Beyond Two-sample-tests: Localizing Data Discrepancies in High-dimensional Spaces

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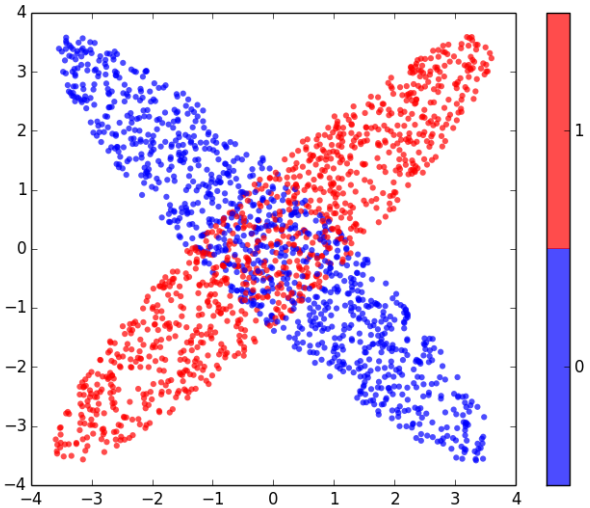
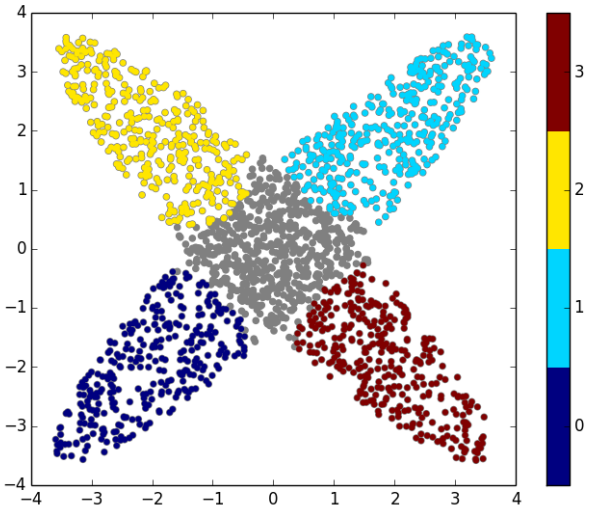




Beyond two-sample tests

Data discrepancies: two-sample problem and effect size

- The two-sample test (TST) approach
  - Two datasets $x^{(n_0)} \equiv \{x_1, \ldots, x_{n_0}\}$ and $y^{(n_1)} \equiv \{y_1, \ldots, y_{n_1}\}$ in $\mathbb{R}^d$
    as i.i.d. samples from two unknown densities f_X and f_Y
  - Hypothesis testing:
    $\mathtt{H}_0 : f_X = f_Y \, a.e.,$
    $\mathtt{H}_1 : \neg \mathtt{H}_0$

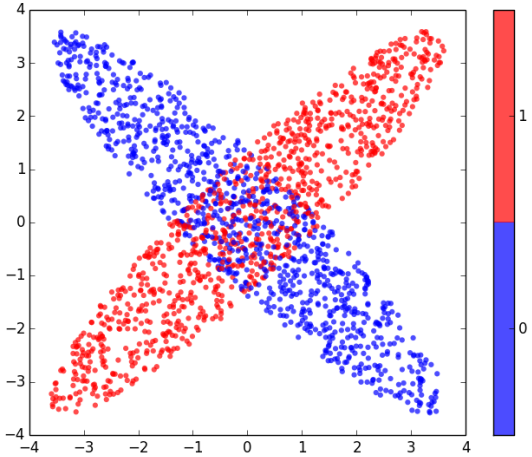
  $\rightarrow$ reject based on p-value: summarizes the difference in one bit!

- Effect size: "quantitative measure of the strength of a phenomenon"
  - p-value: magnitude of the statistical significance?
    for consistent TST: large sample size implies significance
  - effect size: various options for univariate data
    normalized difference between means

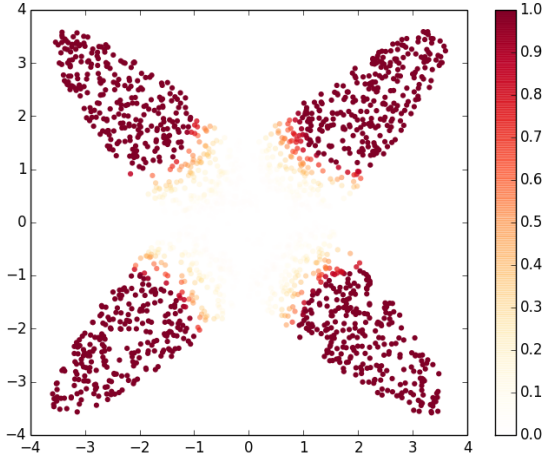
- Towards a notion of nonparametric multivariate effect size:
  - accommodating general discrepancies in $\mathbb{R}^d$
  - amenable to comparisons via some kind of normalization

What do we provide?

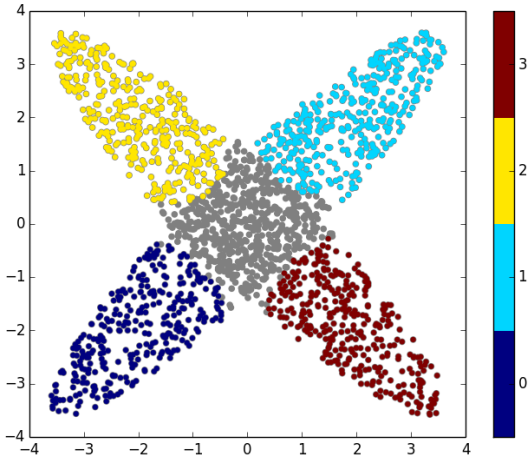
Comparing two point clouds:



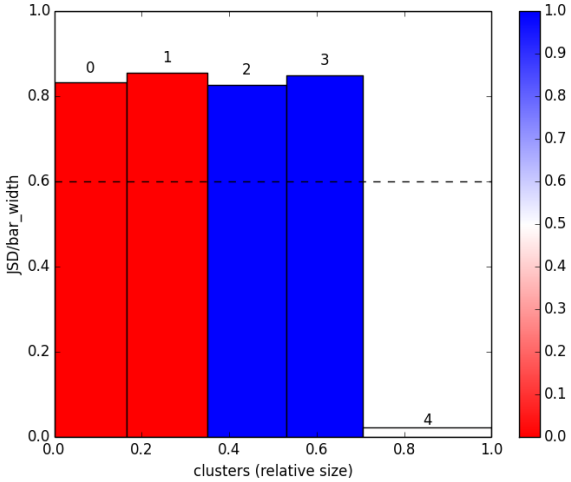
1. compute a local discrepancy,



2. find spatially coherent regions of high discrepancy,



3. provide a cluster based normalized effect size.



Outline of our method: three steps

- **Step 1:** Estimate a measure of local discrepancy at each given point
  - Ingredient: information theory
- **Step 2:** Aggregate local discrepancy in a spatially coherent way, to produce clusters by removing low discrepancy points
  - Ingredient: topological persistence
- **Step 3:** Produce an effect size barplot to summarize the discrepancy profile
- **Aftermath:** Assess the stability of clusters

Beyond two-sample tests

Pre-requisite: Jensen-Shannon divergence

▷ Kullback-Leibler divergence (KLD):

$$\begin{cases} D_{\mathrm{KL}}\left(f \| g\right) \equiv \int_{-\infty}^{\infty} f(x) \log \frac{f(x)}{g(x)} dx \\ \\ D_{\mathrm{KL}}\left(P \| Q\right) \equiv \sum_{l \in \mathcal{A}} P(l) \log \frac{P(l)}{Q(l)} \end{cases}$$

▷ The Jensen-Shannon divergence (JSD): symmetrizes and smoothes the KLD:
Consider $f \equiv (f_X + f_Y)/2$, then

$$JS\left(f_X \| f_Y\right) \equiv \frac{1}{2}\left(D_{\mathrm{KL}}\left(f_X \| f\right) + D_{\mathrm{KL}}\left(f_Y \| f\right)\right)$$

▷ Main properties of JS divergence:

- JSD is symmetric
- JSD is bounded between 0 and 1
- Its square root yields a metric

Step 1: Jensen-Shannon divergence and its decomposition

- Notations: two unknown densities f_X and f_Y, and the associated samples $x^{(n_0)}$ and $y^{(n_1)}$

- Define two random variables:
  - a position variable Z with density $f_Z \equiv f = (f_X + f_Y)/2$
  - a binary label $L \in \{0, 1\}$ with pmf $P(0) = 1/2$,
    indicating from which density (f_X or f_Y) an instance of Z is obtained.

- Equivalently, one defines a random vector:

$$(L, Z) = \begin{cases} (0, X) & \text{with prob. } \frac{1}{2} \\ (1, Y) & \text{with prob. } \frac{1}{2} \end{cases}$$

- Associated conditional and unconditional mass functions:

$$\begin{cases} P(l|z) = \mathbb{P}(L = l | Z = z) \\ P(l) = \mathbb{P}(L = l) = \frac{1}{2} \end{cases}$$

- Lemma: the JSD can be expressed as:

$$JS(f_X \| f_Y) = \int_{\mathbb{R}^d} f_Z(z) D_{\mathrm{KL}}(P(\cdot|z) \| P(\cdot))\, dz$$

Step 1: the local discrepancy

- From
$$JS(f_X \| f_Y) = \int_{\mathbb{R}^d} f_Z(z) D_{\mathrm{KL}}\left(P(\cdot|z) \| P(\cdot)\right) dz$$
- We define the *discrepancy* at location z as
$$\delta(z) \equiv D_{\mathrm{KL}}\left(P(\cdot|z) \| P(\cdot)\right).$$
- Observation:
  - $\delta(z) \in [0,1]$ and $\delta(z) = 0 \Leftrightarrow f_X(z) = f_Y(z)$.
    NB: $P(I) = 1/2$; logarithm in base 2
- Exploiting the discrepancy: $P(I)$ is known but $P(I|z)$ is not:

  we need to estimate $P(I|z)$ at each given location z.

Step 1: random design nonparametric regression

- Consider random variables: location $Z \in \mathbb{R}^d$, and response variable $R \in \mathbb{R}$
- Associated regression function:

$$m(z) \equiv \mathbb{E}\left[R|Z = z\right].$$

- Consider data: $\{(Z_i, R_i)\}_{i=1,\ldots,n}$
- k_n-nearest neighbor regressor: upon sorting samples by increasing distance to the query point z:

$$m_n(z) = \frac{1}{k_n} \sum_{i=1,\ldots,k_n} R_{(i,n)}(z)$$

▷Ref: L. Györfi and A. Krzyzak; A distribution-free theory of nonparametric regression; 2002

▷Ref: S. Kpotufe, NIPS 2011

Step 1: estimation via k-nearest neighbors

- Using the labels as response variable i.e. $R \equiv L$
- Using n i.i.d. realizations of (L, Z): build an estimator $m_n(z)$ for

$$m(z) = \mathbb{E}\left[L|Z = z\right] = P(1|z).$$

- Define the following estimator for $P(l|z)$: if $0 \leq m_n(z) \leq 1$:

$$\hat{P}_n\left(l|z\right) \equiv |1 - l - m_n(z)|.$$

- Thm: Using a k_n-nearest neighbor regressor, s.t. $\frac{k_n}{\log n} \to \infty$ and $\frac{k_n}{n} \to 0$:

$$\hat{\delta}_n(z) \equiv D_{\mathrm{KL}}\left(\hat{P}_n\left(\cdot|z\right)\|P(\cdot)\right) \xrightarrow{n\to\infty} \delta(z) \text{ a.s.}$$

for f-almost all $z \in \mathbb{R}^d$.

The random multiplexer to obtain i.i.d. realizations of (L, Z)

▷ A random sampler produces i.i.d. realizations of (Z, L) from $x^{(n_0)}$ and $y^{(n_1)}$:

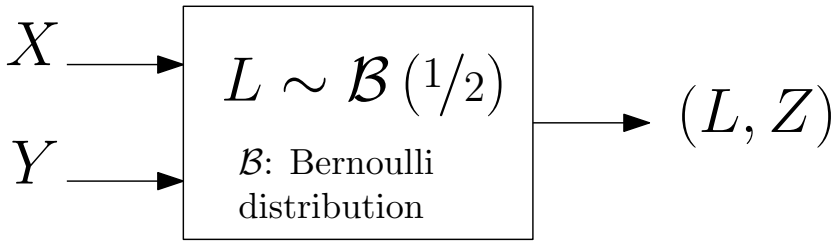


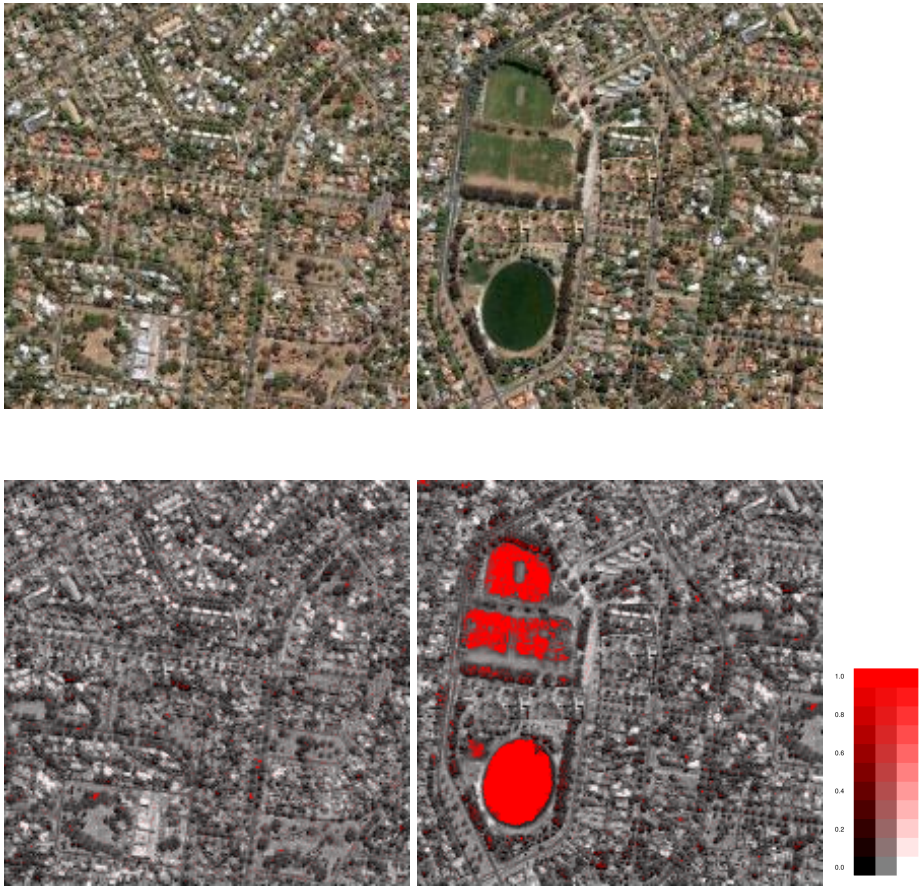
Figure: **Random multiplexer generating pairs (label, position).**

▷ The case of uneven populations:

– the multiplexer will consume faster the *small* population, and halt
– unused samples of the large population remain – detrimental information loss
– resample B times and take the median of estimates, on a per sample basis

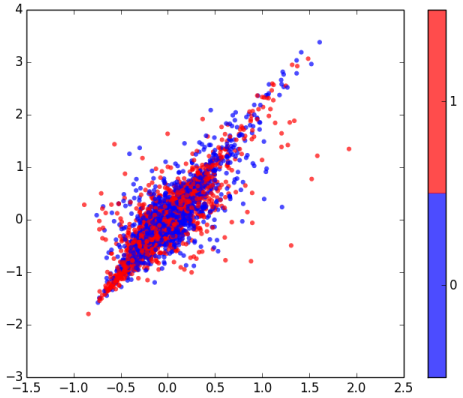
Step 1: Illustration: statistical image comparison

- ▷ Images: taking 2×2 blocks + (R,G,B) color coding: yields points in $\mathbb{R}^{12}$.
- ▷ Discrepancy estimate: using $k_n = n^{1/3}$
- ▷ Discrepancy plot: interpolate gray scale pixel color with red scale representing discrepancy at each pixel (upper left corner of the corresponding block)

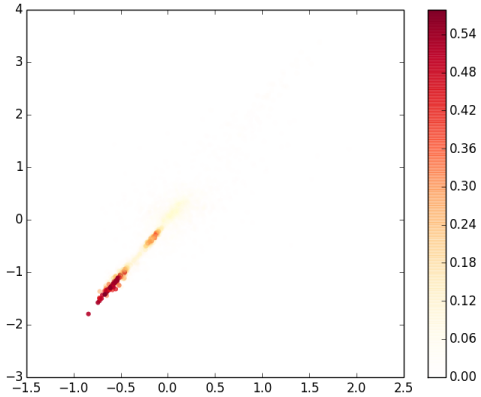


▷ Multidimensional Scaling of parameter space:

The two populations in $\mathbb{R}^2$...



...colored with $\hat{\delta}$:



Beyond two-sample tests

ToMATo: Topological Mode Analysis Tool

Persistence based clustering algorithm

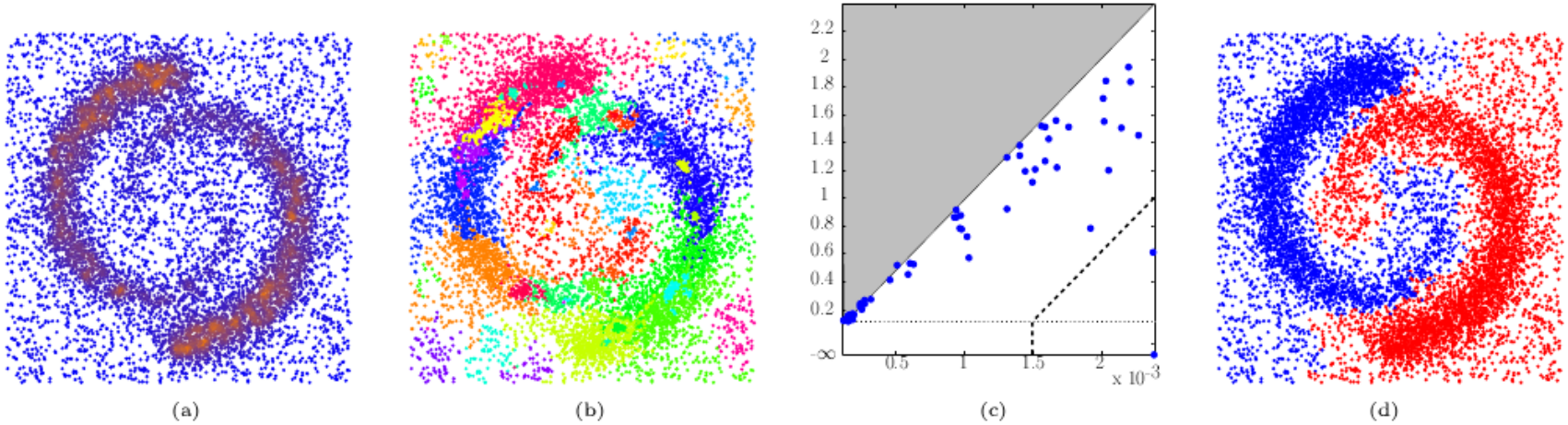
- Mode seeking strategy
  - Input: points sampled on a manifold
  - From a density estimation: height $\equiv$ estimated density
  - Find the persistent modes: one cluster per mode

    Step 1: build G^+

    Step 2: top-down processing yield potential merges between peaks
  - Key benefits

    existence diagram: estimate of the # of clusters

    works in a Riemannian setting—points on a manifold
- W.r.t. Morse theory: persistent maxima and their stable manifolds

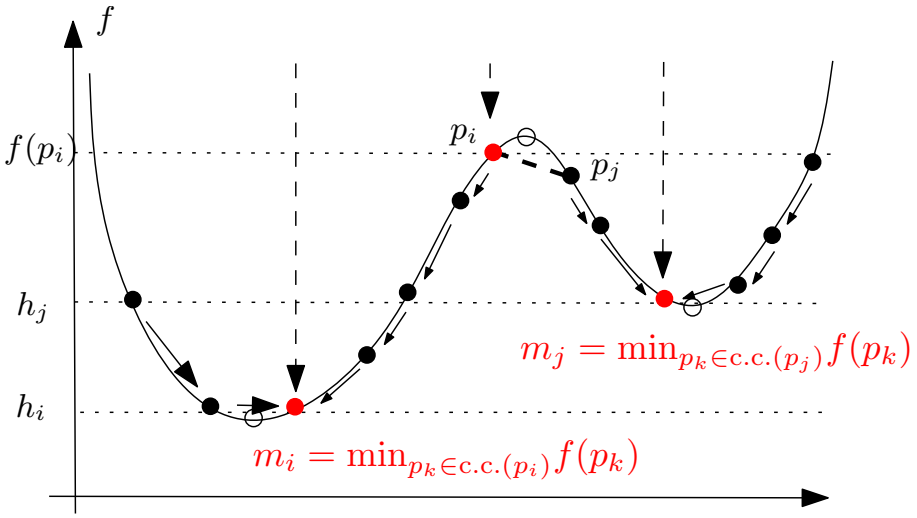


- Ref: Chazal, Guibas, Oudot, Skraba; ACM SoCG 2011

Persistent Minima and Sub-level Set Extraction from Samples: the Tomato Algorithm

- ▷ Input: NNG connecting samples on the landscape
- ▷ Output: DG + persistence diagram + one sub-level set
- ▷ Algorithm: relies on three operations at once, in 2 passes
- – quenches samples to their minima using a NNG discrete quench)
- – finds *bifurcations* i.e. pairs of sample across a *ridge*
- – cancels *non persistent basins* on the fly (Union-Find algorithm)

- – Variant if all samples have been quenched:
  detection of adjacencies between basins (yet: overestimation of barriers)

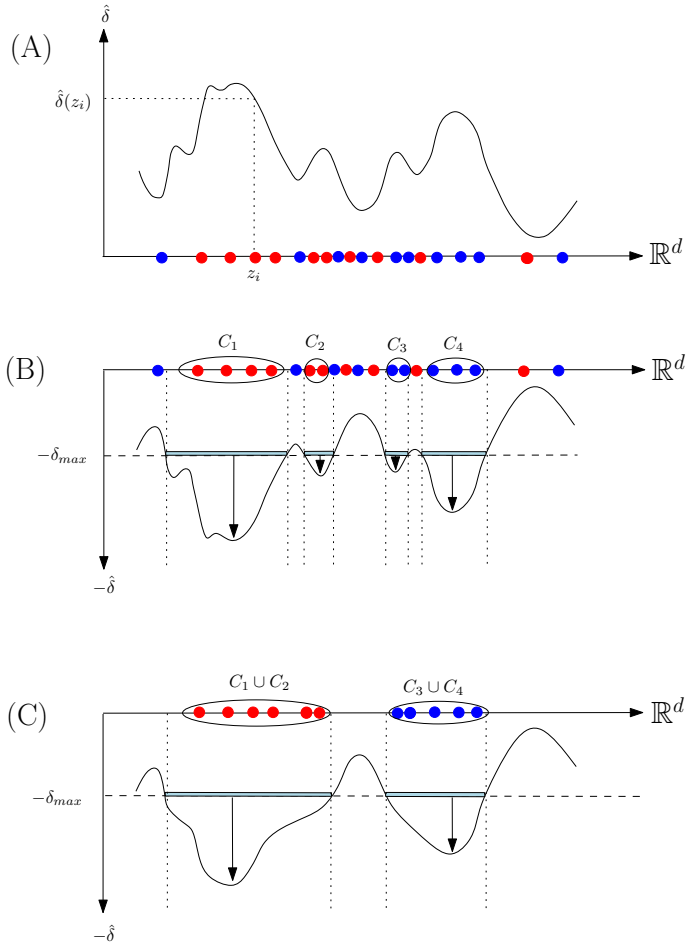


▷Ref: Chazal, Guibas, Oudot, Skraba; ACM SoCG 2011

Beyond two-sample tests

Step 2: Building the clusters from sublevel sets of $-\hat{\delta}(z)$

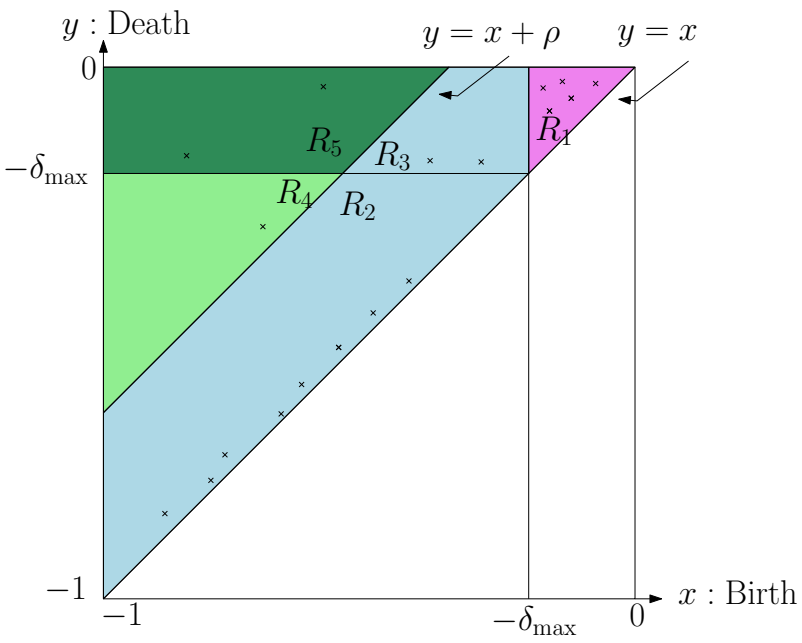
- Ingredients:
  - Height function $-\hat{\delta}(z)$ modeled with nearest neighbor graph
  - Parameter: discrepancy/significance threshold δ_{max}
- Construction:
  - Idea: one cluster $\sim$ one connected component of the sublevel set of $-\hat{\delta}(z)$ defined by δ_{max}
  - Extra ingredient: smoothing the landscape to get rid of small clusters : smoothing using topological persistence at threshold ρ



Step 2: Building the clusters: persistence diagram

▷ Partition of the PD induced by:

- Significance threshold δ_{max}
- Persistence threshold ρ



▷ Local minimum m of $-\hat{\delta}(z)$:

- Selected/rejected: m was born before $-\delta_{max}$.
- Persistent/canceled: persistence$(m) \geq \rho$
- Filtered (un-filtered): the catchment basin of m dies after (before) $-\delta_{max}$.

▷ Observation:

- # clusters : 1 + # points in region R_5 of the PD.
- # persistent local minima : 1 + num points in the region $R_4 \cup R_5$ of the PD.

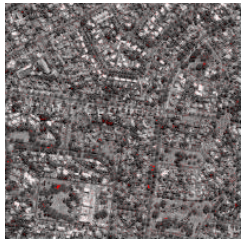
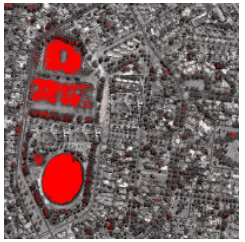
▷Ref: Chazal, Guibas, Oudot, Skraba, J. ACM, 2013

▷Ref: Cazals and D. Cohen-Steiner, CGTA, 2011

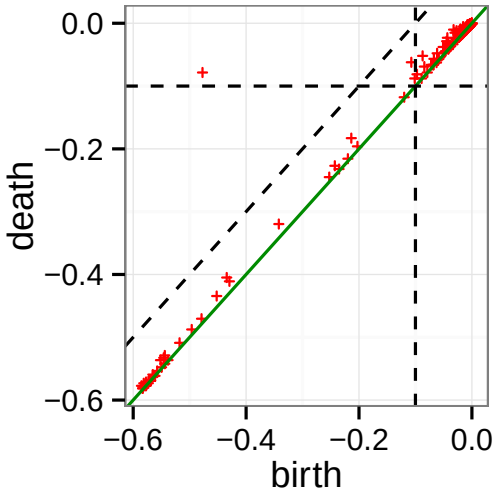
Step 2: Illustration: statistical image comparison

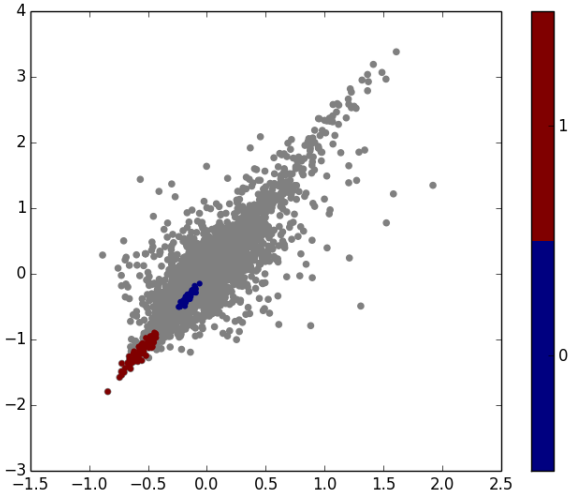
- Images again:



- Parameters: $k = 10$ (NNG), $\rho = 0.1, \delta_{max} = 0.1$





Beyond two-sample tests

Step 3: Effect size: discrepancy profile

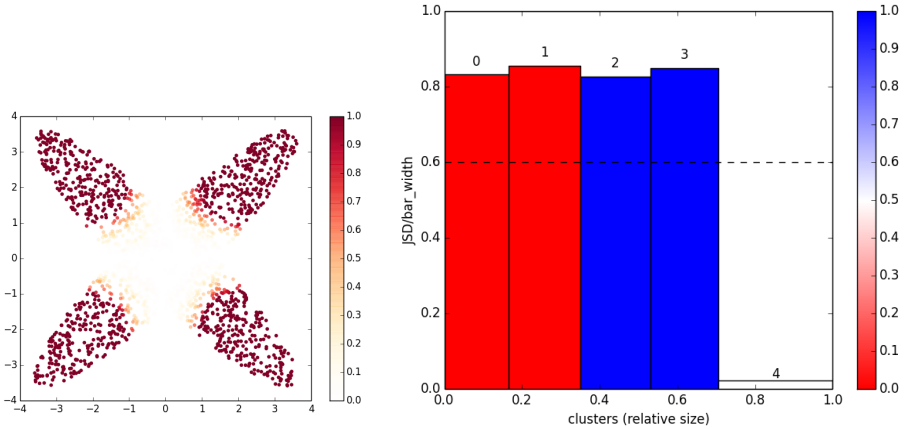
- Global estimated JSD: area under dashed line
- Maximum JSD: area under continuous line (=1)
- Contribution of each cluster C to JSD: area of bar

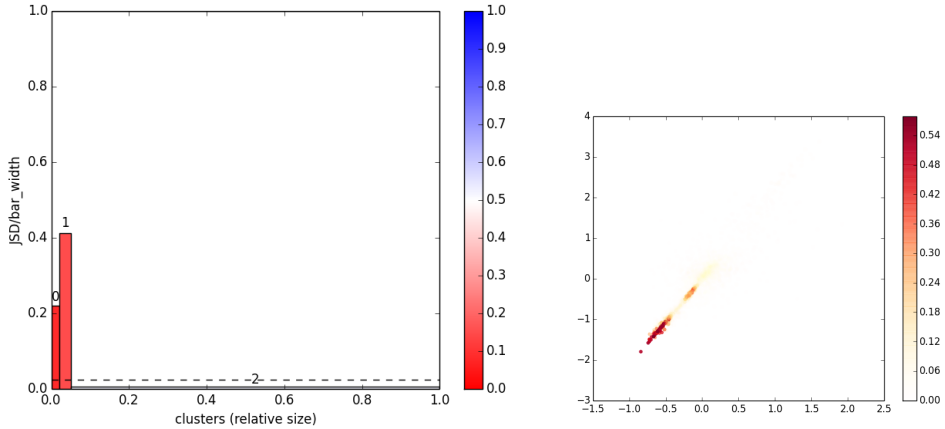
$$JS_C\left(f_X \| f_Y\right) \equiv \frac{1}{n_0 + n_1} \sum_{z \in (x^{(n_0)} \cup y^{(n_1)}) \cap C} \hat{\delta}(z).$$

- Mass of each cluster: bar width
- Population balance in each cluster: bar color (heat map)

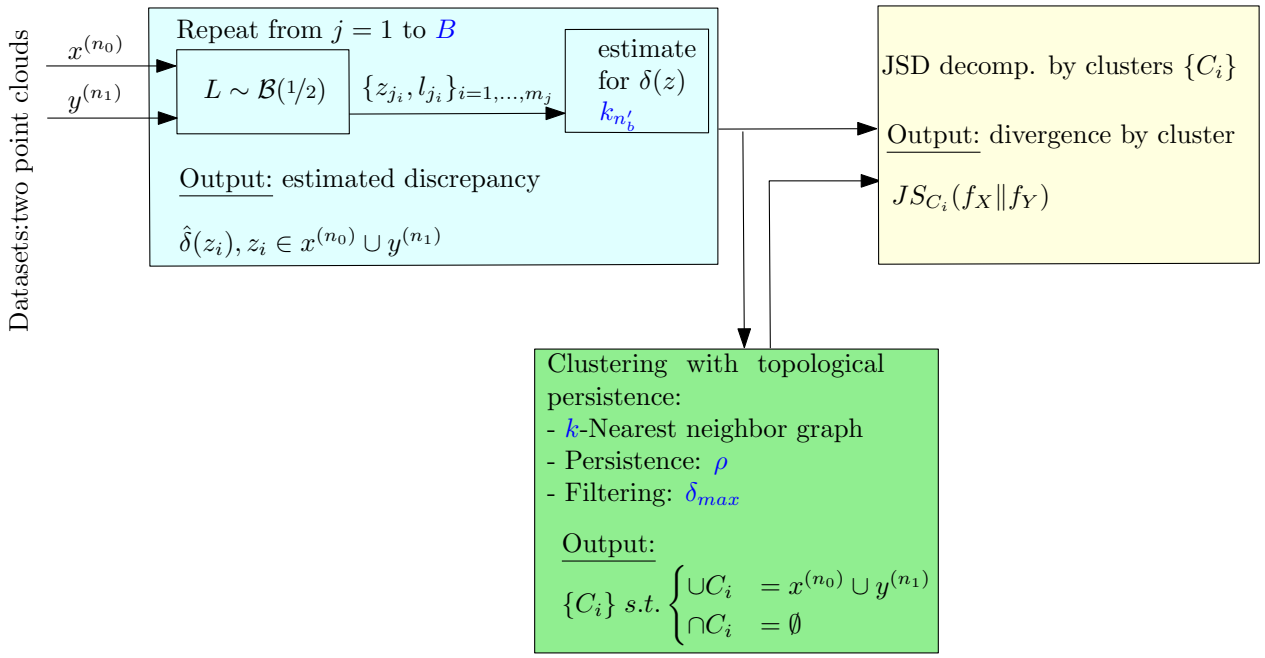
- Ellipses:
  - Large global JSD (dashed line)
  - Contributed by 2+2 balanced clusters

- Images:
  - Smaller global JSD (dashed line)
  - Contributed by 2 clusters





Wrapping-up: workflow

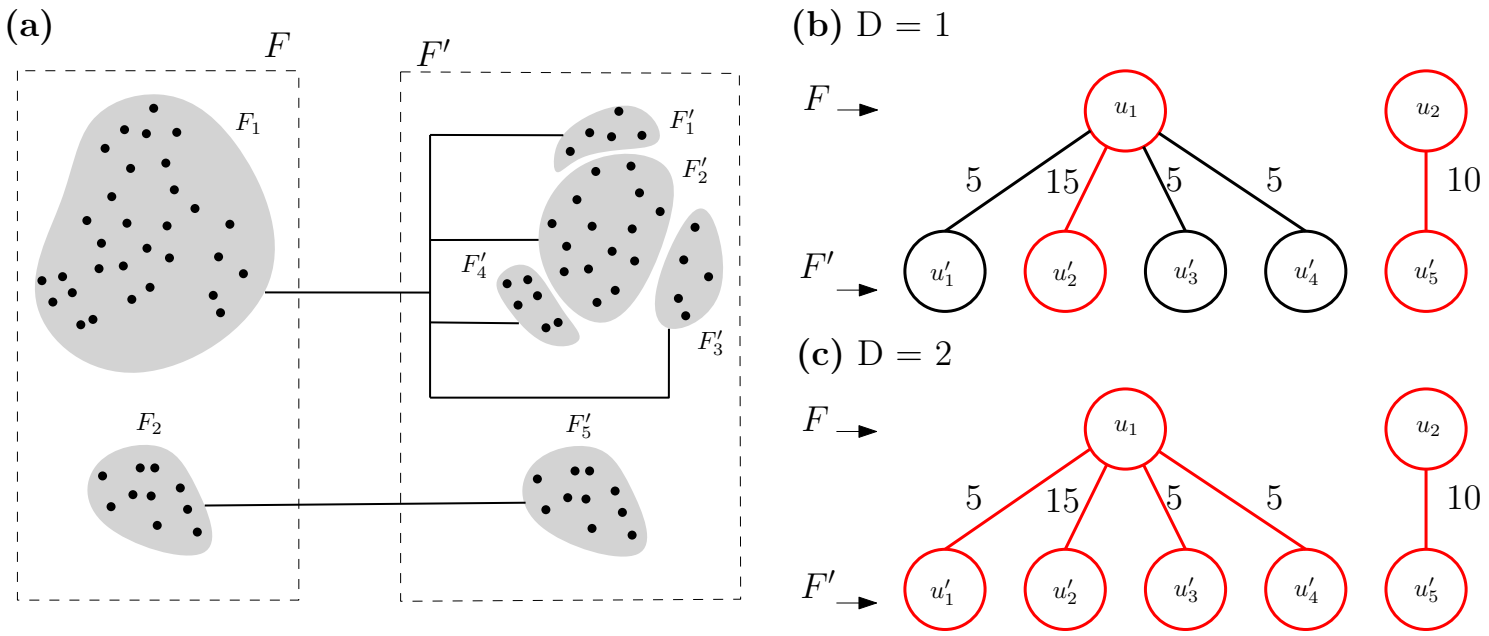


- ▷ Compulsory parameters:
  - k_n: regression parameter
  - δ_{max}: discrepancy significance threshold
  - ρ: persistence threshold
  - k: number of nearest neighbors for the persistence analysis
- ▷ Optional parameter:
  - B: num. repetition in case of unbalanced populations

Beyond two-sample tests

On the stability of clusterings

- Question: are the clusters stable w.r.t. these compulsory parameters?



- General approach: comparing clusterings via clusters of clusters
  - Find a matching between clusters of clusters, called meta-clusters
  - Controlled by a parameter D monitoring the diameter of meta-clusters
    In the example: compare $D = 1$ vs $D = 2$

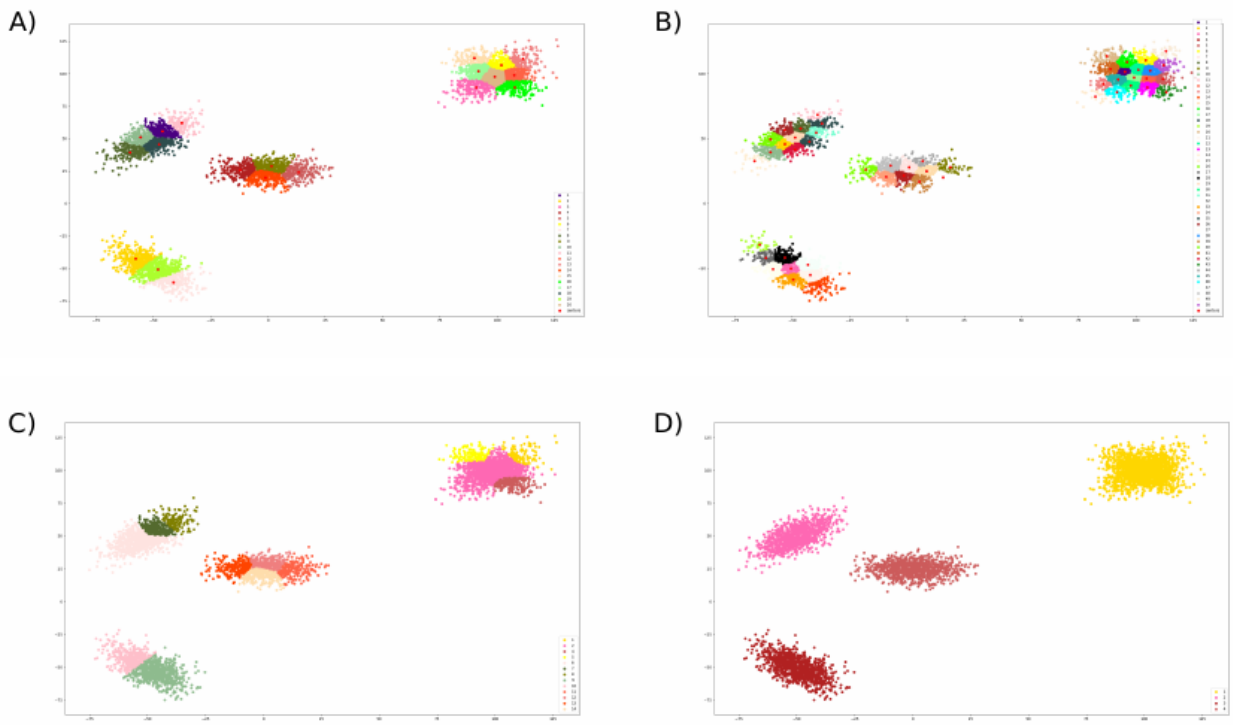
Comparing clusterings: at which *scale* do clusters merge?

What is the *right* number of clusters?

- ▷ Example:
  - Using `k-means++` to cluster 5000 samples from five Gaussian blobs
  - Using D-family matching to infer the *right/natural* # of clusters

(A) k-means++, $k = 20$

(B) k-means++, $k = 50$



(C) $D = 3$, 17 meta clusters, $\Phi_{=}(4)068$

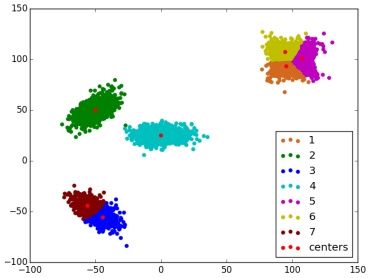
(D) $D = 4$, 4 meta clusters, $\Phi_{=}(5)000$

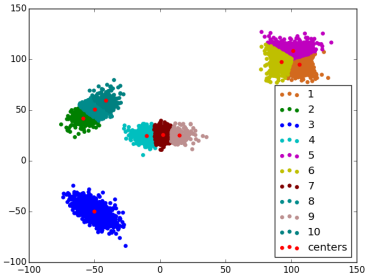
Comparing clusterings using matchings between clusters of clusters

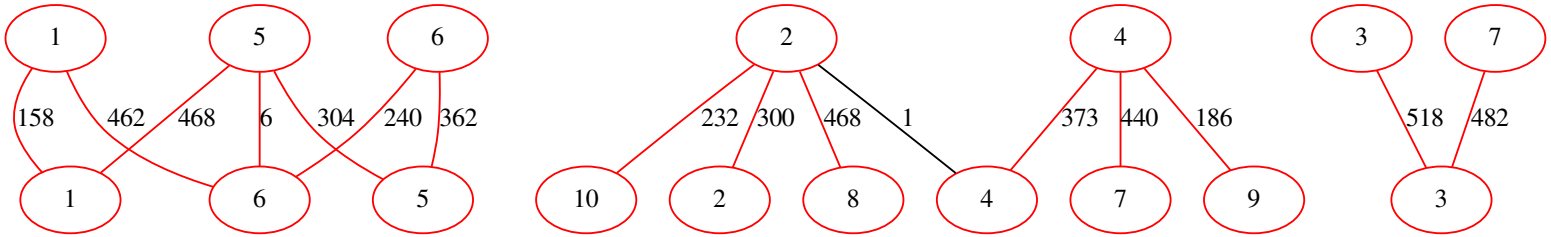
▷ Contributions:

– Formalization of the D-family matching problem
– NP-completeness results and unbounded approximation ratio for simple strategies
  Open: is the problem APX hard?
– Exact polynomial time algos. for selected intersection graphs (trees)
– Heuristics for general graphs
– Extensive experiments (vs. the variation of information)

▷ Stability of kmeans++:







▷Ref: Cazals, Mazauric, Tetley, Watrigant; submitted

Beyond two-sample tests

Conclusions - Outlook

- An elementary method providing a normalized discrepancy based upon (provably correct) estimates of the JS divergence computed on a per point basis
- Merely requires an efficient algorithm for (approximate) nearest neighbors
- By changing the sign of the discreancy: can be used to find clusters of low discrepancy i.e. *coherent regions*
- Can be used as goodness-of-fit tool, by sampling from a given model, then comparing data to spot discrepancies
- Clusters can be post-processed separately: e.g., PCA to find relevant directions
    - See also Mueller and Jaakkola, NIPS 2015

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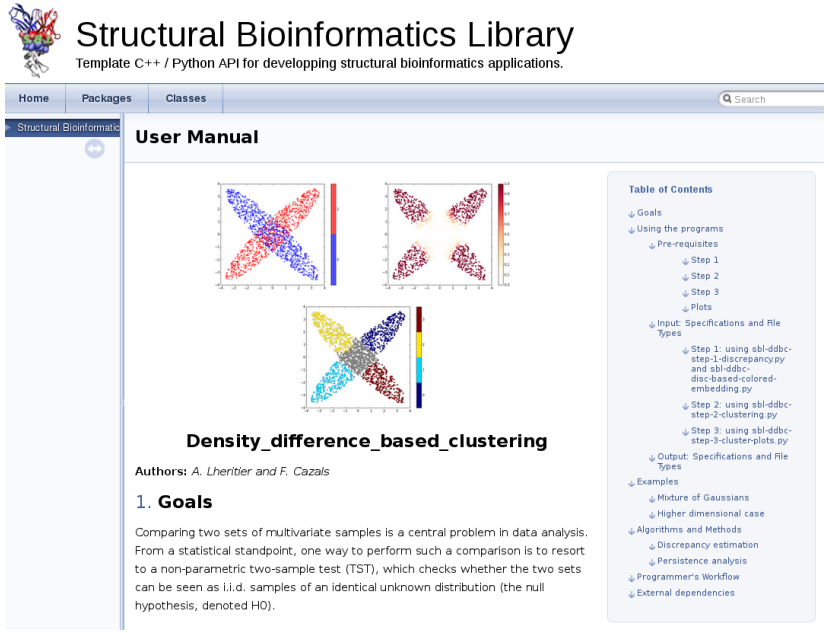

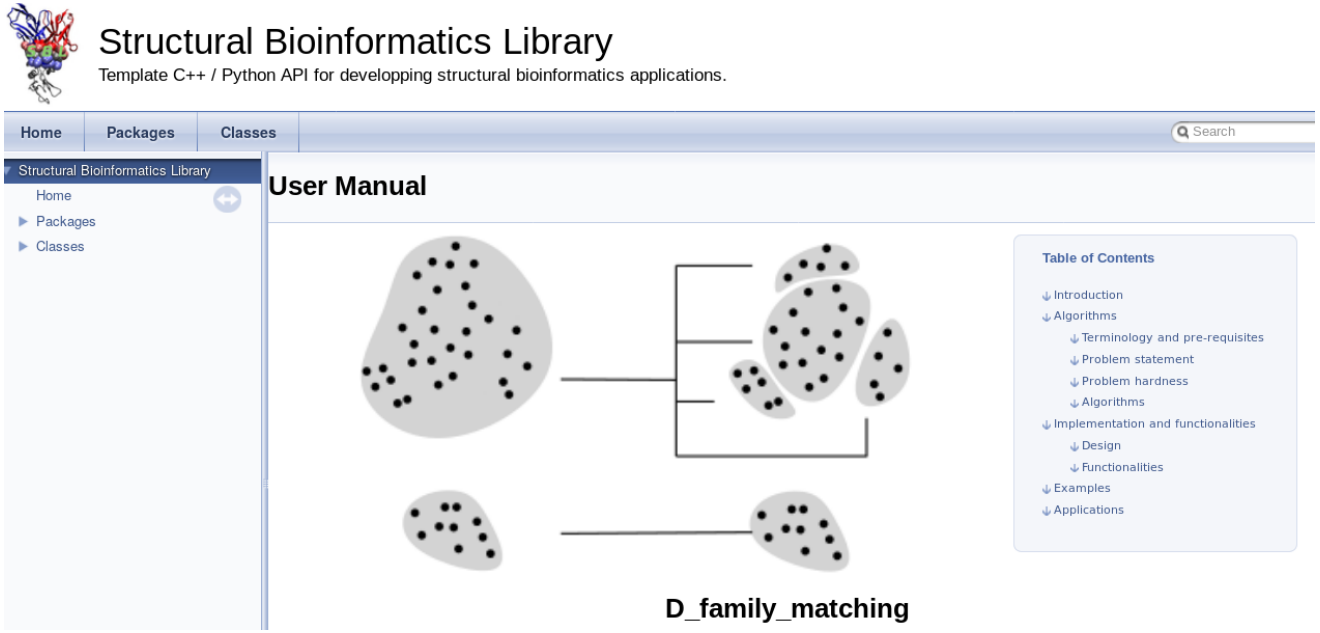

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