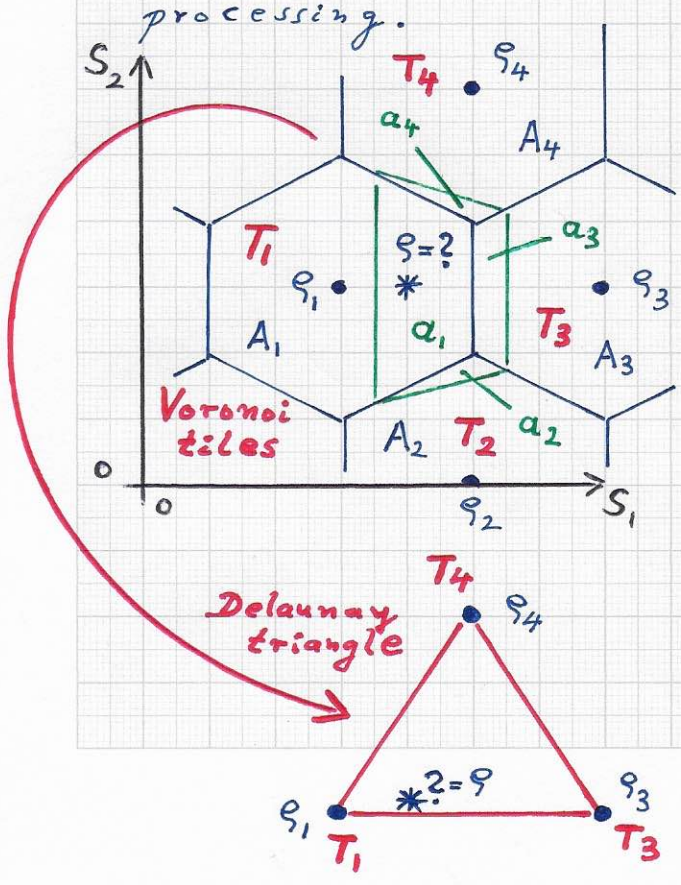
■ OBJECT AND MATERIAL EIGENFUNCTIONS - Cont'd.

• Laplacian eigenfunctions and neural networks:...

The mentioned paper by Peterka et al. on density estimation of particle data focuses on PHYSICAL particle data – i.e., the data lie in 3D space. Our dataset consists of S-tuple data in a potentially high-dimensional space. Thus, one must keep in mind that some of the density estimation schemes discussed by Peterka et al. are not appropriate for high-dimensional S-tuple data due to the rapid increase of computational cost with increasing number of dimensions. Nevertheless, we briefly describe some of the main aspects of these density estimation approaches as they can be adapted to the demands of efficient high-dimensional S-tuple processing.



The figure (left) sketches relevant concepts for the 2D case. Points/particles '•' in S-domain space have associated density values $\varrho_1, \ldots, \varrho_4$. The points '•' have associated **tiles** $T_1, \ldots, T_4$ in their Voronoi tessellation. **Tile** T_i has area A_i; thus, the density of a "unit mass point" is $\varrho_i = 1/A_i$. The Voronoi tessellation and its dual, the Delaunay tessallation (triangulation) support several methods for defining and computing $\varrho(*)$.

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■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd

• Laplacian eigenfunctions and neural networks:... The three "natural ways" to calculate a density estimate $\varrho(*)$ for the $-tuple $*$ are the following:

i) **Tile T_i** contains the point $*$; define $\varrho(*) = \varrho_i$. The resulting density function $\varrho(s_1, s_2)$ is piecewise constant and discontinuous.

ii) **Sibson interpolation** "inserts" $*$ into the Voronoi tessellation – "cutting out" sub-regions from certain tiles with specific areas; here, the areas are $a_1, \ldots, a_4$. Sibson interpolation defines $\varrho(*)$ as

$$\varrho(*) = \sum_{i=1}^{4} a_i \varrho_i \Big/ \sum_{i=1}^{4} a_i \quad .$$

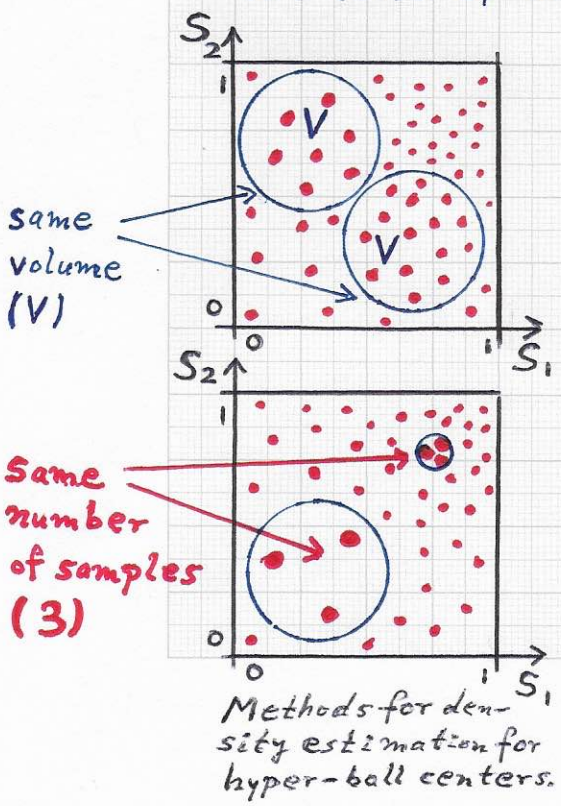
The resulting density function $\varrho(s_1, s_2)$ is continuous.

iii) "Usually," the dual Delaunay tessellation is given as a simplicial complex, i.e., as a **Delaunay triangulation**. Thus, one can perform **linear interpolation** over the triangle that contains $*$. Considering the figure from the previous page, $\varrho(*)$ is obtained by linearly interpolating ϱ_1, ϱ_3 and ϱ_4, i.e., "$\varrho(*) = LinInt(\varrho_1, \varrho_3, \varrho_4)$". The resulting density function $\varrho(s_1, s_2)$ is piecewise linear and thus continuous.

This discussion of Voronoi and Delaunay based ideas regarding density function construction is "educational" – but not "generally practical."

■ OBJECT AND MATERIALS EIGENFUNCTIONS - Cont'd.

• Laplacian eigenfunctions and neural networks:... First, the tessellations (Voronoi, Delaunay) become too complex as far as data structure and processing requirements are concerned; for $-domains beyond 3D space, other simpler approaches are necessary. Second, they do not "smooth" local $-tuple data sufficiently; one is generally interested in a density function construction scheme that uses local subsets of point/particle data to smooth the "non-smooth nature" inherent in a given discrete sample dataset. Thus, density function estimation schemes should involve "smoothing kernels" of data-appropriate radius/width to achieve the desired level of discrete data smoothing while still preserving the level of detail and local behavior that should remain.



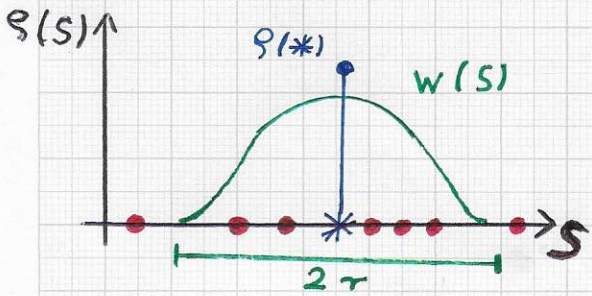
Methods for density estimation for hyper-ball centers.

• The two figures (Left) illustrate two fundamental ideas for local neighborhood-based density estimation, keeping in mind the desire for smoothing and simplicity even for high-dimensional settings. One approach (top) uses a fixed, constant hyper-volume as kernel domain to estimate a density value for the center of the respective hyper-ball. The other approach (bottom) uses a fixed, constant number of discrete samples per hyper-ball.

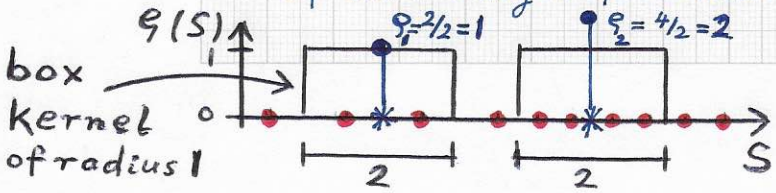
■ OBJECT AND MATERIAL EIGENFUNCTIONS - Cont'd.

• Laplacian eigenfunctions and neural networks:...

This second approach – using a constant number of samples per hyper-ball – is also known in "smoothed particle hydrodynamics" (SPH), where continuum phenomena are computationally simulated via discrete, not-connected particle sets. In the SPH context, the particle model assigns actual physical properties to each particle, including mass. Further, a particle primitive has an associated weight / kernel function with a finite disk (2D) or ball (3D) domain, defining interactions with other particles in a local neighboorhood.



The figure (left) illustrates the basic idea for density estimation for a location '*' in a 1D S-domain. A density estimate ρ(*) is calculated by determining the radius r of a 1D hyper-ball that contains the specified number of samples (5) in its interior. A positive weight / kernel function w(s) with a 2r-wide finite domain is used to estimate ρ(*) in a weighted fashion, with '*' being the center of the weight functions domain. The left figure (bottom) shows a simple example for the first approach: The box convolution kernel yields $\rho_1 = 1$ and $\rho_2 = 2$.



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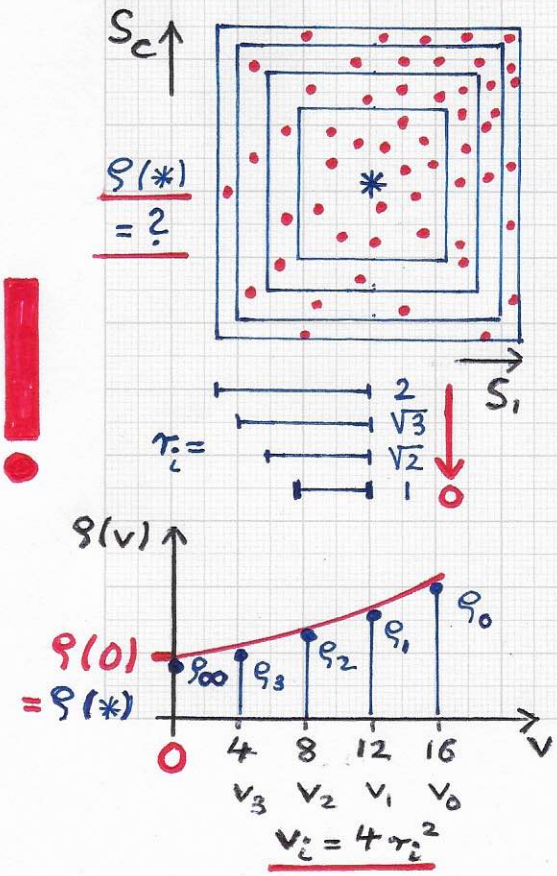
■ Laplacian eigenfunctions and neural networks:...

● Extrapolation — Richardson extrapolation specifically — can be considered for density value estimation as well. Density (="mass/volume") at a point can be understood as a LIMIT in our context: We count S-tuples in a "C-ball" (C-dimensional hyper-ball) to estimate density for the center of the "C-ball". Thus, one can use a sequence of "C-balls" with decreasing volumes, count S-tuples inside the decreasing volumes, and view the density at the common center of all these "C-balls" as a LIMIT value — obtained when extrapolating the sequence of counted numbers to the volume zero. The figures (left) sketch the concept. The concept is not truly Richardson extrapolation in the sense that a "geometrically decreasing stepsize" of a numerical scheme produces increasingly better estimates; rather, a sequence of shrinking "C-balls" generates increasingly local density estimates. The sequence of hyper-volumes V_i generates "C-ball" density estimates ϱ_i for the S-tuple location '*'. One must practically evaluate whether this extrapolation concept can indeed be turned into a proper Richardson method.



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