Vectorizing PD for Machine Learning

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Acknowledgment

Contents of the slide (including figures) are based on the book:

- Baris Coskunuzer and Cneyt Grcan Akora. Topological Methods in Machine Learning: A Tutorial for Practitioners

Background

Ultimate goal:

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Vectorization:

- Convert PDs into vectors where each component has a fixed meaning (e.g., an *image*)

- *Fixed* vectorization:
  - A *fixed* mapping from a PD to a vector (which may involve a *hyperparameter choice*)
  - All described vectorization methods are applicable to *any* type of data (they simply transform a given PD into a vector)
  - However, the effectiveness and common usage of certain vectorization methods can vary depending on the *data type* and the *density or sparsity* of the PDs

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  - If you want the features in all the dimensions, you can concatenate all vectors $v_0 \| v_1 \| \ldots \| v_d$ assuming the maximum dimension is d
  - Alternatively, you can convert the PD of all dimensions, PD_*, into a single vector v_*

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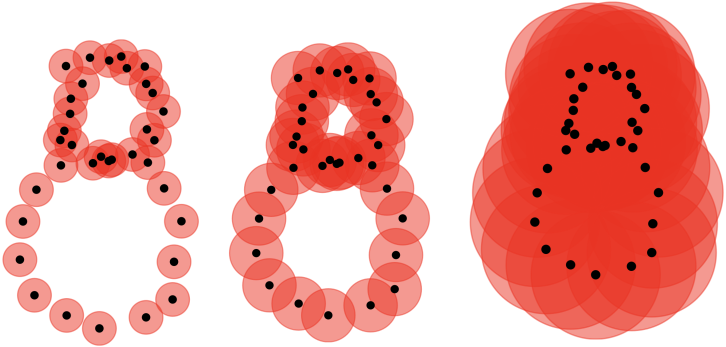
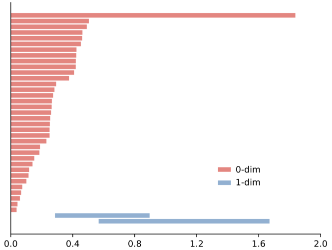
- $n, \alpha_1, \alpha_2, \ldots, \alpha_n$ are the *hyperparameters* that you need to determine in practice (e.g., we could let $n = 50$)

Example



(a) $\epsilon = 0.4$ (c) $\epsilon = 0.7$ (e) $\epsilon = 2$



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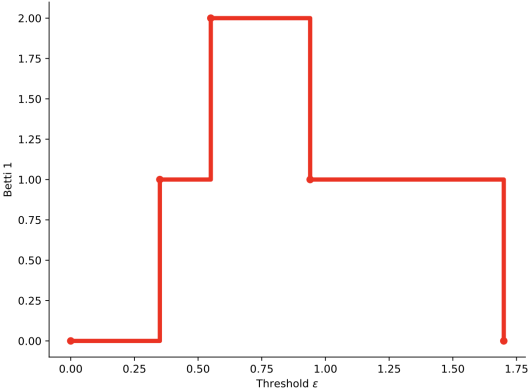
- $\vec{\beta}_1 = [0, 0, 2, 1, 0]$



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Some advantages of Betti vectors:

- While being able to be derived from persistence diagrams, Betti vectors *do not* require the computation of persistence diagrams.
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- While being able to be derived from persistence diagrams, Betti vectors *do not* require the computation of persistence diagrams.
- Indeed, there are computationally more effective ways to produce Betti vectors.
- Another favorable aspect of Betti vectors is their *ease of interpretation*: Simply put, $\beta_p(K_\alpha)$ is equal to the number of p-dimensional holes in K_α.

Persistence Landscapes

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- Consider a persistence diagram $PD_p = \{(b_i, d_i)\}$
- For each $(b_i, d_i) \in PD_p$, first define its generating function

$$\Lambda_i : [0, \infty) \to \mathbb{R},$$

which is a piece-wise linear function obtained by two line segments connecting $(b_i, 0)$ and $(d_i, 0)$ to $(\frac{b_i+d_i}{2}, \frac{d_i-b_i}{2})$

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- Observe that the longer the interval $[b_i, d_i)$ is, the "higher" and "wider" the generating function Λ_i is (so longer bars are emphasized)

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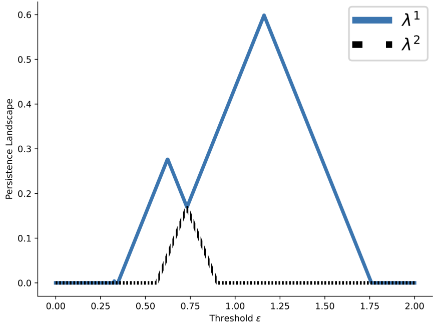
- E.g.: λ^1 and λ^2 for PD_1 of the previous 8-shaped point cloud:



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- Also note that λ^1 and λ^2 are the most commonly used to produce the vectors, and the vectors are used with concatenation in the applications

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- The Silhouette function $\Psi_q : [0, \infty) \to \mathbb{R}$ is defined as the weighted sum of the Λ_i's:

$$\Psi_q(\alpha) = \frac{\sum_{i=1}^{N} w_i \Lambda_i(\alpha)}{\sum_{i=1}^{N} w_i},$$

where w_i is the weight of the function Λ_i

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- The weight w_i for a Λ_i is typically taken as $(d_i - b_i)^p$, so Ψ_q becomes:
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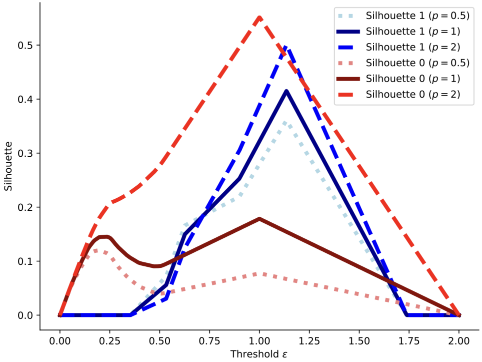

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- If the persistence diagram has a few points and the goal is to emphasize these significant features, $p = 2$ would be a good choice
- If there are many points in PD and the key information comes from smaller features, $1/2$ can be used

Persistence Curve

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We have:

- "$[\cdots]$" encloses a "vector" which produces a real value for each $(b,d) \in PD(\alpha)$
- Given the vector, T then provides a "aggregate" (e.g., sum, mean, or max)

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- By selecting different combinations of Λ and T, one can generate various functional summaries of the PD, each potentially highlighting different aspects of the data
- Specifically, all previous vectorization methods can be considered as special cases of Persistence Curves by choosing a certain Λ and T
- E.g., let

$$\Lambda_{(b,d)}(t) = \begin{cases} 0 & \text{if } t \notin [b,d] \\ t-b & \text{if } t \in [b, \frac{b+d}{2}] \\ d-t & \text{if } t \in (\frac{b+d}{2}, d] \end{cases}$$

and T be the k^{th}-max function, then we get the persistence landscape

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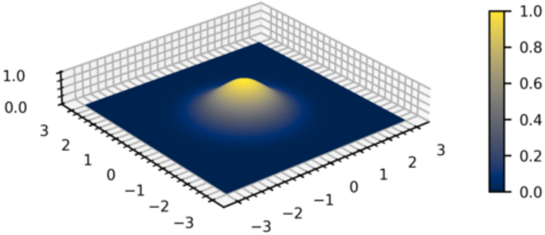
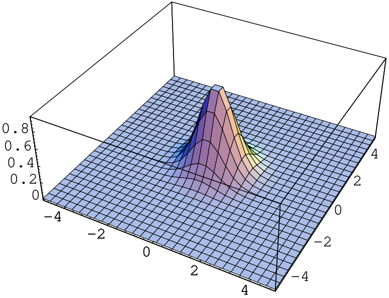
- A Gaussian function is a relaxation of it but in 2D. We don't need the integral to be 1 and the function always has the same height:

$$\phi(x) = \exp\left(-\frac{\|x-\mu\|_2^2}{\sigma^2}\right)$$

where μ is still the "mean" (center) and σ^2 is the "width" (spread) now

Gaussian functions





(Figure from handwiki and wolfram mathworld)

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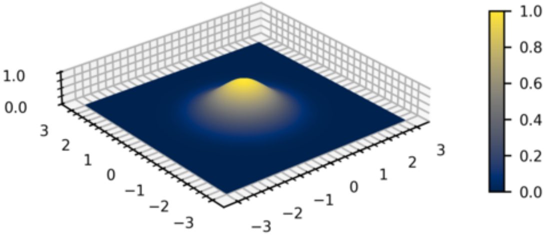

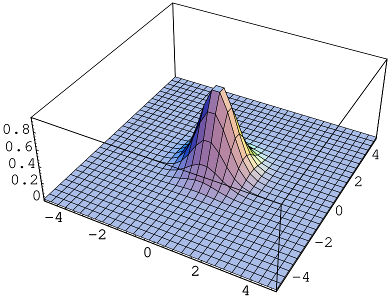

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- So the function value is basically just an indication of how far a point x is from the center μ (instead of directly using the inverse distance $1/\|x-\mu\|_2$)

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- The Persistence Image of PD is a 2D function $pi : \mathbb{R}^2 \to \mathbb{R}$:
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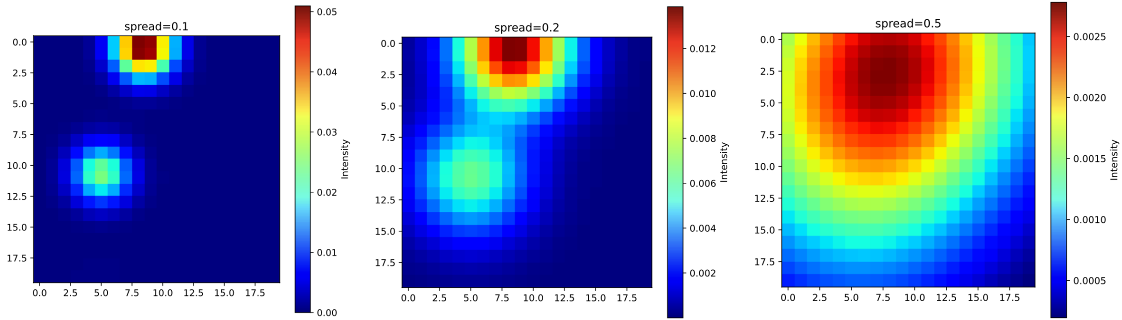
- w_i is typically $(d_i - b_i)^p$

Example

- For the two points in the 1st PD of the previous 8-shaped point cloud:



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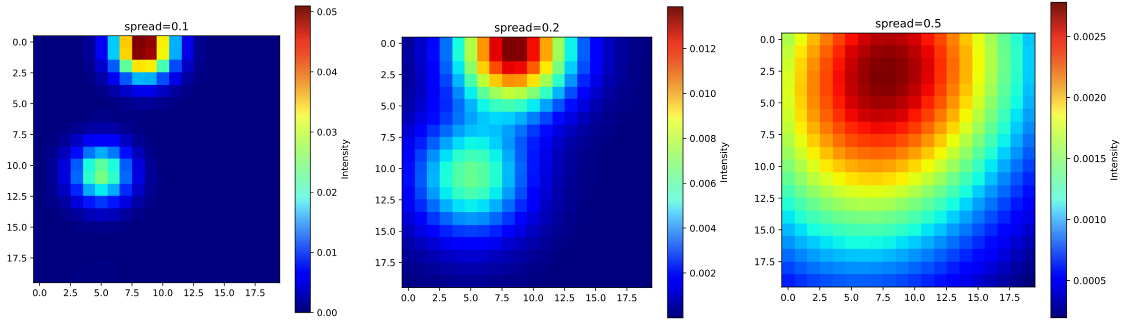

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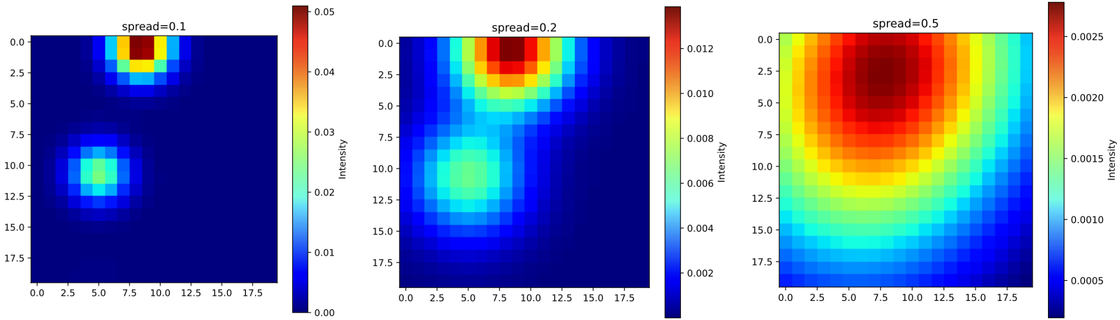

- So it's just a 2D function indicating the "positions" of the points in a PD
- Notice: $pi : \mathbb{R}^2 \rightarrow \mathbb{R}$ as defined is still a continuous function
- As in the previous vectorizations, we still need to discretize it into a 2D image: by doing some sampling on a 2D grid (which is another hyperparameter)

Question

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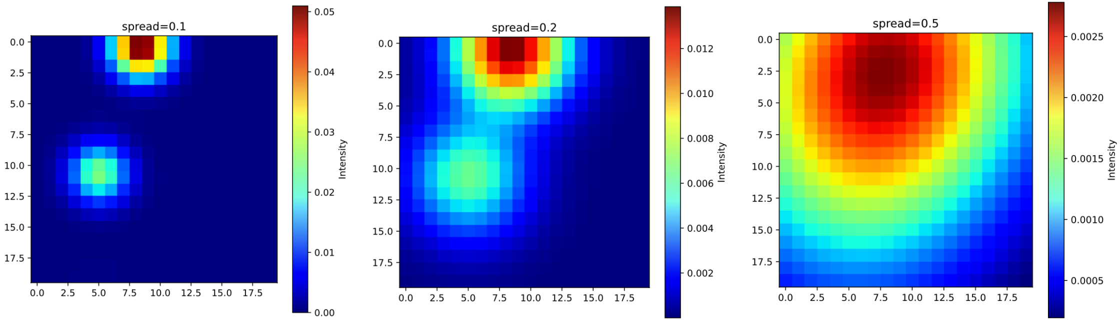

- Why don't (can't) we use a 2D image to directly encode a PD (which is in 2D)?

Kernel Methods for Integrating PD into ML framework

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  where $\phi(x_1, x_2)$ is the Gaussian kernel:

$$\phi(x_1, x_2) = \exp\left(-\frac{\|x_1 - x_2\|_2^2}{\sigma^2}\right)$$

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- Although kernel methods can yield better results in some settings, they can be computationally intensive and impractical for large datasets due to the high computational costs associated with computing the kernel matrix
- In particular, computing kernels takes quadratic time in the number of diagrams, while vectorizing PDs takes only linear time

Stability of vectorizations

- In most applications, the stability of vectorization is vital for statistical and inferential tasks
- Essentially stability means that a small change in the persistence diagram (PD) should not lead to a significant change in its vectorization
- In particular, if two PDs, D_1 and D_2, are close, their corresponding vectorizations, $\vec{v}(D_1)$ and $\vec{v}(D_2)$, should also be close
- This ensures that the vectorization process preserves the structural properties of the data
- Therefore, when two persistence diagrams are similar, it implies that the datasets share similar shape characteristics (due to the stability of PD we learned before)
- If these datasets are intuitively expected to belong to the same class, their vectorizations should likewise remain close

Stability of vectorizations

- To measure the stability, we utilize the Wasserstein distance (which is more general)
- A vectorization technique $\vec{v}$ is said to be stable if it satisfies:

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- Among the methods described earlier, persistence landscapes, silhouettes, persistence images, and most kernel methods are stable vectorizations, while Betti functions are generally unstable

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- Note that most vectorizations are computationally efficient and require minimal time compared to the computation of PDs

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- The resolution parameter sets the number of pixels in the persistence image, thus determining the output dimension of the vectorization
- Higher resolution captures finer detail but at a higher computational cost