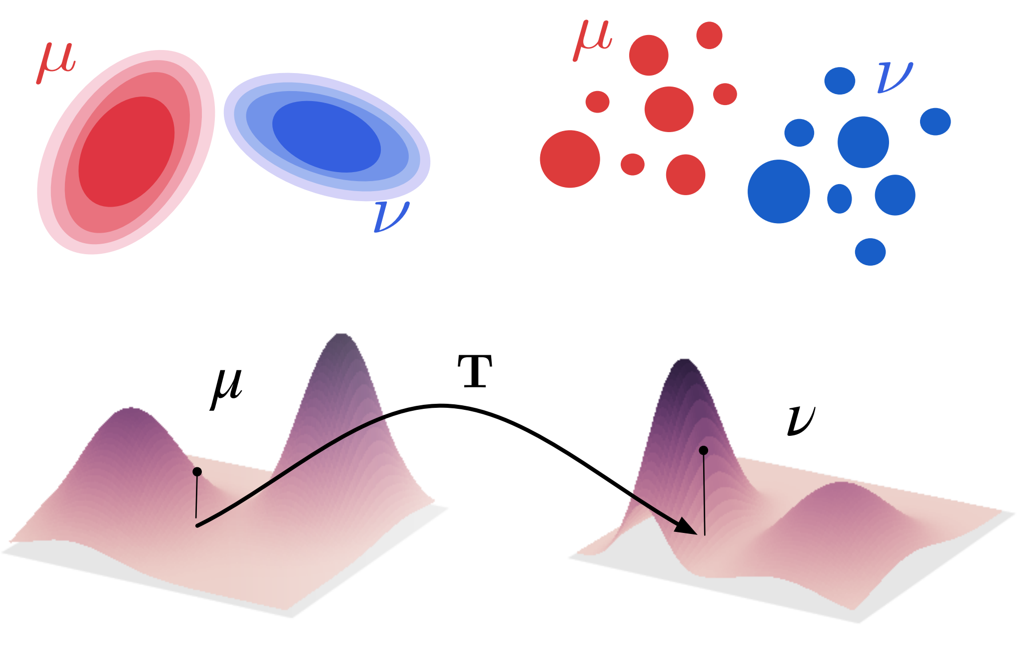






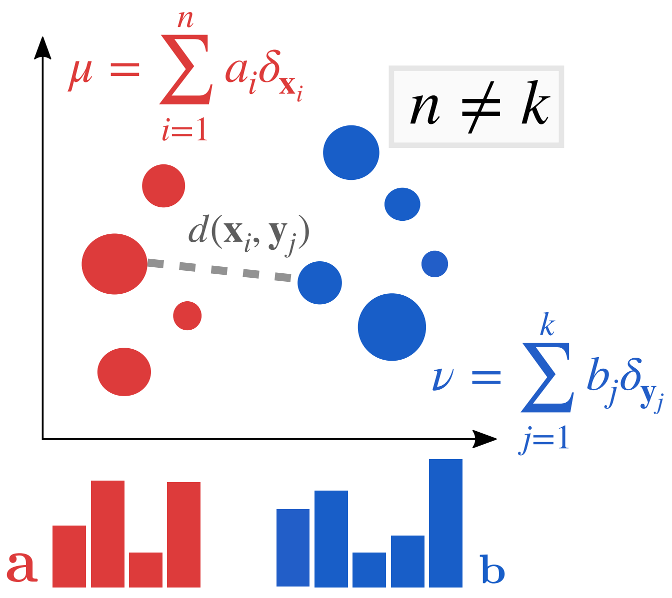
(Shekhar et al., 2016)

From linear Optimal Transport to Gromov-Wasserstein



From Wasserstein to Gromov-Wasserstein

✦ Classical optimal transport (in a nutshell)



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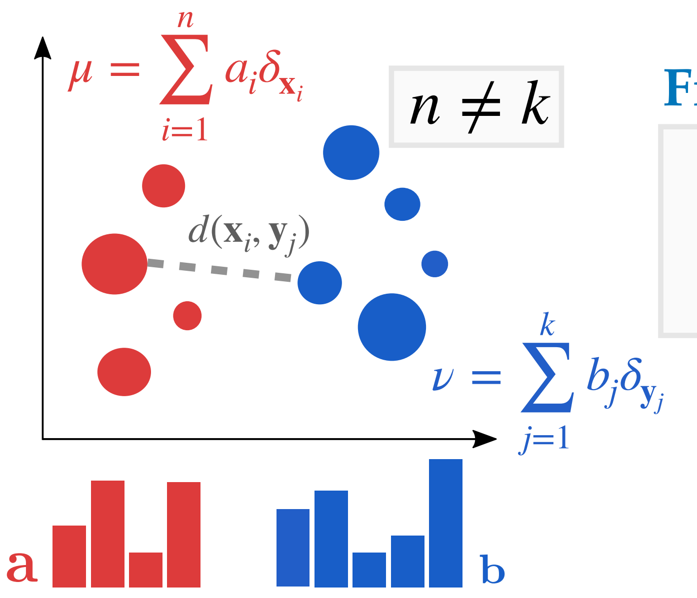

Find plan $T \in \mathbb{R}_+^{n \times k}$

$$\min_T \sum_{ij} d(\mathbf{x}_i, \mathbf{y}_j) T_{ij}$$

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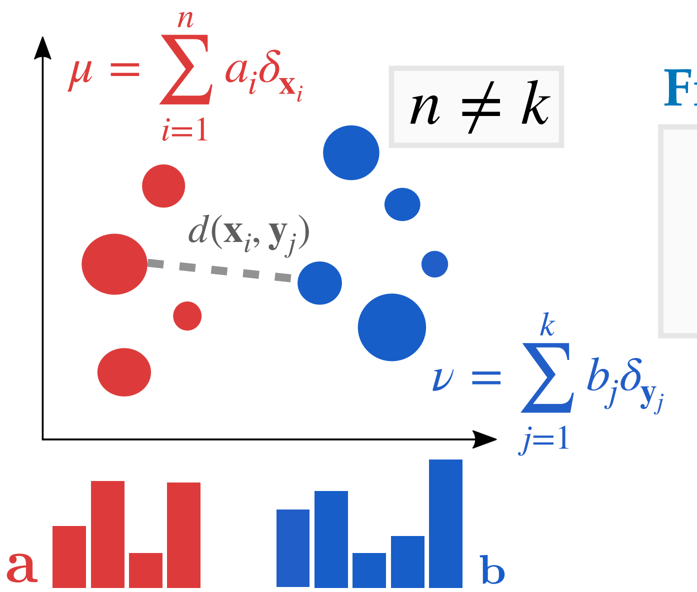

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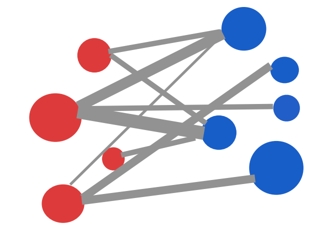
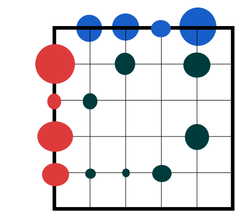
which constraints ?

Coupling $\Pi(a, b)$

$$T^\top 1_n = a$$
$$T 1_k = b$$





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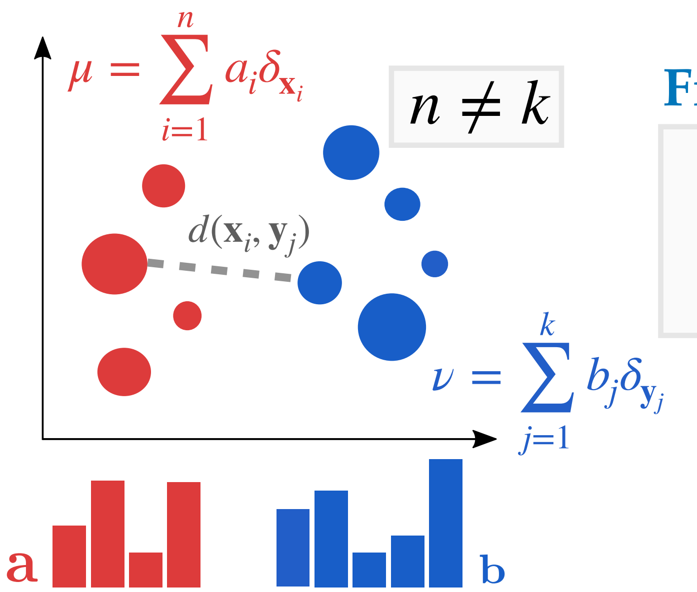

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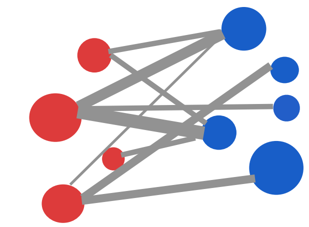
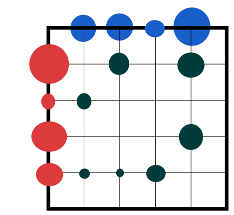




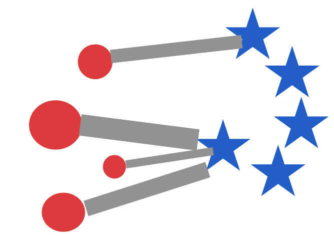
$T \in [0,1]^{n \times k}$

Semi-relaxed coupling

$$T^\top 1_n = a$$

$\sim$ `assign` in k-means

$$\sim \min_b \min_{T \in \Pi(a,b)} \sum_{ij} d(\mathbf{x}_i, \mathbf{y}_j) T_{ij}$$



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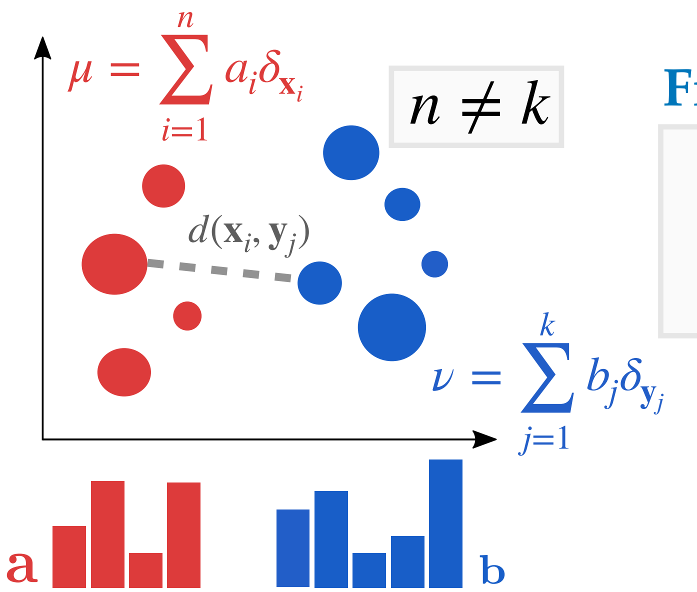

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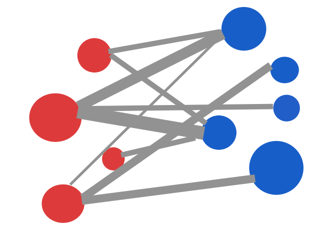

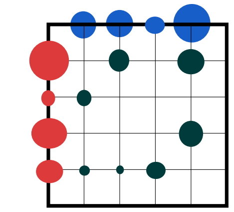

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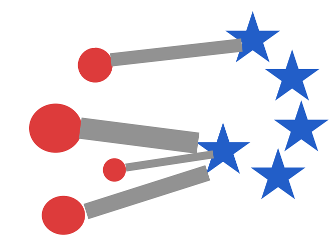
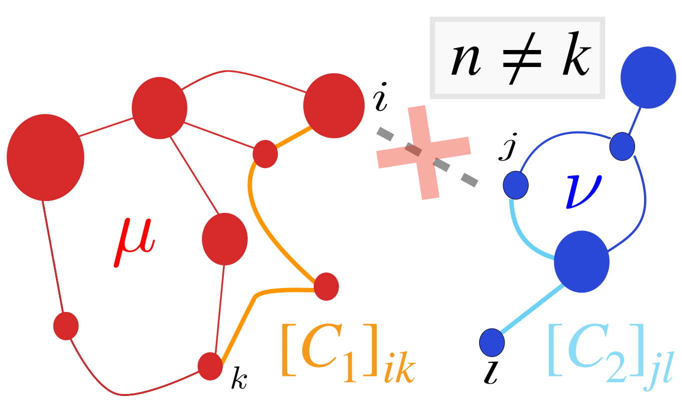


✦ Gromov-Wasserstein



(Sturm, 2012)

(Mémoli, 2011)

From Wasserstein to Gromov-Wasserstein

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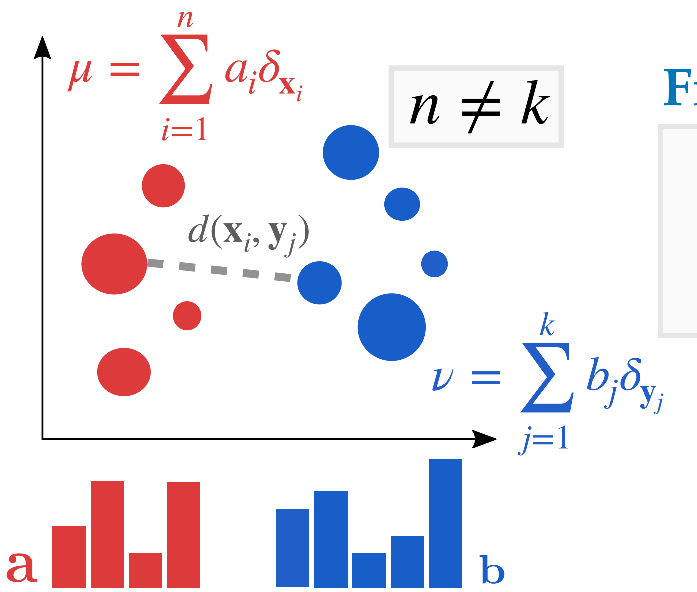

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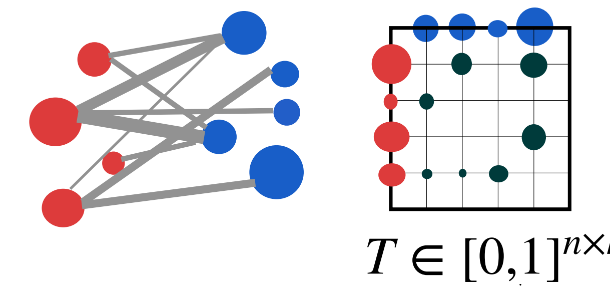

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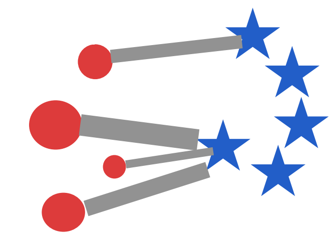

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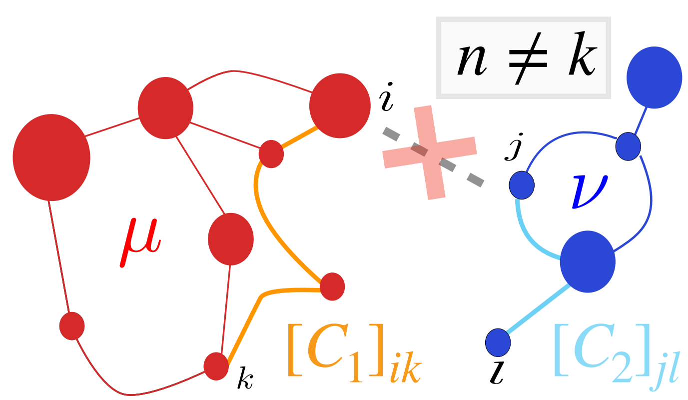


(Sturm, 2012)

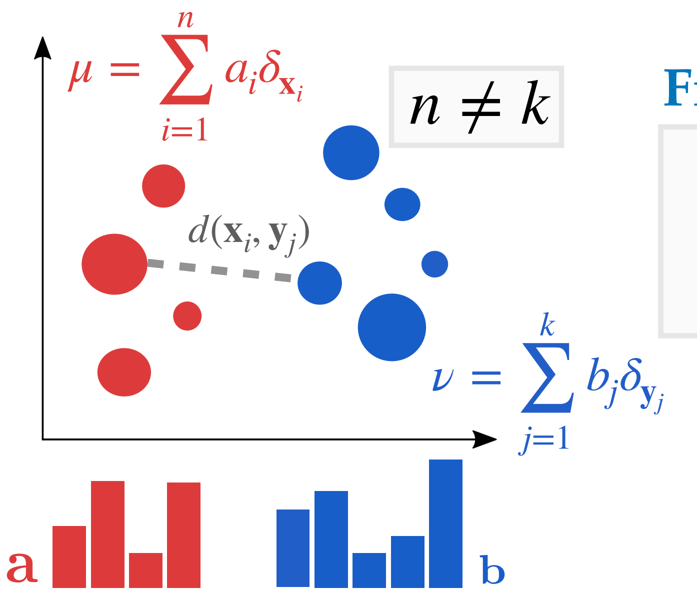
(Mémoli, 2011)

Quadratic OT: find the plan

$$\min_{T \in \Pi(a,b)} \sum_{ijkl} L\left([C_1]_{ik}\ ,\ [C_2]_{jl} \right) T_{ij} T_{kl}$$

From Wasserstein to Gromov-Wasserstein

✦ Classical optimal transport (in a nutshell)



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→ **Coupling** $\Pi(a, b)$

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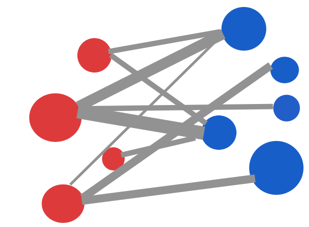

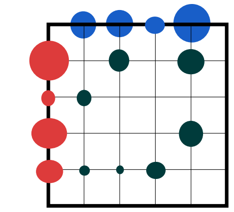

$T \in [0,1]^{n \times k}$

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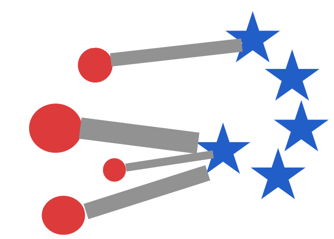

✦ Gromov-Wasserstein

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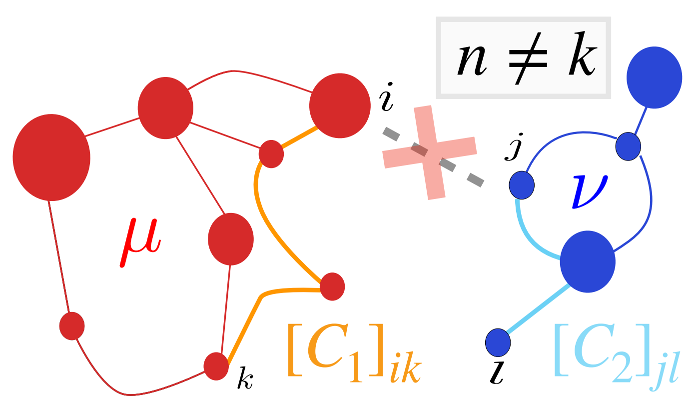

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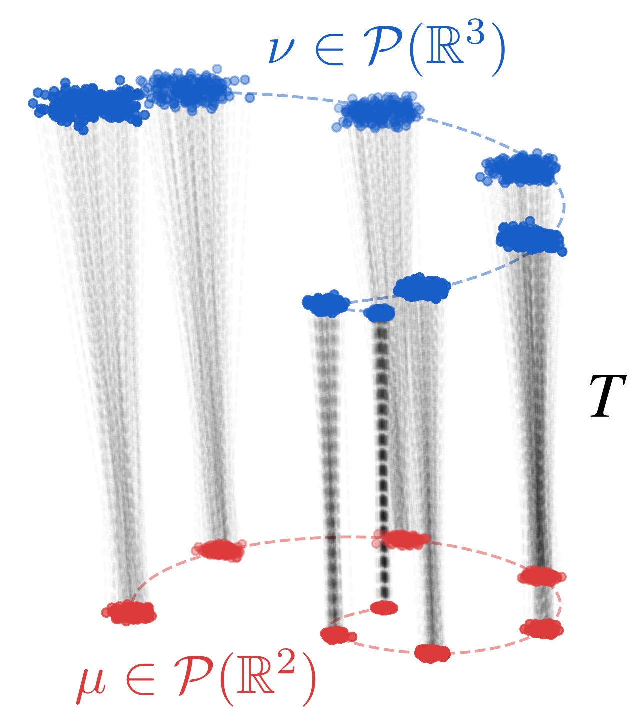
$$\min_{T \in \Pi(a,b)} \sum_{ijkl} L\Big([C_1]_{ik}\ ,\ [C_2]_{jl}\Big)\, T_{ij} T_{kl}$$

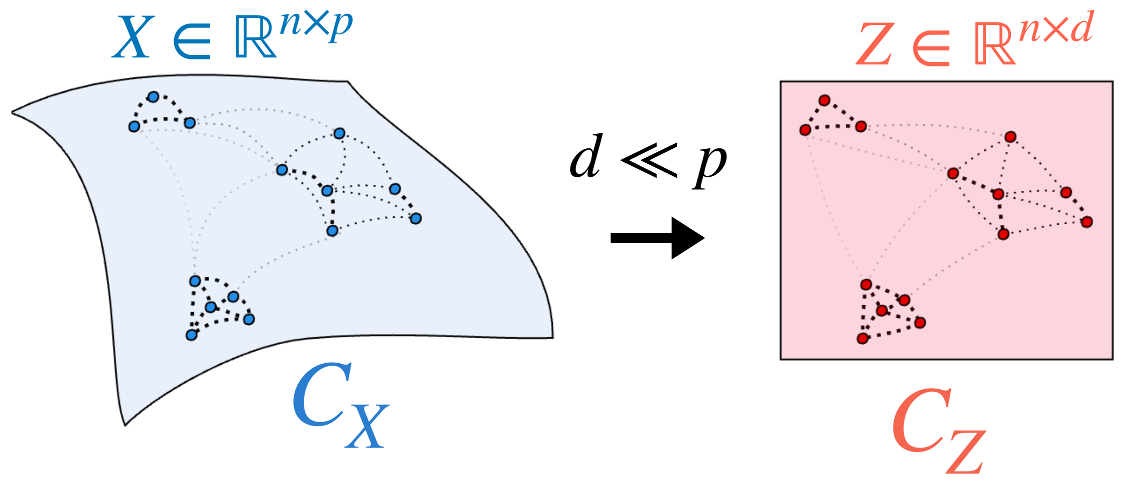
- ✦ L measures distortion

$$\Big|[C_1]_{ik} - [C_2]_{jl}\Big|^2$$

- ✦ Goal : **preserving pairwise connectivity**
- ✦ Distance w.r.t. isomorphisms
- ✦ Difficult quadratic problem (NP-hard)



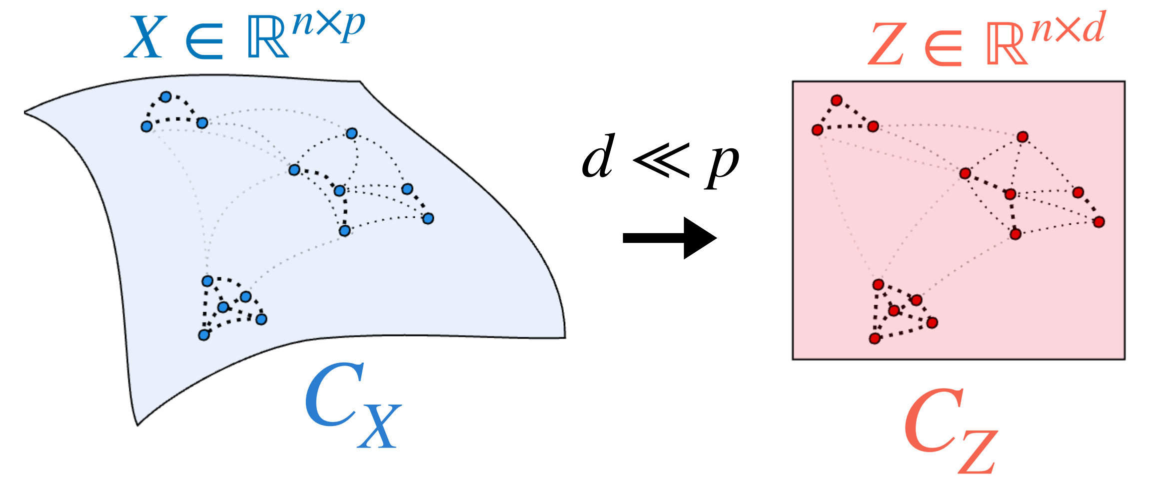
DR as OT in disguise



✦ Dimension reduction

$$\min_{Z \in \mathbb{R}^{n \times d}} \sum_{i,j=1}^{n} L\left([C_X]_{ij} \, , \, [C_Z]_{ij} \right)$$

DR as OT in disguise



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equiv

Permutation equivariance

$\forall P, C_{PZ} = PC_ZP^\top$

$$\min_{Z\in\mathbb{R}^{n\times d}} \min_{\sigma\in S_n} \sum_{i,j=1}^{n} L\left([C_X]_{ij}\ ,\ [C_Z]_{\sigma(i)\sigma(j)}\right)$$

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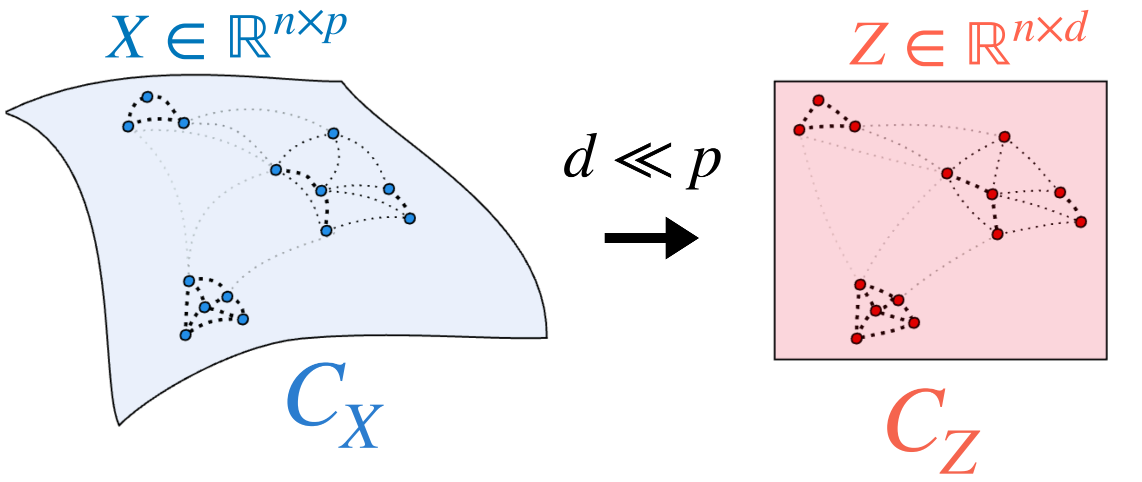

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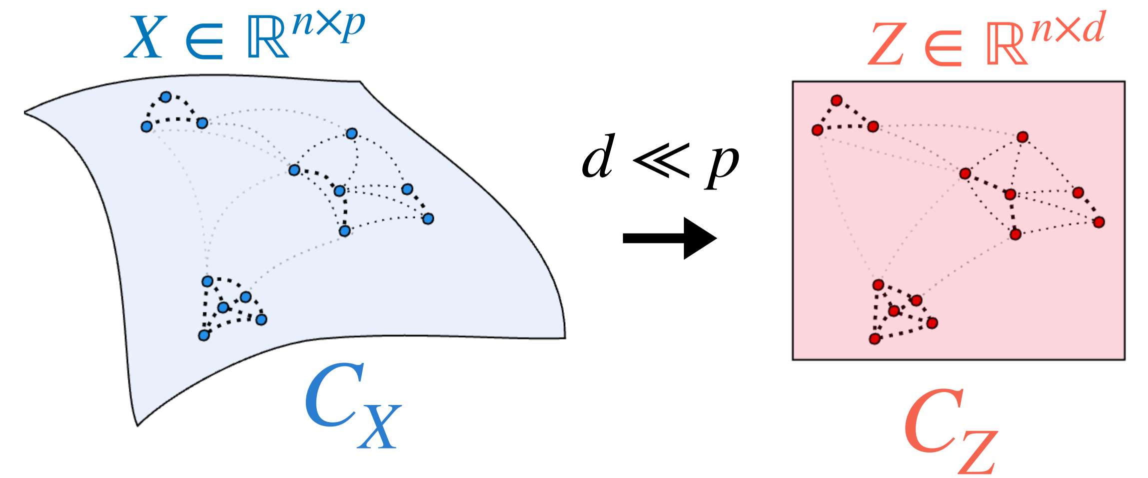

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?

✦ Gromov-Wasserstein projection

$$\min_{Z\in\mathbb{R}^{n\times d}} \min_{T\in\Pi(\frac{1_n}{n},\frac{1_n}{n})} \sum_{ijkl} L\Big([C_X]_{ik}\ ,\ [C_Z]_{jl}\Big) T_{ij}T_{kl}$$

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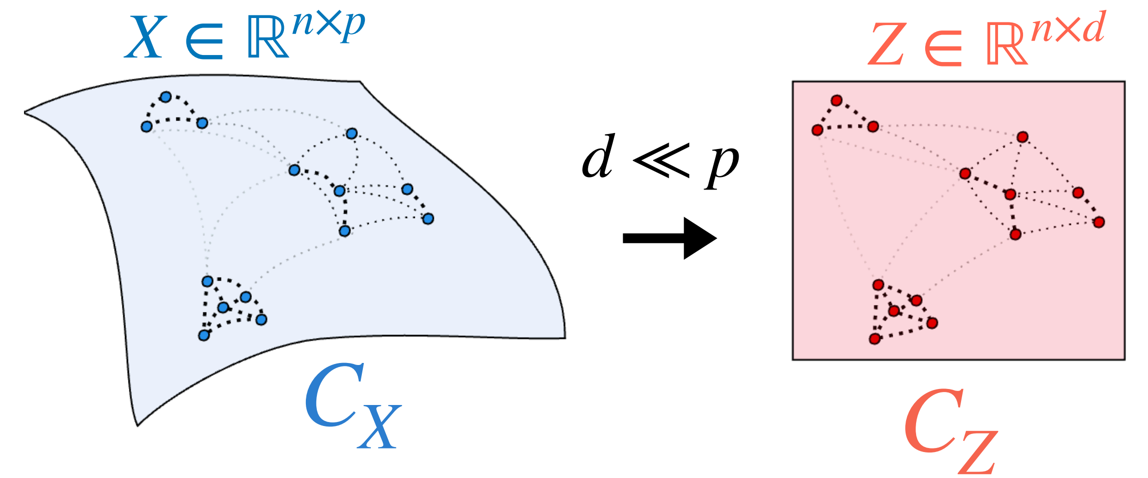

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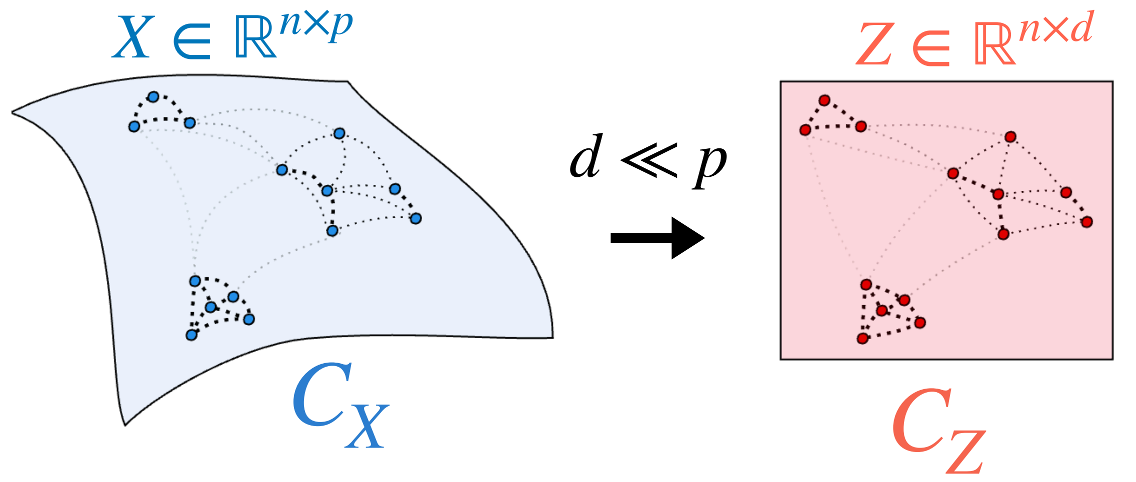
✦ Equivalence holds for

Spectral methods

- C_X any matrix, $L = |\cdot|^2$, $C_Z = ZZ^\top$

DR as OT in disguise



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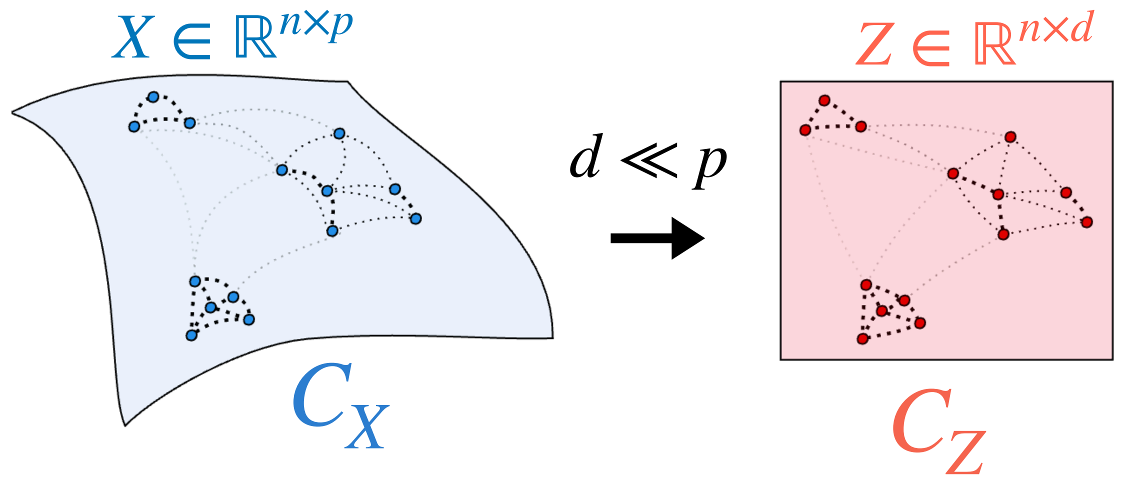

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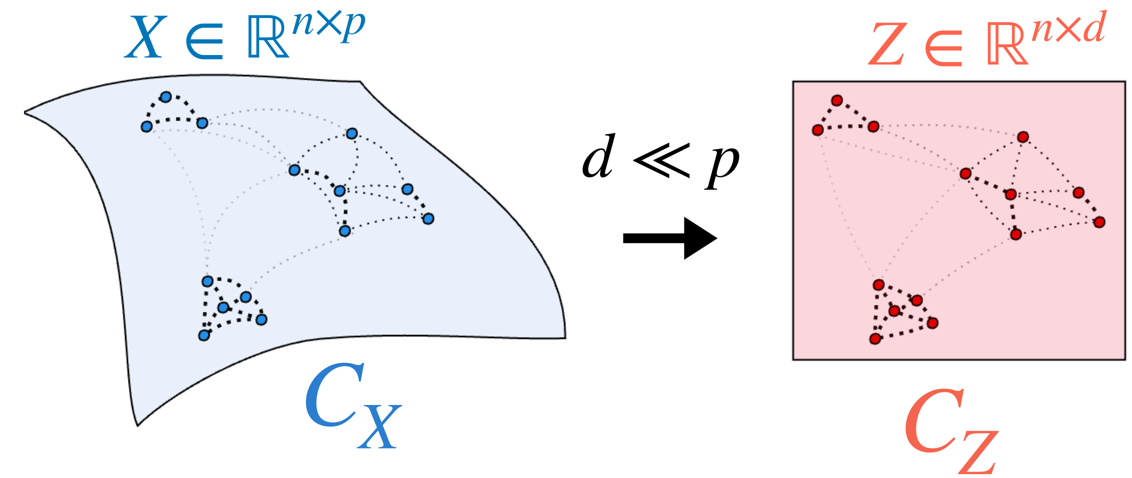
Neighbor embedding methods

✦ C_X is CPD, $L = KL$

$C_Z = \mathrm{diag}(\alpha_Z)\ K_Z\ \mathrm{diag}(\beta_Z)$

where $\log(K_Z)$ is CPD

DR as OT in disguise



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where $\log(K_Z)$ is CPD

e.g. $K_Z = \exp(-\|\mathbf{z}_i - \mathbf{z}_j\|_2^2)$ and its usual normalizations

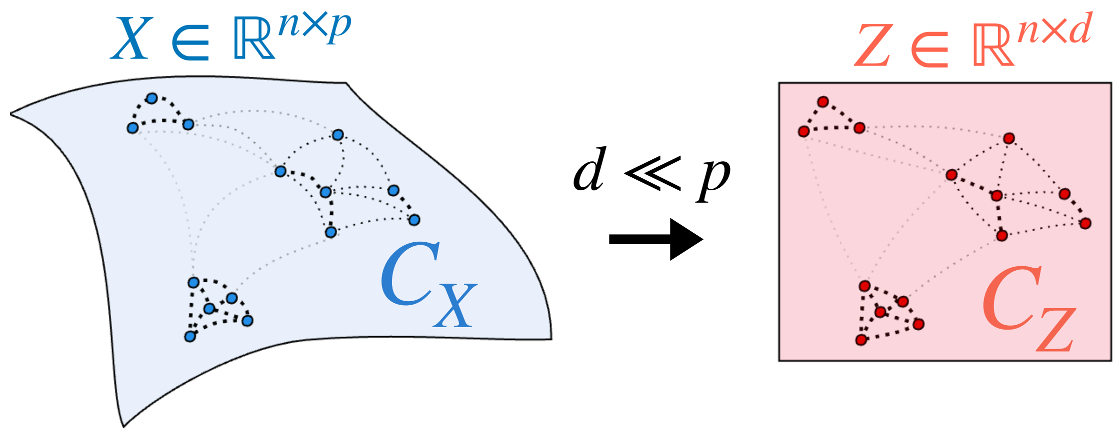
$1_n^\top K_Z 1_n = 1$, $K_Z 1_n = 1_n$, $K_Z^\top 1_n = 1_n$ + $K_Z 1_n = 1_n$

(Sinkhorn & Knopp, 1967)

Beware that C_X is not always CPD.

Distributional reduction

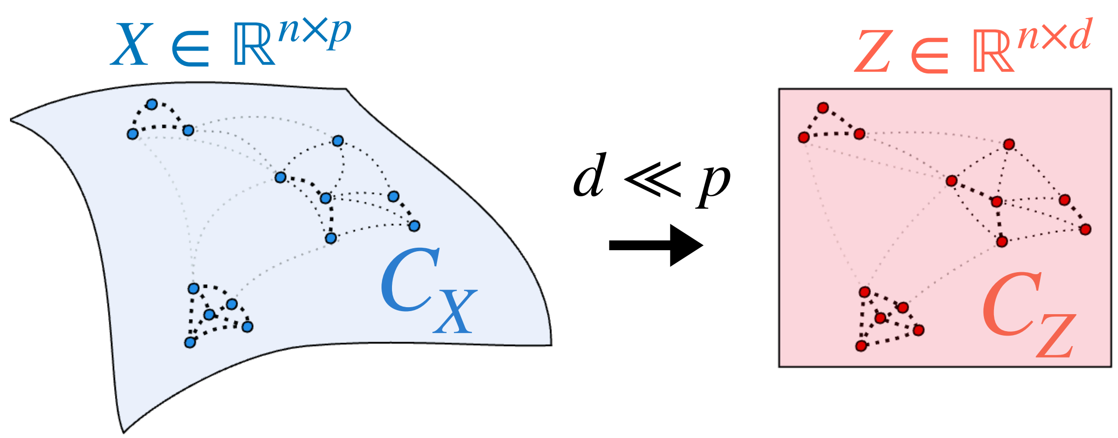
Distributional Reduction



$$\sim \quad \min_{Z \in \mathbb{R}^{n \times d}} \mathrm{GW}_L\left(C_X, C_Z, \frac{1_n}{n}, \frac{1_n}{n}\right)$$

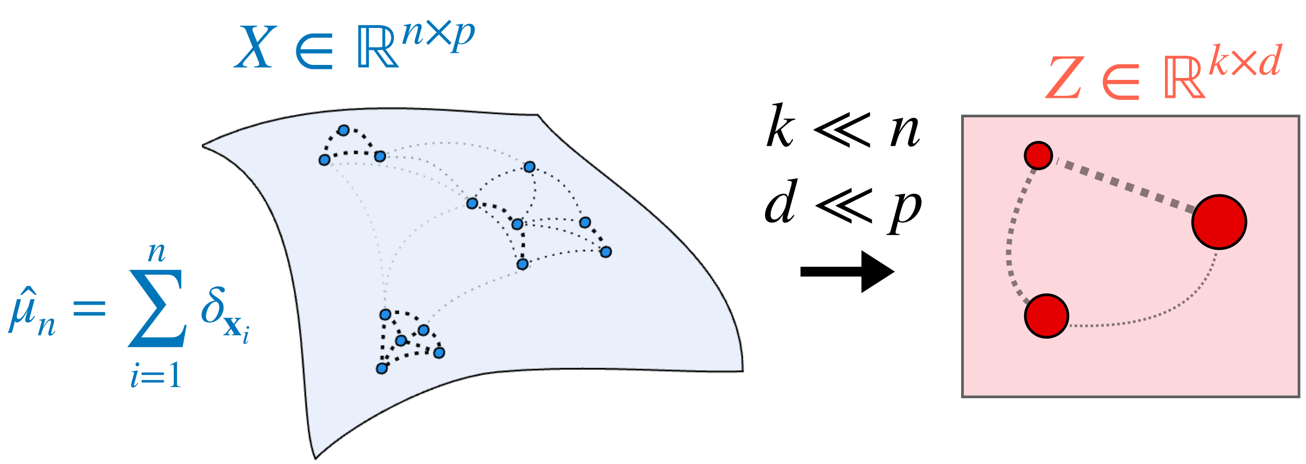
$$\sim \quad \min_{\nu = \frac{1}{n}\sum_{i=1}^{n} \delta_{\mathbf{x}_i}} \mathrm{GW}_L(\hat{\mu}_n, \nu)$$

Distributional Reduction

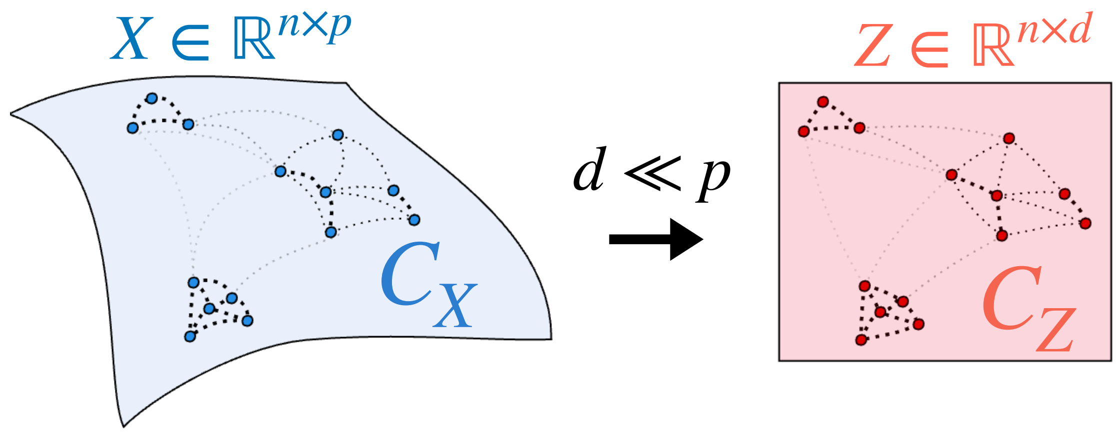


$$\sim \quad \min_{Z\in\mathbb{R}^{n\times d}} \mathrm{GW}_L\left(C_X, C_Z, \frac{1_n}{n}, \frac{1_n}{n}\right)$$

$$\sim \quad \min_{\nu=\frac{1}{n}\sum_{i=1}^{n}\delta_{\mathbf{x}_i}} \mathrm{GW}_L(\hat{\mu}_n, \nu)$$



Distributional Reduction



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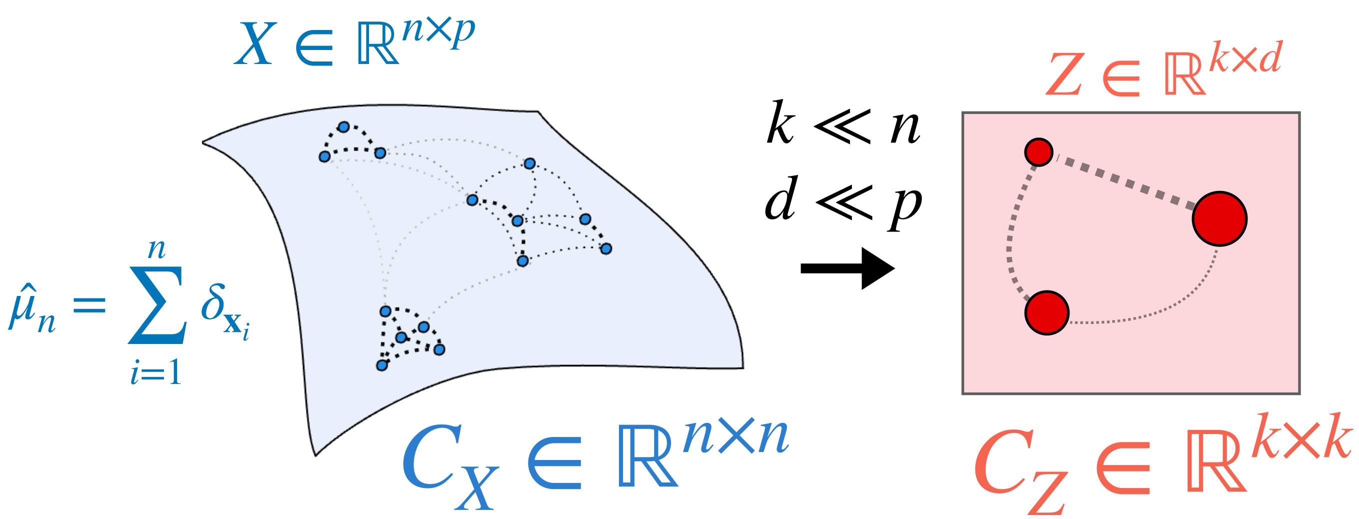
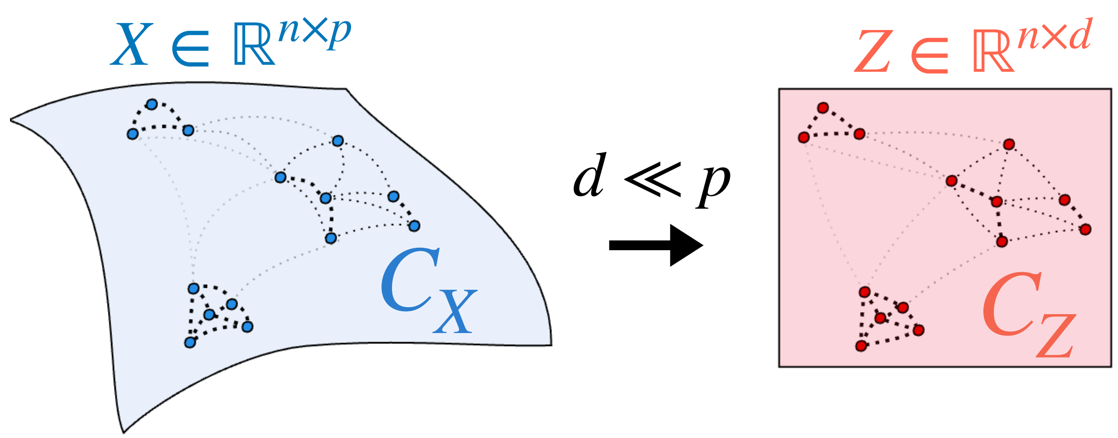


✦ **GW projection**

$$\min_{\nu\in\mathscr{P}_k(\mathbb{R}^d)} \mathrm{GW}(\hat{\mu}_n, \nu) \qquad \nu = \sum_{j=1}^{k} b_j \delta_{\mathbf{z}_j}$$

Distributional Reduction



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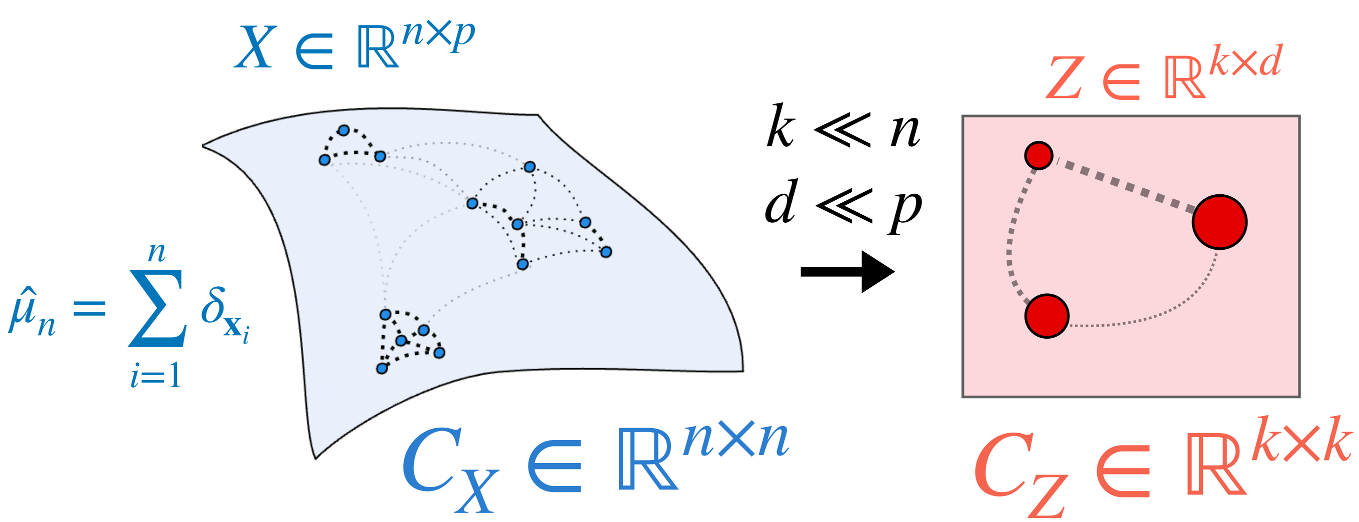

✦ **Optimization problem**

$$\min_{Z\in\mathbb{R}^{k\times d}} \min_{b\in\Sigma_k} \mathrm{GW}_L\left(C_X, C_Z, \frac{1_n}{n}, b\right)$$

- Find **few prototypes** in **low dim.**
- Find the weights / cluster size

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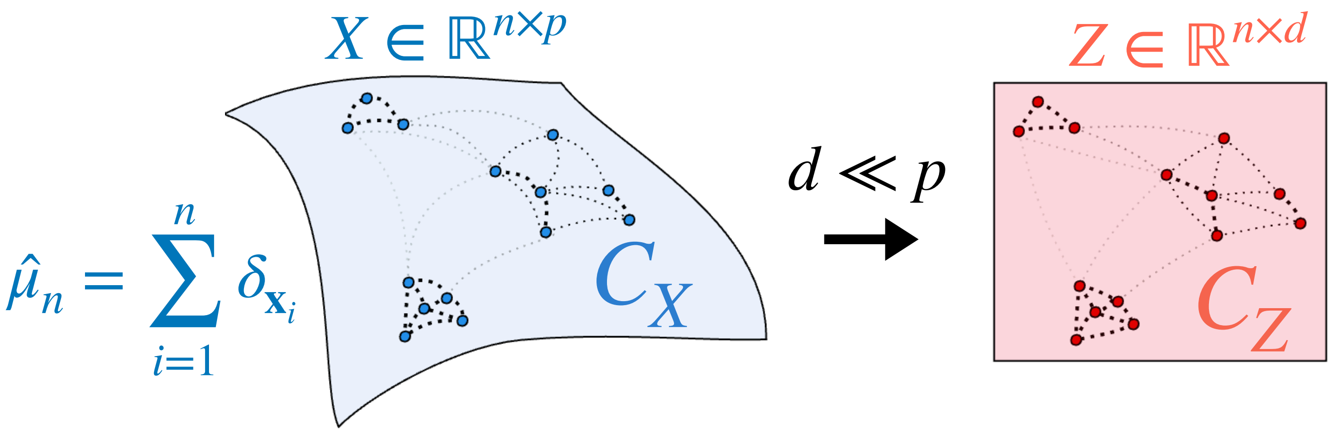

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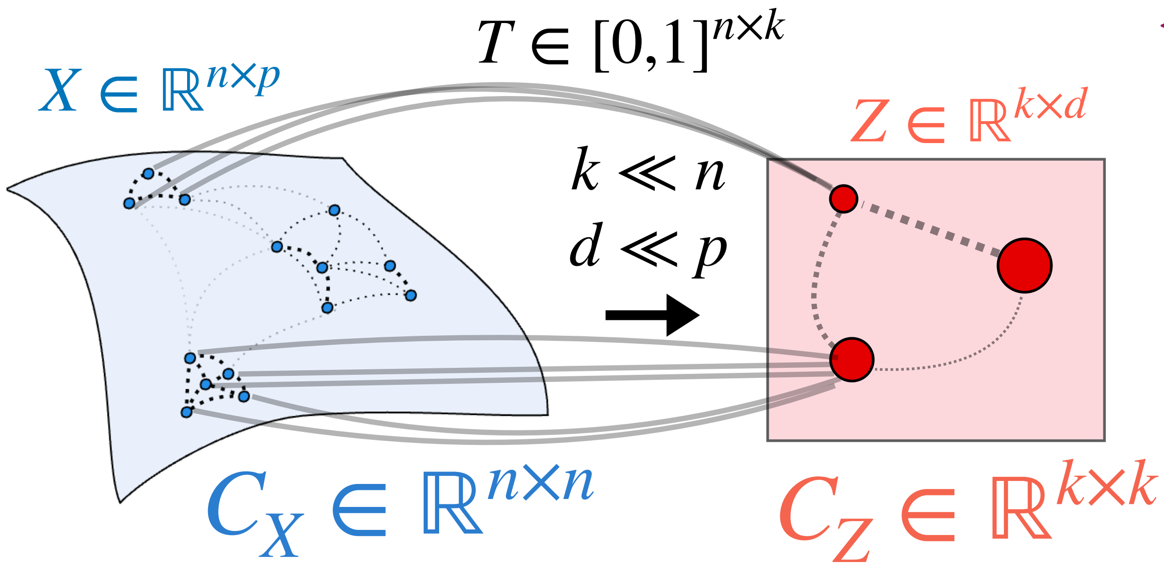

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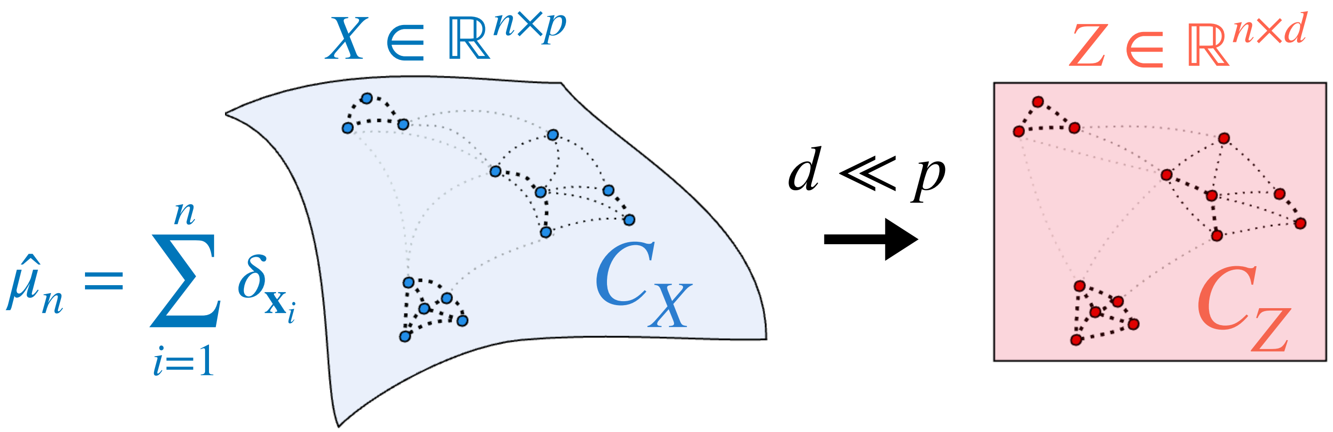
Distributional Reduction



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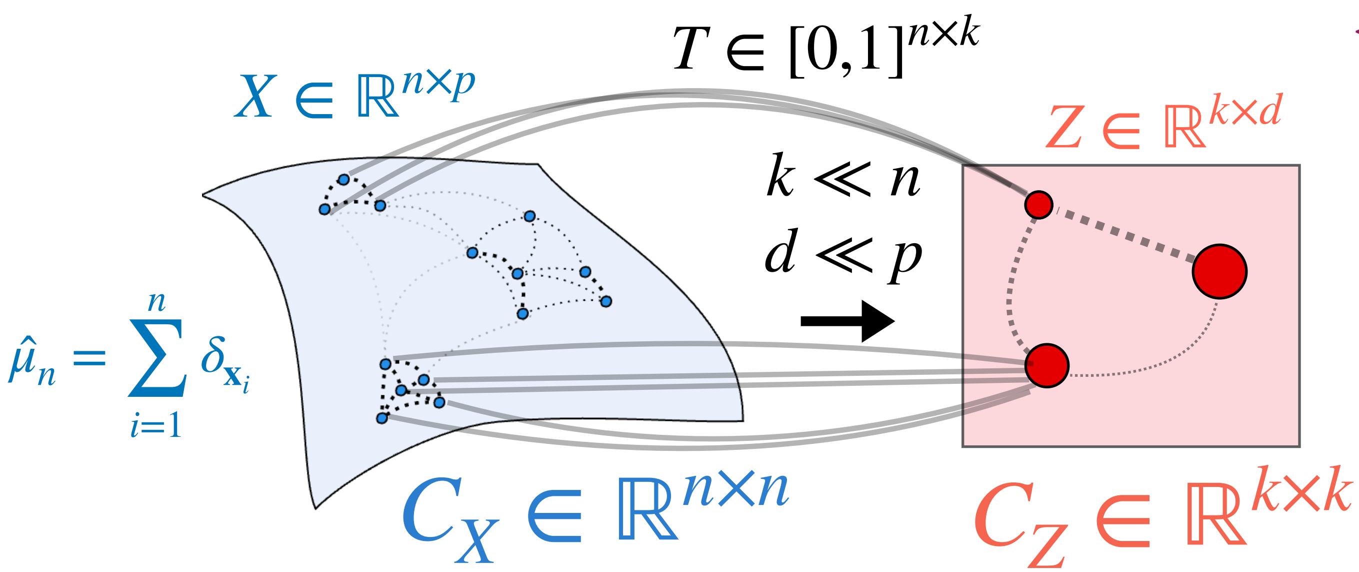

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✦ A semi-relaxed objective

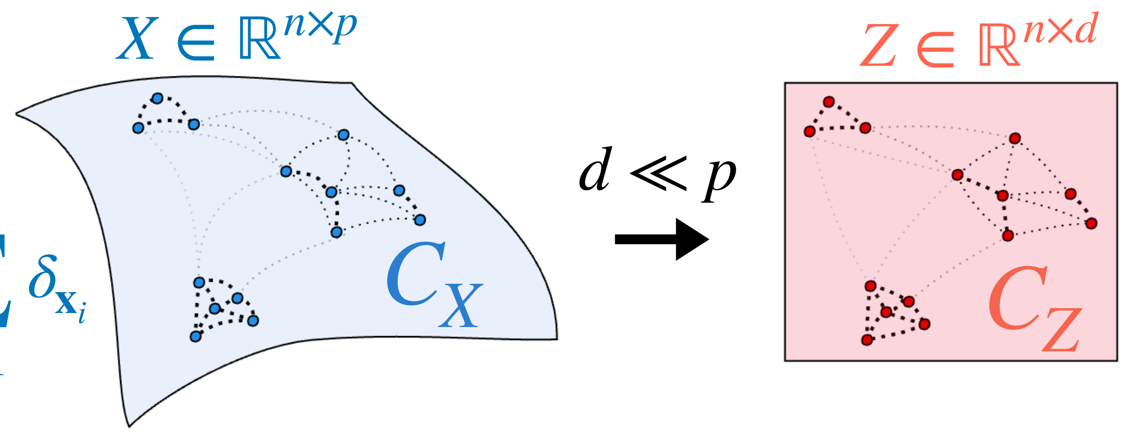
(Vincent-Cuaz et al., 2022)

$$\min_{Z \in \mathbb{R}^{n \times d}} \min_{T : T 1_k = \frac{1_n}{n}} \sum_{ijkl} L\left([C_X]_{ik}, [C_Z]_{jl}\right) T_{ij} T_{kl}$$

→ easier than GW

Distributional Reduction

$$\hat{\mu}_n = \sum_{i=1}^{n} \delta_{\mathbf{x}_i}$$



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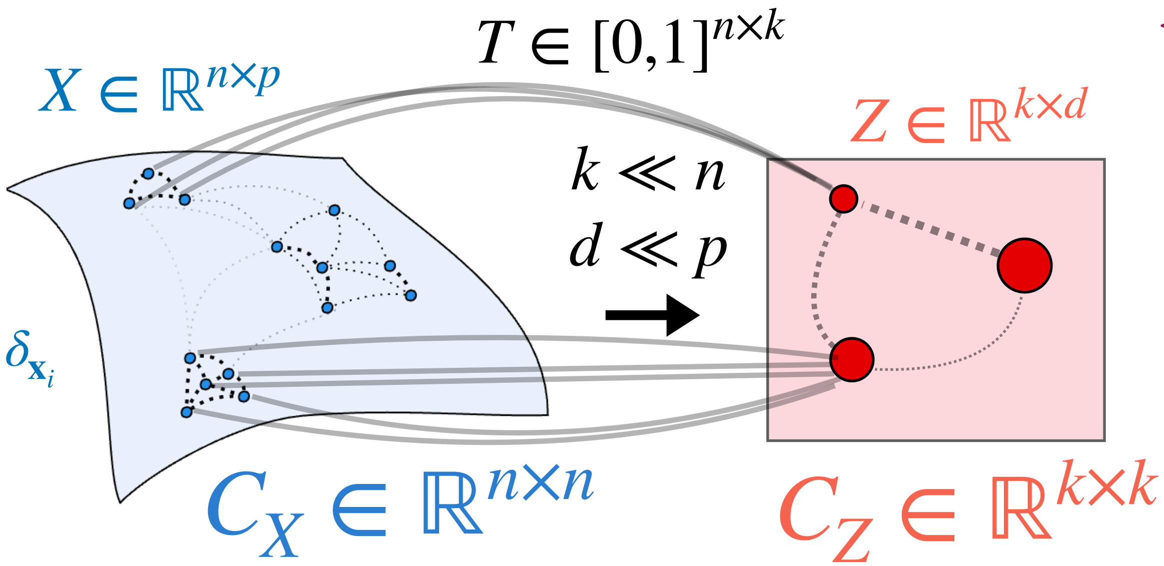

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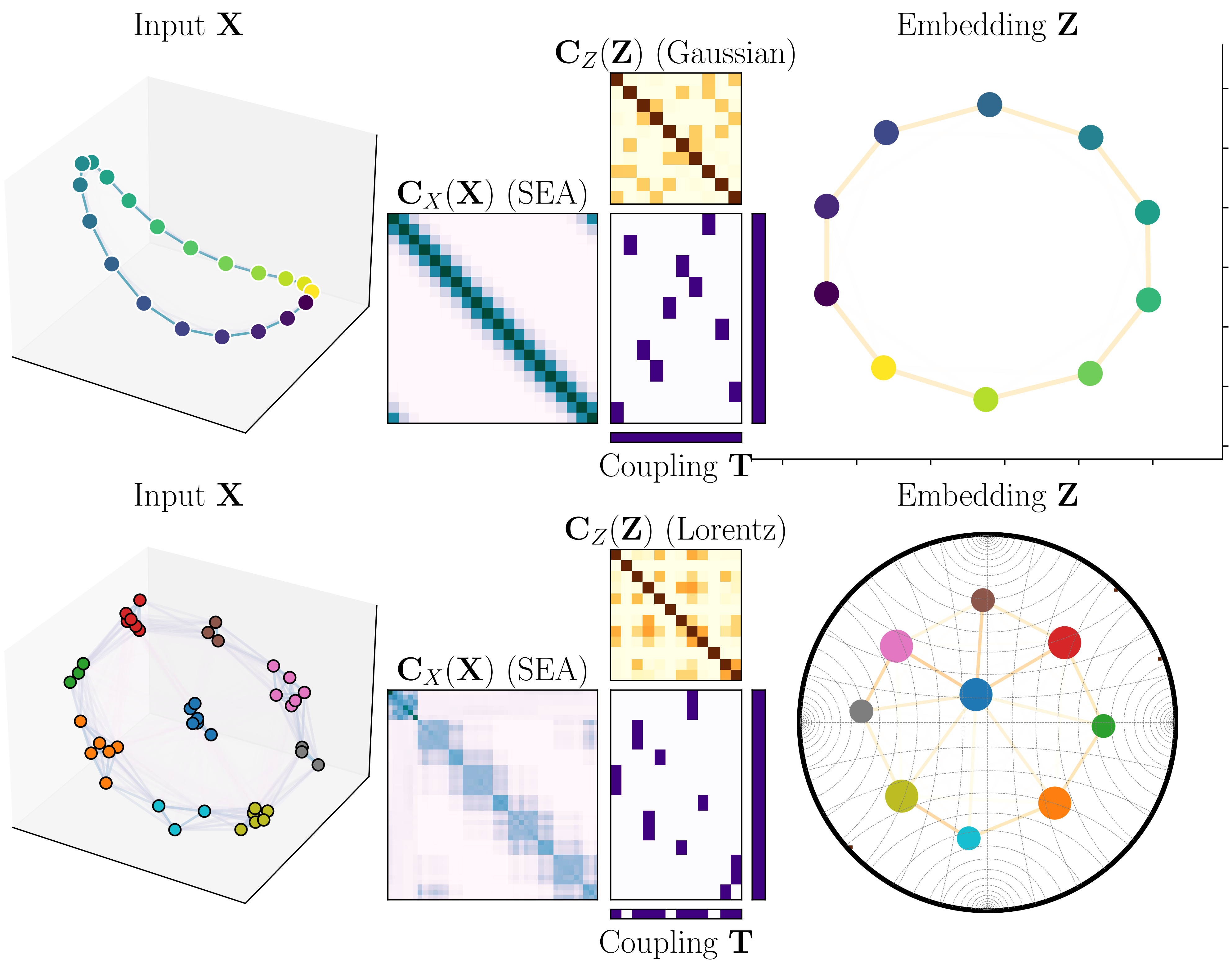
→ easier than GW

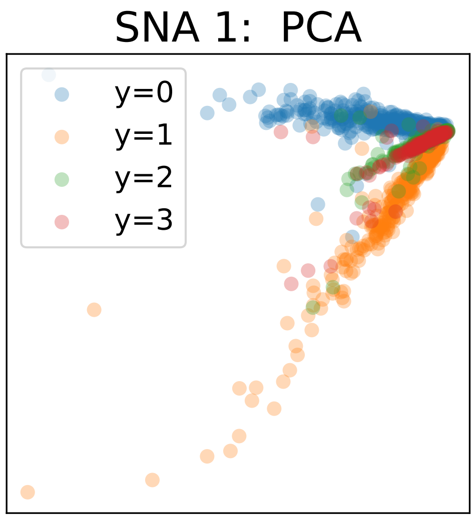
- Non-convex problem
- BCD: alternates optim in Z, in T
- Optim in T: CG solver in $O(n^2 k)$ for $L \in \{\mathrm{KL}, |\cdot|^2\}$
- With low-rank structures $O(nkr + n^2)$

Distributional Reduction



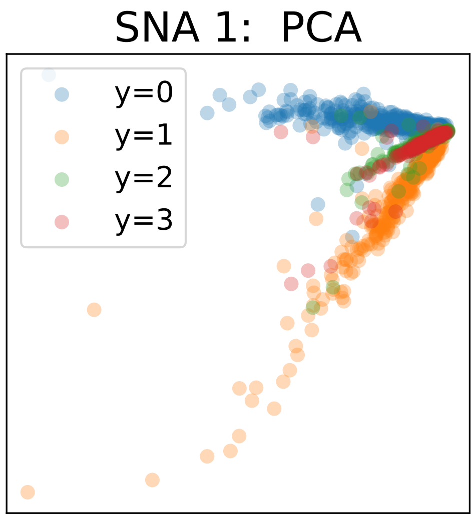
Distributional Reduction

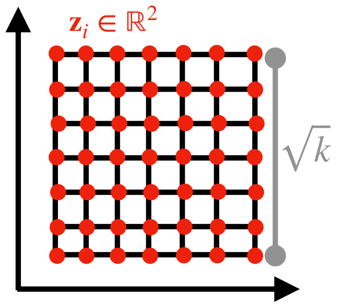
✦ **Single-cell dataset** (Chen et al., 2019) Only solve $\min_{b \in \Sigma_k} \mathrm{GW}_L(C_X, C_Z, \frac{1_n}{n}, b)$



Distributional Reduction

✦ **Single-cell dataset** (Chen et al., 2019) Only solve $\min_{b \in \Sigma_k} \mathrm{GW}_L(C_X, C_Z, \frac{1_n}{n}, b)$ with $C_X = XX^\top$ and $C_Z = ZZ^\top$ **fixed on a grid** $Z \in \mathbb{R}^{k \times 2}$





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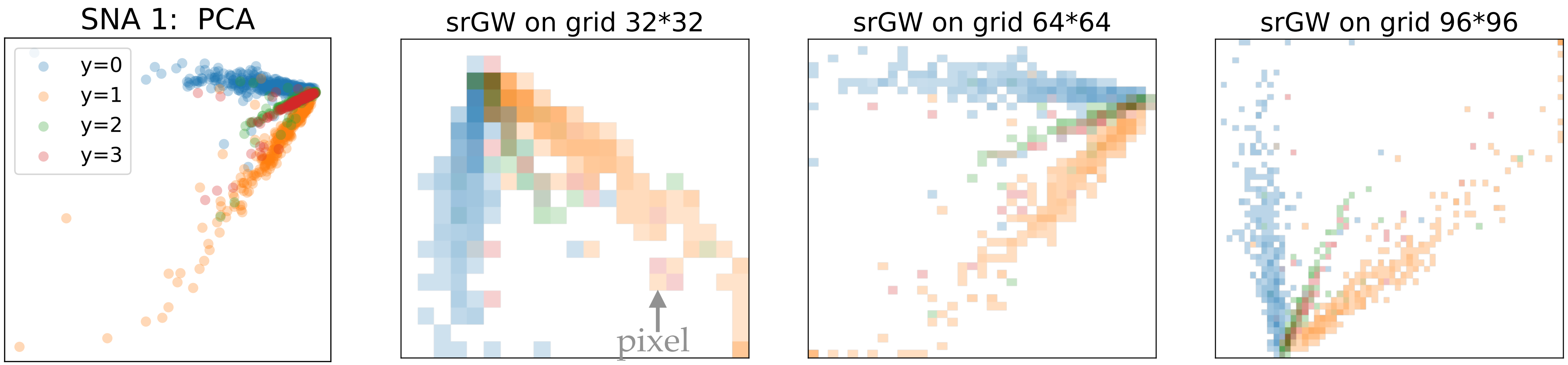
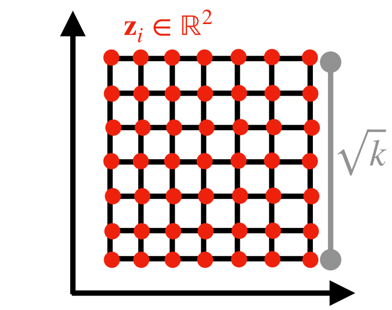


dataset as an image



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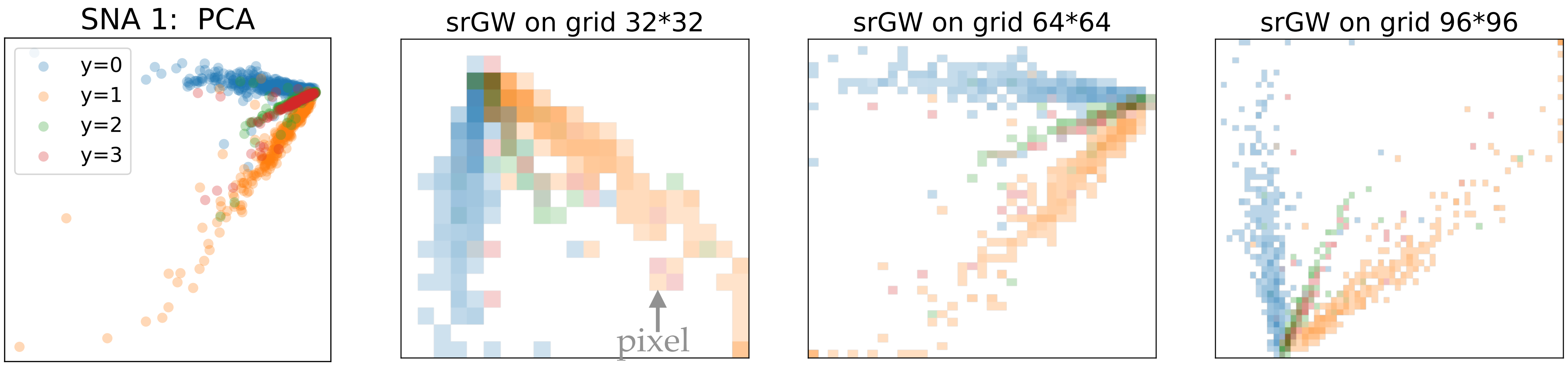
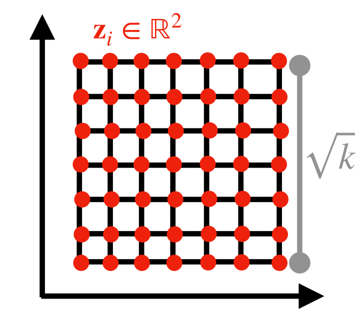
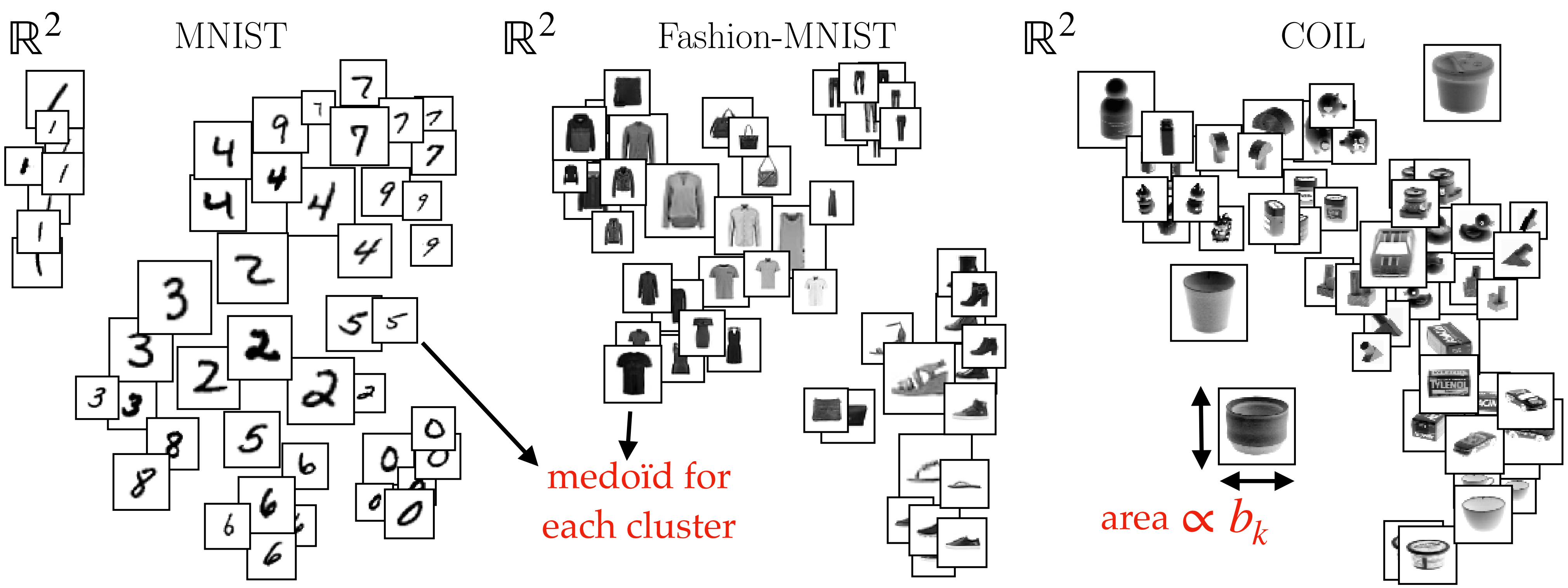




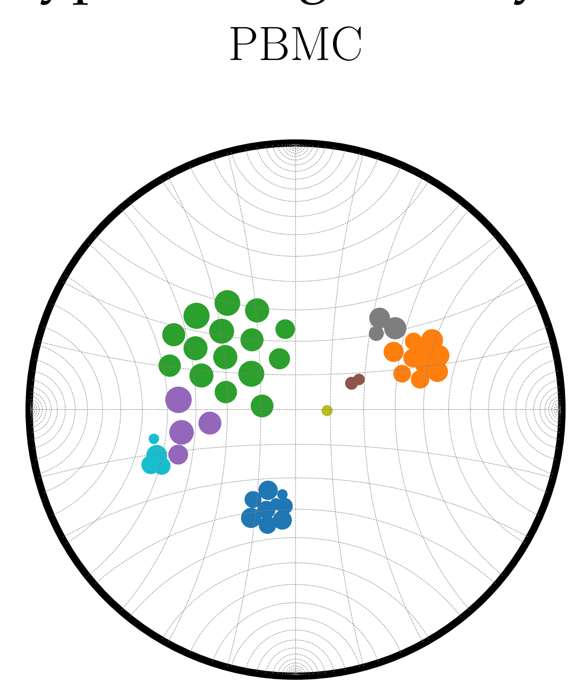
dataset as an image

✦ Image datasets

C_X symmetric entropic aff. (Van Assel et al., 2023) C_Z Student t-kernel

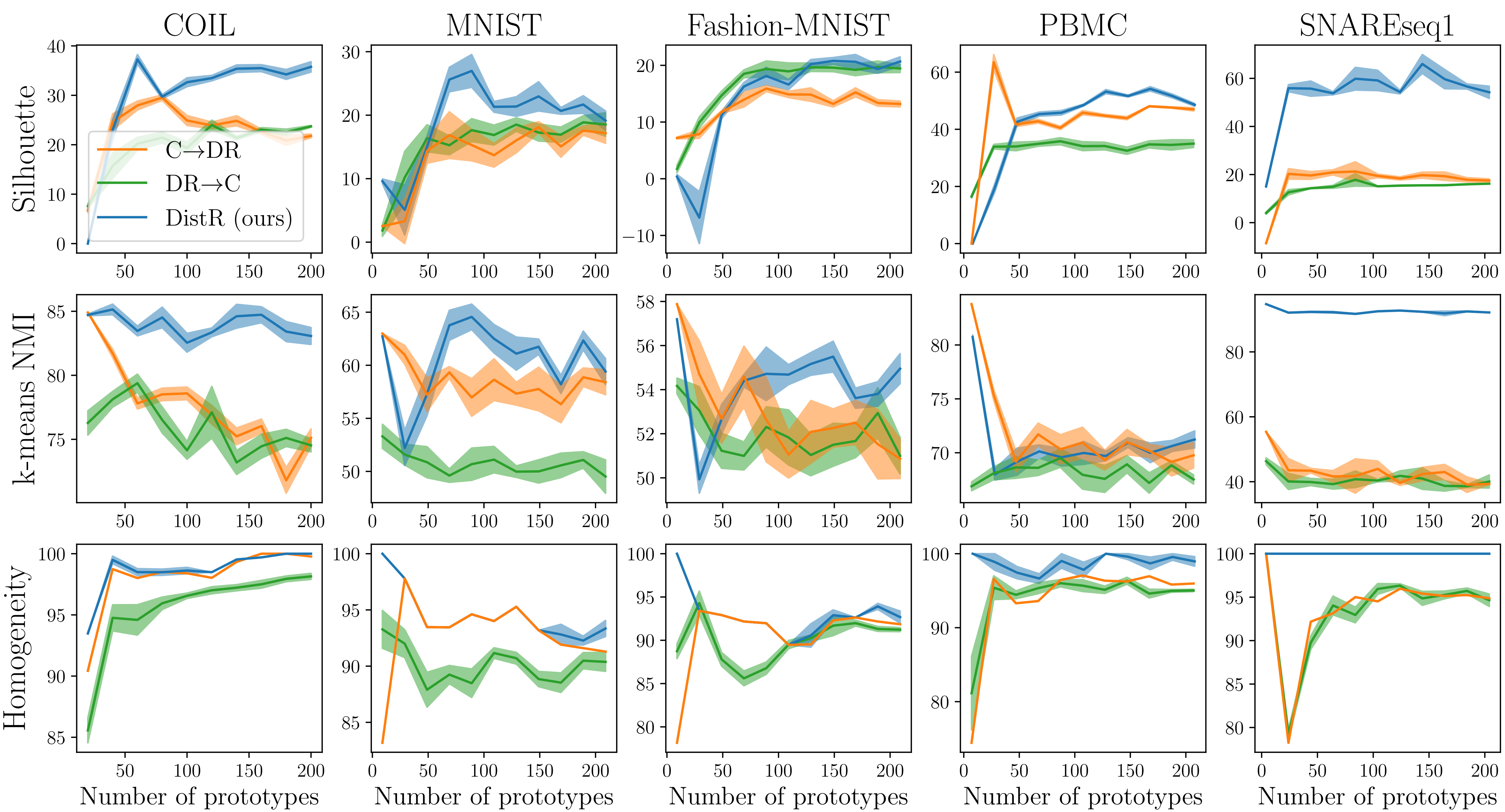


Hyperbolic geometry



Distributional Reduction

✦ Comparison with DR then clustering or clustering then DR



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